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A High-Order Efficient Optimised Global Hybrid Method for Singular Two-Point Boundary Value Problems

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Abstract. An optimised global hybrid block method for second order singular boundary value problems with two boundary conditions is developed. A special attention is paid to the problems having solutions with singularities at the left end of the interval considered. The method is a combination of the optimised hybrid formulas in [43] and a new set of formulas. The ad hoc procedure is used just to pass the singularity and the main formulas are applied to obtain approximations at other discrete points. Numerical experiments show that the method is a good alternative for the problems studied.

AMS subject classifications: 65L10, 65L10

Key words: Singular boundary value problem, hybrid methods, block methods, optimisation technique.

1. Introduction

Two-point boundary value problems occur in various applications, including fluid flow, shock waves and geophysical models. The problems can be categorised as singular and singularly perturbed ones and we refer the reader to [4] for more information about BVPs. In the present work we are concerned with numerical solution of two-point singular boundary value problems (SBVPs) for ODEs. Such problems frequently occur in practical phenomena such as reaction-diffusion processes, chemical kinetics, physiological processes, thermal-explosion theory, electro hydro-dynamics and shallow membrane caps theory [5, 9, 11, 13, 15, 16, 18, 23]. Since it is not always possible to find closed form solutions of SBVPs, these

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problems are usually tackled numerically. Second order two-point SBVPs have a great scientific significance, so that they attracted attention of many researchers. Here we consider the singular boundary value problem

$$z''(x) = f\big(x, z(x), z'(x)\big), \quad x \in [a,b], \tag{1.1}$$

subject to one of the following types of boundary conditions (BCs):

$$\begin{aligned} &\text{Dirichlet: } z(a) = z_a,\ z(b) = z_b,\\ &\text{Neumann: } z'(a) = z'_a,\ z'(b) = z'_b \text{ or}\\ &\text{Mixed: } g_1\big(z(a), z'(a)\big) = \nu_a,\ g_2\big(z(b), z'(b)\big) = \nu_b. \end{aligned} \tag{1.2}$$

We also assume that the function f in (1.1) has a singularity at the left end of the integration interval — i.e. at the point $x = a$. Different codes have appeared in the literature in order to numerically deal with special cases of SBVPs. Thus, Russell and Shampine [39] presented various numerical methods for solving SBVPs, Roul *et al.* proposed a high-order numerical scheme based on a quartic B-spline optimal collocation method for nonlinear SBVPs, Pandey *et al.* [27,28] considered second and fourth order finite difference methods, and Abukhaled [1] employed a second order B-spline collocation scheme for special SBVPs. Other approaches to solving SBVPs are discussed in [5,9,11–23,25–28,35–40,44].

The present work deals with the development and analysis of a method combining two approaches — viz. hybrid and block methods specifically used in numerical integrators of the initial value problems for ODEs [10,24]. For more details on hybrid and block methods for solving different types of differential equations one can consult [6,14,30–34,42] and references therein. The paper at hand, is an extension of our earlier work. More precisely, we combine an optimised hybrid block method for second order ODEs studied in [43] with an ad hoc set of formulas used to treat singularities at the left end of the integration intervals.

The subsequent sections are as follows. In Section 2, the main and an ad hoc formulas are presented. Section 3 deals with the convergence of the method. In Section 4, we discuss the implementation of the method. Numerical experiments are carried out in Section 5, and concluding remarks are given in Section 6.

2. Main and Ad Hoc Formulas

Here we present the main formulas and an ad hoc strategy for the SBVP (1.1).

2.1. Main formulas

In order to derive the main formulas, we discretise the interval $[a,b]$ as

$$a = x_0 < x_1 < x_2 < \cdots < x_N = b,$$

where $x_n = x_0 + nh$, $n = 0,1,\dots,N$ and $h = x_{n+1} - x_n$ is the stepsize. Let z_n be an approximation of the true solution $z(x)$ at x_n, i.e. $z_n \approx z(x_n)$. On the two-step block interval

$[x_n, x_{n+2}]$ with $n > 0$ we approximate the true solution of (1.1) by the following interpolating polynomial:

$$z(x) \approx \psi(x) = \sum_{j=0}^{8} \eta_j \psi_j(x), \tag{2.1}$$

where $\psi_j(x) = (x - x_n)^j$ and η_j are unknown coefficients. In order to find η_j, we impose interpolating and collocation conditions — viz.

(i) $z_n = \psi(x_n)$,

(ii) $z'_n = \psi'(x_n)$,

(iii) $f_{n+i} = \psi''(x_{n+i}), \quad i = 0, p, 1, q, 2$,

(iv) $g_{n+i} = \psi'''(x_{n+i}), \quad i = 0, 2$.

Note that z_n and z'_n are approximations of $z(x_n)$ and $z'(x_n)$, respectively,

$$f_{n+i} \approx f\big(x_{n+i}, z(x_{n+i}), z'(x_{n+i})\big),$$
$$g_{n+i} \approx g\big(x_{n+i}, z(x_{n+i}), z'(x_{n+i})\big)$$

with

$$g(x, z, z') = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial z} z' + \frac{\partial f}{\partial z'} f(x, z, z').$$

The above interpolation and collocation conditions lead to a system of nine equations with nine unknowns. In the resulting system, the points x_{n+p} and x_{n+q} are referred to as intra-step points in the block $[x_n, x_{n+2}]$ with the restriction $0 < p < 1 < q < 2$. Hence, we have a system of nine equations with nine unknowns and two parameters corresponding to two intra-step points in the block $[x_n, x_{n+2}]$. The system obtained can be solved by any Computer Algebra System — e.g. by MATLAB or MATHEMATICA. We used MATHEMATICA thus obtaining the unknown coefficients η_j, $j = 0, 1, 2, \ldots, 8$. Substituting η_j in (2.1), we obtain the following approximation formula:

$$\begin{aligned} z(x) \approx \psi(x) = {} & \alpha_0(x) z_n + \alpha_1(x) h z'_n + h^2 \sum_i \beta_i(x) f_{n+i} \\ & + h^3 \sum_j \gamma_j(x) g_{n+j}, \quad i = 0, p, 1, q, 2, \quad j = 0, 2. \end{aligned} \tag{2.2}$$

The coefficients $\alpha_0(x), \alpha_1(x), \beta_i(x), \gamma_j(x)$ depend on continuous variable x. In order to get the main formulas at the end point of $[x_n, x_{n+2}]$, we evaluate the approximation $z(x) \approx \psi(x)$ and its first derivative at x_{n+2}. These approximations, $z_{n+2} = \psi(x_{n+2})$ and $z'_{n+2} = \psi'(x_{n+2})$ are expressed in terms of unknown parameters p and q corresponding respectively to the points x_{n+p} and x_{n+q} in the block $[x_n, x_{n+2}]$. Now we have to find appropriate values for these parameters. For this, one can use the following optimisation strategy:

Step 1. Expand z_{n+2} and z'_{n+2} into Taylor series about $x = x_n$ and get the truncation errors

$$\mathscr{L}[z(x_{n+2});h] = \frac{(2-3pq)z^{(9)}(x_n)h^{(9)}}{99225} + \mathcal{O}\big(h^{10}\big), \tag{2.3}$$

$$\mathscr{L}[z'(x_{n+2});h] = \frac{(2-p-q)z^{(9)}(x_n)h^{8}}{33075} + \mathcal{O}\big(h^{9}\big). \tag{2.4}$$

Step 2. Equating the principal terms in (2.3) and (2.4) to zero yields

$$2-3pq=0,$$
$$2-p-q=0.$$

Step 3. Now, solving this system, we find optimised values of p and q, viz.

$$p = 1-\frac{\sqrt{3}}{3} \simeq 0.42265, \quad q = 1+\frac{\sqrt{3}}{3} \simeq 1.57735.$$

Note that the system in Step 2 corresponds to two curves symmetric with respect to the diagonal $p = q$. Hence, it has a unique solution if $0 < p < 1 < q < 2$.

In order to show the influence of these values of p and q, we substitute them in (2.3) and (2.4), thus obtaining

$$\mathscr{L}[z(x_{n+2});h] = \frac{-z^{(11)}(x_n)h^{11}}{58939650} + \mathcal{O}\big(h^{12}\big),$$
$$\mathscr{L}[z'(x_{n+2});h] = \frac{z^{(12)}(x_n)h^{11}}{589396500} + \mathcal{O}\big(h^{12}\big).$$

The above expressions confirm the suitability of p and q found. We note that such choice of p and q adds two accuracy orders in the approximation of $z(x_{n+2})$ and three accuracy orders in the approximation of $z'(x_{n+2})$. Now, using (2.2), we get the following formulas at the end point of the block $[x_n, x_{n+2}]$

$$\begin{aligned} z_{n+2} = z_n + 2hz'_n + \frac{h^2}{105}\big(&37f_n + (54+18\sqrt{3})f_{n+p} + 64f_{n+1} \\ &+ (54-18\sqrt{3})f_{n+q} + f_{n+2} + 2hg_n\big), \end{aligned} \tag{2.5}$$
$$z'_{n+2} = z'_n + \frac{h}{105}\big(19f_n + 54f_{n+p} + 64f_{n+1} + 54f_{n+q} + 19f_{n+2} + h(g_n - g_{n+2})\big).$$

Additional formulas. Up to now, we established only two approximations of the true solution and its derivative at the point x_{n+2}. However, one needs more equations because of the presence of ten unknowns $z_n, z_{n+p}, z_{n+1}, z_{n+q}, z_{n+2}, z'_n, z'_{n+p}, z'_{n+1}, z'_{n+q}, z'_{n+2}$ in (2.5). Therefore, we evaluate (2.2) and its first derivative at the points $x_{n+p}, x_{n+1}, x_{n+q}$, so that

$$z_{n+p} = z_n + \frac{(3+\sqrt{3})hz'_n}{3(2+\sqrt{3})} + \frac{h^2}{11340(2+\sqrt{3})}\Big((1801+559\sqrt{3})f_n + (630+315)f_{n+p}$$

$$
\begin{aligned}
&+(400-376\sqrt{3})f_{n+1}+(990-477\sqrt{3})f_{n+q}-(41+21\sqrt{3})f_{n+2}\\
&+h\Big((107+36\sqrt{3})g_n+(7+4\sqrt{3})g_{n+2}\Big)\Big),\\
z_{n+1}={}&z_n+hz'_n+\frac{h^2}{6720}\Big(1171f_n+(945+576\sqrt{3})f_{n+p}+280f_{n+1}\\
&+(945-576\sqrt{3})f_{n+q}+19f_{n+2}+h(67g_n-3g_{n+2})\Big),\\
z_{n+q}={}&z_n+\frac{(-3+\sqrt{3})hz'_n}{3(-2+\sqrt{3})}+\frac{h^2}{11340(-2+\sqrt{3})}\Big((-1801+559\sqrt{3})f_n\\
&-(990+477\sqrt{3})f_{n+p}-(400+376\sqrt{3})f_{n+1}+(-630+315\sqrt{3})f_{n+q}\\
&+(41-21\sqrt{3})f_{n+2}+h\Big((-107+36\sqrt{3})g_n+(-7+4\sqrt{3})g_{n+2}\Big)\Big),\\
z'_{n+p}={}&z'_n+\frac{h}{3780(2+\sqrt{3})}\Big((1726+885\sqrt{3})f_n+(1656+780\sqrt{3})f_{n+p}\\
&+(96-320\sqrt{3})f_{n+1}+(396-60\sqrt{3})f_{n+q}-(94+25\sqrt{3})f_{n+2}\\
&+h\Big((124+65\sqrt{3})g_n+(16+5\sqrt{3})g_{n+2}\Big)\Big),\\
z'_{n+1}={}&z'_n+\frac{h}{1680}\Big(257f_n+(432+315\sqrt{3})f_{n+p}+512f_{n+1}+(432-315\sqrt{3})f_{n+q}\\
&+47f_{n+2}+8h(g_n-g_{n+2})\Big),\\
z'_{n+q}={}&z'_n+\frac{h}{3780(-2+\sqrt{3})}\Big((885\sqrt{3}-1726)f_n-(396+60\sqrt{3})f_{n+p}\\
&-(96+320\sqrt{3})f_{n+1}+(780\sqrt{3}-1656)f_{n+q}+(94-25\sqrt{3})f_{n+2}\\
&+h\Big((65\sqrt{3}-124)g_n+(5\sqrt{3}-16)g_{n+2}\Big)\Big).
\end{aligned}
\tag{2.6}
$$

Remark 2.1. Formulas (2.5)-(2.6) form a two-step hybrid block-type method with two optimised intra-step points that will be considered for $n = 1(2)N-2$, where $N \geq 3$ is an odd integer. All these formulas can be used starting from the second sub-interval, whereas for the first subinterval they are not applicable because of the singularity. For the sub-interval $[x_0, x_1]$, we develop an ad hoc set of formulas.

2.2. Ad hoc formulas in the first step

In order to establish ad hoc formulas for the sub-interval $[x_0, x_1]$ to bypass the singularity, one has to use a procedure similar to the one used for formulas (2.5)-(2.6) but with appropriately changed interpolation and collocation conditions. Consider the following approximation:

$$
z(x) \approx \phi(x) = \sum_{j=0}^{5} \kappa_j \phi_j(x) \tag{2.7}
$$

of the true solution of (1.1) by an interpolating polynomial on the subinterval $[x_n, x_{n+1}]$ with $\phi_j(x) = (x - x_n)^j$ and unknown coefficients κ_j. In order to determine coefficients κ_j, we impose the following interpolating and collocation conditions:

(i) $z_n = \phi(x_n)$,

(ii) $z'_n = \phi'(x_n)$,

(iii) $f_{n+i} = \phi''(x_{n+i}), \quad i = r, s, t, 1$

for intermediate points corresponding to the parameters $0 < r < s < t < 1$.

Proceeding in a similar way as in the previous section, we obtain the ad hoc formulas for $[x_0, x_1]$, viz.

$$\begin{aligned} z_r &= z_0 + 0.0885\,hz'_0 + h^2(+0.0053f_r - 0.0024\,f_s + 0.0015\,f_t - 0.0006f_1), \\ z_s &= z_0 + 0.4094hz'_0 + h^2(0.0695\,f_r + 0.0161\,f_s - 0.0024f_t + 0.0006f_1), \\ z_t &= z_0 + 0.7876hz'_0 + h^2(0.1545f_r + 0.1448f_s + 0.0111f_t - 0.0003f_1), \\ z_1 &= z_0 + hz'_0 + h^2(0.2009f_r + 0.2292f_s + 0.0698\,f_t), \\ z'_r &= z'_0 + h(0.1129f_r - 0.0403f_s + 0.0258f_t - 0.0099f_1), \\ z'_s &= z'_0 + h(0.2343f_r + 0.2068f_s - 0.0478f_t + 0.0160f_1), \\ z'_t &= z'_0 + h(0.2166f_r + 0.4061f_s + 0.1890f_t - 0.0241f_1), \\ z'_1 &= z'_0 + h(0.2204f_r + 0.3881f_s + 0.3288f_t + 0.0625f_1), \end{aligned} \tag{2.8}$$

where

$$\begin{aligned} r &= 0.088587959512703947395546143769 45, \\ s &= 0.409466864440734710864926252068 82, \\ t &= 0.787659461760847056025241889875 99. \end{aligned}$$

2.3. Complete optimised global hybrid block method

Combining the main formulas (2.5)-(2.6) for $n = 1(2)N - 2$ and the ad hoc formulas (2.8), we arrive at a complete optimised global hybrid block method. Applying this complete global method to the SBVP (1.1) yields $4N + 6$ discrete approximations

$$\begin{aligned} &\left\{z_0, z_r, z_s, z_t, z_1, z_{1+p}, z_2, z_{1+q}, z_3, z_{3+p}, z_4, z_{3+q}, \ldots, z_N\right\}, \\ &\left\{z'_0, z'_r, z'_s, z'_t, z'_1, z'_{1+p}, z'_2, z'_{1+q}, z'_3, z'_{3+p}, z'_4, z'_{3+q}, \ldots, z'_N\right\}. \end{aligned}$$

On the other hand, the Eqs. (2.5)-(2.6) for $n = 1(2)N - 2$ and the formulas (2.8) comprise $4N + 4$ equations. Adding two given boundary conditions (1.2) leads to a system of $4N + 6$ equations with $4N + 6$ unknowns. The details of this method are presented below.

3. Theoretical Analysis

Here we will discuss the accuracy and convergence of the complete method for solving SBVPs (1.1), starting with the accuracy of the main formulas (2.5)-(2.6).

3.1. Order of accuracy

The two-step block formulas (2.5)-(2.6) may be written in the matrix form

$$\mathbf{\Lambda_1\ Z_n = h\ \Lambda_2\ Z'_n + h^2\ \Lambda_3\ F_n + h^3\ \Lambda_4\ G_n}, \tag{3.1}$$

where $\mathbf{\Lambda_1}, \mathbf{\Lambda_2}, \mathbf{\Lambda_3}$ and $\mathbf{\Lambda_4}$ are 8×5 matrices with constant coefficients. One can readily get these coefficients from (2.5)-(2.6). Here, $\mathbf{Z_n}, \mathbf{Z'_n}, \mathbf{F_n}$ and $\mathbf{G_n}$ are

$$\begin{aligned}
\mathbf{Z_n} &= (z_n, z_{n+p}, z_{n+1}, z_{n+q}, z_{n+2})^T, \\
\mathbf{Z'_n} &= (z'_n, z'_{n+p}, z'_{n+1}, z'_{n+q}, z'_{n+2})^T, \\
\mathbf{F_n} &= (f_n, f_{n+p}, f_{n+1}, f_{n+q}, f_{n+2})^T, \\
\mathbf{G_n} &= (g_n, g_{n+p}, g_{n+1}, g_{n+q}, g_{n+2})^T.
\end{aligned}$$

Assume that $Y(x)$ is an analytical function. Consider the following difference operator associated with the formulas (2.5)-(2.6):

$$\begin{aligned}
\mathscr{L}[Y(x_n);h] = \sum_j \bar{\alpha}_j Y(x_n+jh) - h\bar{\beta}_j Y'(x_n+jh) - h^2\bar{\gamma}_j Y''(x_n+jh) \\
- h^3\bar{\delta}_j Y'''(x_n+jh), \quad j = 0, p, 1, q, 2,
\end{aligned} \tag{3.2}$$

where $\bar{\alpha}_j, \bar{\beta}_j, \bar{\gamma}_j, \bar{\delta}_j$ are the j-th columns of $\mathbf{\Lambda_1}, \mathbf{\Lambda_2}, \mathbf{\Lambda_3}$ and $\mathbf{\Lambda_4}$, respectively. The main method (2.5)-(2.6) and the difference operator (3.2) are said to be of order k if using the Taylor series expansion of $Y(x_n+jh), Y'(x_n+jh), Y''(x_n+jh)$ and $Y'''(x_n+jh)$ about the point x_n, we obtain

$$\mathscr{L}[Y(x_n);h] = \bar{\nu}_0 Y(x_n) + \bar{\nu}_1 hY'(x_n) + \bar{\nu}_2 h^2 Y''(x_n) + \cdots + \bar{\nu}_m h^m Y^{(m)}(x_n) + \ldots$$

with $\bar{\nu}_0 = \bar{\nu}_1 = \bar{\nu}_2 = \cdots = \bar{\nu}_{k+1} = \mathbf{0}$ and $\bar{\nu}_{k+2} \neq 0$. Here, $\bar{\nu}_i$ are vectors and $\bar{\nu}_{k+2}$ is named as the vector of error constants. For the hybrid block formulas (2.5) -(2.6), we have, $\bar{\nu}_0 = \bar{\nu}_1 = \cdots = \bar{\nu}_8 = \mathbf{0}$, and

$$\bar{\nu}_9 = \left(\frac{-1}{1837080\sqrt{3}}, 0, \frac{1}{1837080\sqrt{3}}, 0, \frac{-1}{612360}, \frac{1}{362880}, \frac{-1}{612360}, 0\right)^T.$$

This implies at least seventh-order of accuracy of formulas (2.5)-(2.6).

Remark 3.1. Similar considerations lead to the accuracy estimates of the ad hoc formulas. The local truncation errors of these formulas give

$$\begin{aligned}
\mathscr{L}[z(x_r);h] &= 2.8055562 \times 10^{-6} z^{(6)}(x_0)h^6 + \mathscr{O}(h^7), \\
\mathscr{L}[z(x_s);h] &= 9.1616770 \times 10^{-7} z^{(6)}(x_0)h^6 + \mathscr{O}(h^7), \\
\mathscr{L}[z(x_t);h] &= -2.9624031 \times 10^{-6} z^{(6)}(x_0)h^6 + \mathscr{O}(h^7), \\
\mathscr{L}[z(x_1);h] &= 1.4172335 \times 10^{-7} z^{(8)}(x_0)h^8 + \mathscr{O}(h^9),
\end{aligned}$$

$$\begin{aligned}
&\mathscr{L}[z'(x_r);h] = 0.0000458z^{(6)}(x_0)h^5 + \mathscr{O}\big(h^6\big),\\
&\mathscr{L}[z'(x_s);h] = -0.0000481z^{(6)}(x_0)h^5 + \mathscr{O}\big(h^6\big),\\
&\mathscr{L}[z'(x_t);h] = 0.0000260z^{(6)}(x_0)h^5 + \mathscr{O}\big(h^6\big),\\
&\mathscr{L}[z'(x_1);h] = -2.0246\times 10^{-8}z^{(9)}(x_0)h^8 + \mathscr{O}\big(h^9\big).
\end{aligned}$$

3.2. Convergence analysis

We want to have the approximations obtained by our method to tend to the true solutions when step-size tends to zero. Now we establish a convergence result for the complete hybrid block method.

Definition 3.1. Let $z(x)$ be the true solution of the Eq. (1.1) supplemented by any boundary condition (1.2), and $\{z_j\}_{j=0}^N$ be the approximations of $z(x)$ derived by the global hybrid block method. The numerical method has k-th order of convergence if there exists a constant C such that for all sufficiently small h one has

$$\max_{0\le j\le N} \|z(x_j) - z_j\| \le Ch^k.$$

The definition implies that

$$\max_{0\le j\le N} \|z(x_j) - z_j\| \to 0 \quad \text{as} \quad h \to 0.$$

Theorem 3.1 (Convergence theorem)**.** *The global hybrid block method of the approximate solution of the SBVP* (1.1) *supplemented by any boundary condition* (1.2) *has* 7*-th order of convergence.*

Proof. For definiteness, let us consider the Eq. (1.1) along with boundary conditions of the Dirichlet-type. Other situations can be studied analogously. Assume that the true known values are given by the boundary conditions — i.e. $z_0 = z(x_0) = z_a$ and $z_N = z(x_N) = z_b$. The other unknowns in the global hybrid block method are

$$\begin{aligned}
&\big\{z_r, z_s, z_t, z_1, z_{1+p}, z_2, z_{1+q}, z_3, z_{3+p}, z_4, z_{3+q}, \ldots, z_{N-1}, z_{N-2+q}\big\},\\
&\big\{z'_0, z'_r, z'_s, z'_t, z'_1, z'_{1+p}, z'_2, z'_{1+q}, z'_3, z'_{3+p}, z'_4, z'_{3+q}, \ldots, z'_{N-2+q}, z'_N\big\}.
\end{aligned}$$

First, we describe the matrices arising in the method. Let D be the $(4N+4)\times(4N+4)$ matrix defined as

$$D = \begin{pmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{pmatrix},$$

where D_{11} and D_{21} are $(2N+2)\times(2N+1)$ sub-matrices,

$$D_{11} = \begin{pmatrix} \bar{D}_{11} & & & & \\ \bar{D}_{21} & \bar{D}_{22} & & & \\ & & \ddots & & \\ & & & \bar{D}_{k-1\,k-1} & \\ & & & \bar{D}_{k\,k-1} & \bar{D}_{k\,k} \end{pmatrix}$$

with $k=(N+1)/2$, $\bar{D}_{ii}=Id_4, i=1,\ldots,k-1$,

$$\bar{D}_{kk}=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\\0&0&0\end{pmatrix},\quad \bar{D}_{i\,i-1}=\begin{pmatrix}0&0&0&-1\\0&0&0&-1\\0&0&0&-1\\0&0&0&-1\end{pmatrix},\quad i=2,\ldots,k,$$

and D_{21} is a null matrix.

The $(2N+2)\times(2N+3)$ sub-matrices D_{12} and D_{22} have the form

$$D_{12}=h\begin{pmatrix}\tilde{D}_{11}&&&&\\&\tilde{D}_{22}&&&\\&&\ddots&&\\&&&\tilde{D}_{k-1\,k-1}&\\&&&&\tilde{D}_{k\,k}\end{pmatrix},\quad k=\frac{N+1}{2},$$

$$\tilde{D}_{11}=\begin{pmatrix}-0.0885&0&0&0\\-0.4894&0&0&0\\-0.7876&0&0&0\\-1&0&0&0\end{pmatrix},\quad \tilde{D}_{i\,i}=\begin{pmatrix}\alpha_1&0&0&0\\\alpha_2&0&0&0\\\alpha_3&0&0&0\\\alpha_4&0&0&0\end{pmatrix},\quad i=2,\ldots,k-1,$$

$$\tilde{D}_{k\,k}=\begin{pmatrix}\alpha_1&0&0&0&0\\\alpha_2&0&0&0&0\\\alpha_3&0&0&0&0\\\alpha_4&0&0&0&0\end{pmatrix},$$

$$\alpha_1=-\frac{(3+\sqrt{3})}{3(2+\sqrt{3})},\quad \alpha_2=-1,\quad \alpha_3=-\frac{(-3+\sqrt{3})}{3(-2+\sqrt{3})},\quad \alpha_4=-2,$$

$$D_{22}=\begin{pmatrix}\hat{D}_{11}&\hat{D}_{12}&&&\\&\hat{D}_{22}&&&\\&&\ddots&&\\&&&\hat{D}_{k-1\,k-1}&\hat{D}_{k-1\,k}\\&&&&\hat{D}_{k\,k}\end{pmatrix},\quad k=\frac{N+1}{2},$$

$$\hat{D}_{i\,i}=\begin{pmatrix}-1&1&0&0\\-1&0&1&0\\-1&0&0&1\\-1&0&0&0\end{pmatrix},\quad i=1,\ldots,k-1,\quad \hat{D}_{k\,k}=\begin{pmatrix}-1&1&0&0&0\\-1&0&1&0&0\\-1&0&0&1&0\\-1&0&0&0&1\end{pmatrix},$$

$$\hat{D}_{i\,i+1}=\begin{pmatrix}0&0&0&0\\0&0&0&0\\0&0&0&0\\1&0&0&0\end{pmatrix},\quad i=1,\ldots,k-2,\quad \hat{D}_{k-1\,k}=\begin{pmatrix}0&0&0&0&0\\0&0&0&0&0\\0&0&0&0&0\\1&0&0&0&0\end{pmatrix}.$$

Further, let

$$X = \begin{pmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{pmatrix}$$

be the $(4N+4)\times(4N+6)$ matrix with $(2N+2)\times(2N+3)$ sub-matrices X_{ij} defined by

$$X_{11} = h\left(\begin{array}{c|cccc} & \bar{X}_{11} & & & \\ & \bar{X}_{21} & \bar{X}_{22} & & \\ 0 & & \ddots & & \\ & & & \bar{X}_{k-1\,k-1} & \\ & & & \bar{X}_{k\,k-1} & \bar{X}_{k\,k} \end{array}\right), \quad k = \frac{N+1}{2},$$

$$\bar{X}_{11} = \begin{pmatrix} -0.0053 & 0.0024 & -0.0015 & 0.0006 \\ -0.0695 & -0.0161 & 0.0024 & -0.0006 \\ -0.1545 & -0.1448 & -0.0111 & 0.0003 \\ -0.2009 & -0.2292 & -0.0698 & 0 \end{pmatrix},$$

$$\bar{X}_{i\,i} = \begin{pmatrix} a_2 & a_3 & a_4 & a_5 \\ b_2 & b_3 & b_4 & b_5 \\ c_2 & c_3 & c_4 & c_5 \\ d_2 & d_3 & d_4 & d_5 \end{pmatrix}, \quad \bar{X}_{i\,i-1} = \begin{pmatrix} 0 & 0 & 0 & a_1 \\ 0 & 0 & 0 & b_1 \\ 0 & 0 & 0 & c_1 \\ 0 & 0 & 0 & d_1 \end{pmatrix}, \quad i = 2, \dots, k$$

with

$$a_1 = -\frac{(1801+559\sqrt{3})}{11340(2+\sqrt{3})}, \quad b_1 = -\frac{1171}{6720},$$
$$c_1 = -\frac{(-1801+559\sqrt{3})}{11340(-2+\sqrt{3})}, \quad d_1 = -\frac{37}{105},$$
$$a_2 = -\frac{(630+315)}{11340(2+\sqrt{3})}, \quad b_2 = -\frac{(945+576\sqrt{3})}{6720},$$
$$c_2 = \frac{(990+477\sqrt{3})}{11340(-2+\sqrt{3})}, \quad d_2 = -\frac{(54+18\sqrt{3})}{105},$$
$$a_3 = -\frac{(400-376\sqrt{3})}{11340(2+\sqrt{3})}, \quad b_3 = -\frac{280}{6720},$$
$$c_3 = \frac{(400+376\sqrt{3})}{11340(-2+\sqrt{3})}, \quad d_3 = -\frac{64}{105},$$
$$a_4 = -\frac{(990-477\sqrt{3})}{11340(2+\sqrt{3})}, \quad b_4 = -\frac{(945-576\sqrt{3})}{6720},$$
$$c_4 = -\frac{(-630+315\sqrt{3})}{11340(-2+\sqrt{3})}, \quad d_4 = -\frac{(54-18\sqrt{3})}{105},$$
$$a_5 = \frac{(41+21\sqrt{3})}{11340(2+\sqrt{3})}, \quad b_5 = -\frac{19}{6720},$$

$$c_5 = -\frac{(41-21\sqrt{3})}{11340(-2+\sqrt{3})}, \quad d_5 = -\frac{1}{105},$$

$$X_{12} = h^2 \left(\begin{array}{c|ccccc} & \tilde{X}_{11} & & & & \\ & \tilde{X}_{21} & \tilde{X}_{22} & & & \\ 0 & & & \ddots & & \\ & & & & \tilde{X}_{k-1\,k-1} & \\ & & & & \tilde{X}_{k\,k-1} & \tilde{X}_{k\,k} \end{array} \right), \quad k = \frac{N+1}{2},$$

$\tilde{X}_{11}$ is a zero square matrix of order 4,

$$\tilde{X}_{i\,i} = \begin{pmatrix} 0 & 0 & 0 & m_1 \\ 0 & 0 & 0 & m_2 \\ 0 & 0 & 0 & m_3 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \tilde{X}_{i\,i-1} = \begin{pmatrix} 0 & 0 & 0 & l_1 \\ 0 & 0 & 0 & l_2 \\ 0 & 0 & 0 & l_3 \\ 0 & 0 & 0 & l_4 \end{pmatrix}, \quad i = 2, \ldots, k,$$

$$l_1 = -\frac{(107+36\sqrt{3})}{11340(2+\sqrt{3})}, \quad l_2 = \frac{-67}{6720}, \quad l_3 = -\frac{(-107+36\sqrt{3})}{11340(-2+\sqrt{3})}, \quad l_4 = -\frac{2}{105},$$

$$m_1 = -\frac{(7+4\sqrt{3})}{11340(2+\sqrt{3})}, \quad m_2 = \frac{3}{6720}, \quad m_3 = -\frac{(-7+4\sqrt{3})}{11340(-2+\sqrt{3})},$$

$$X_{21} = \left(\begin{array}{c|ccccc} & \hat{X}_{11} & & & & \\ & \hat{X}_{21} & \hat{X}_{22} & & & \\ 0 & & & \ddots & & \\ & & & & \hat{X}_{k-1\,k-1} & \\ & & & & \hat{X}_{k\,k-1} & \hat{X}_{k\,k} \end{array} \right), \quad k = \frac{N+1}{2},$$

$$\hat{X}_{11} = \begin{pmatrix} -0.1129 & 0.0403 & -0.0258 & 0.0099 \\ -0.2343 & -0.2068 & 0.0478 & -0.0161 \\ -0.2166 & -0.4061 & -0.1890 & 0.0241 \\ -0.2204 & -0.3881 & -0.3288 & -0.0625 \end{pmatrix},$$

$$\hat{X}_{i\,i} = \begin{pmatrix} n_2 & n_3 & n_4 & n_5 \\ o_2 & o_3 & o_4 & o_5 \\ p_2 & p_3 & p_4 & p_5 \\ q_2 & q_3 & q_4 & q_5 \end{pmatrix}, \quad \hat{X}_{i\,i-1} = \begin{pmatrix} 0 & 0 & 0 & n_1 \\ 0 & 0 & 0 & o_1 \\ 0 & 0 & 0 & p_1 \\ 0 & 0 & 0 & q_1 \end{pmatrix}, \quad i = 2, \ldots, k,$$

with

$$n_1 = -\frac{(1726+885\sqrt{3})}{3780(2+\sqrt{3})}, \quad o_1 = -\frac{257}{1680}, \quad p_1 = -\frac{(-1726+885\sqrt{3})}{3780(-2+\sqrt{3})}, \quad q_1 = -\frac{19}{105},$$

$$n_2 = -\frac{(1656+780\sqrt{3})}{3780(2+\sqrt{3})}, \quad o_2 = -\frac{(432+315\sqrt{3})}{1680}, \quad p_2 = \frac{(396+60\sqrt{3})}{3780(\sqrt{3}-2)}, \quad q_2 = -\frac{54}{105},$$

$$n_3 = -\frac{(96-320\sqrt{3})}{3780(2+\sqrt{3})}, \quad o_3 = -\frac{512}{1680}, \quad p_3 = \frac{(96+320\sqrt{3})}{3780(-2+\sqrt{3})}, \quad q_3 = -\frac{64}{105},$$
$$n_4 = -\frac{(396-60\sqrt{3})}{3780(2+\sqrt{3})}, \quad o_4 = -\frac{(432-315\sqrt{3})}{1680}, \quad p_4 = \frac{(1656-780\sqrt{3})}{3780(\sqrt{3}-2)}, \quad q_4 = -\frac{54}{105},$$
$$n_5 = \frac{(94+25\sqrt{3})}{3780(2+\sqrt{3})}, \quad o_5 = -\frac{47}{1680}, \quad p_5 = -\frac{(94-25\sqrt{3})}{3780(-2+\sqrt{3})}, \quad q_5 = -\frac{19}{105},$$

$$X_{22} = h\left(\begin{array}{c|ccccc} & \breve{X}_{11} & & & & \\ & \breve{X}_{21} & \breve{X}_{22} & & & \\ 0 & & & \ddots & & \\ & & & & \breve{X}_{k-1\,k-1} & \\ & & & & \breve{X}_{k\,k-1} & \breve{X}_{k\,k} \end{array}\right), \quad k = \frac{N+1}{2},$$

$\breve{X}_{1\,1}$ is a zero square matrix of order 4,

$$\breve{X}_{i\,i} = \begin{pmatrix} 0 & 0 & 0 & v_1 \\ 0 & 0 & 0 & v_2 \\ 0 & 0 & 0 & v_3 \\ 0 & 0 & 0 & v_4 \end{pmatrix}, \quad \breve{X}_{i\,i-1} = \begin{pmatrix} 0 & 0 & 0 & t_1 \\ 0 & 0 & 0 & t_2 \\ 0 & 0 & 0 & t_3 \\ 0 & 0 & 0 & t_4 \end{pmatrix}, \quad i = 2, \ldots, k,$$

with

$$t_1 = -\frac{(124+65\sqrt{3})}{3780(2+\sqrt{3})}, \quad t_2 = -\frac{8}{1680}, \quad t_3 = -\frac{(-124+65\sqrt{3})}{3780(-2+\sqrt{3})}, \quad t_4 = \frac{-1}{105},$$
$$v_1 = -\frac{(16+5\sqrt{3})}{3780(2+\sqrt{3})}, \quad v_2 = \frac{8}{1680}, \quad v_3 = -\frac{(-16+5\sqrt{3})}{3780(-2+\sqrt{3})}, \quad v_4 = \frac{1}{105}.$$

Now, let $z(x)$ be the true solution of the SBVP. We define the $(4N+4)$-vector Z and $(4N+6)$-vector $\mathscr{F}$ by

$$\begin{aligned} Z &:= \Big(z(x_r), z(x_s), z(x_t), z(x_1), z(x_{1+p}), z(x_2), \ldots, \\ &\qquad z(x_{N-1}), z(x_{N-2+q}), z'(x_0), z'(x_r), \ldots, z'(x_N)\Big)^T, \\ \mathscr{F} &:= \Big(f\big(x_0, z(x_0), z'(x_0)\big), f\big(x_r, z(x_r), z'(x_r)\big), \ldots, \\ &\qquad f\big(x_N, z(x_N), z'(x_N)\big), g\big(x_0, z(x_0), z'(x_0)\big), \\ &\qquad g\big(x_r, z(x_r), z'(x_r)\big), \ldots, g\big(x_N, z(x_N), z'(x_N)\big)\Big)^T. \end{aligned}$$

The representation of the global system corresponding to the optimised global method, whose solutions are the exact values, can be written as

$$D_{(4N+4)\times(4N+4)} Z_{4N+4} + hX_{(4N+4)\times(4N+6)} \mathscr{F}_{4N+6} + C_{4N+4} = \mathscr{L}(h)_{4N+4}. \tag{3.3}$$

In the above expression the subscripts denote the dimensions of the corresponding matrices. The vector C_{4N+4} contains the known values — i.e.

$$C_{4N+4} = (-z_a, -z_a, -z_a, -z_a, 0, \ldots, 0, z_b, 0, \ldots, 0)^T,$$

and the vector $\mathscr{L}(h)_{4N+4}$ contains the local truncation errors from

$$\mathscr{L}(h) = \begin{pmatrix} 2.8055562 \times 10^{-6} z^{(6)}(x_0)h^6 + \mathscr{O}(h^7) \\ \cdots \\ 1.4172335 \times 10^{-7} z^{(8)}(x_0)h^8 + \mathscr{O}(h^9) \\ \dfrac{1}{1837080\sqrt{3}} z^{(9)}(x_1)h^9 + \mathscr{O}(h^{10}) \\ \dfrac{-1}{14515200} z^{(10)}(x_1)h^{10} + \mathscr{O}(h^{11}) \\ \dfrac{-1}{1837080\sqrt{3}} z^{(9)}(x_1)h^9 + \mathscr{O}(h^{10}) \\ \cdots \\ \cdots \\ \dfrac{-1}{58939650} z^{(11)}(x_{N-2})h^{11} + \mathscr{O}(h^{12}) \\ 0.000045852 z^{(6)}(x_0)h^5 + \mathscr{O}(h^6) \\ \cdots \\ -2.0246 \times 10^{-8} z^{(9)}(x_0)h^8 + \mathscr{O}(h^9) \\ \dfrac{1}{612360} z^{(9)}(x_1)h^8 + \mathscr{O}(h^9) \\ \dfrac{-1}{362880} z^{(9)}(x_1)h^8 + \mathscr{O}(h^9) \\ \dfrac{1}{612310} z^{(9)}(x_1)h^8 + \mathscr{O}(h^9) \\ \cdots \\ \cdots \\ \dfrac{1}{589396500} z^{(12)}(x_{N-2})h^{11} + \mathscr{O}(h^{12}) \end{pmatrix}.$$

Now, consider the system of approximate values of the problem — viz.

$$D_{(4N+4)\times(4N+4)}\bar{Z}_{4N+4} + hX_{(4N+4)\times(4N+6)}\bar{\mathscr{F}}_{4N+6} + C_{4N+4} = 0, \tag{3.4}$$

where

$$\bar{Z}_{4N+4} = \left(z_r, z_s, z_t, z_1, z_{1+p}, z_2, z_{1+q}, z_3, z_{3+p}, z_4, \ldots, z_{N-2+q}, z_0', z_r', \ldots, z_N'\right)^T,$$

is the vector of approximate values of Z_{4N+4} and $\bar{\mathscr{F}}_{4N+6}$ is given by

$$\bar{\mathscr{F}}_{4N+4} = \left(f_0, f_r, f_s, f_t, f_1, f_{1+p}, f_2, \ldots, f_N, g_0, g_r, g_s, g_t, g_1, g_{1+p}, g_2, \ldots, g_N\right)^T.$$

Subtracting (3.4) from (3.3) yields

$$D\mathscr{E} + hX(\mathscr{F} - \bar{\mathscr{F}}) = \mathscr{L}(h), \tag{3.5}$$

where the vector $\mathscr{E} = Z - \bar{Z} = (E_r, E_s, E_t, E_1, E_{1+p}, E_2, \dots, E_{N-2+q}, E'_0, E'_r, \dots, E'_N)^T$ contains the errors at intra-step and nodal points.

Using the Mean Value Theorem, for $i = 0, r, s, t, 1, 1+p, 2, 1+q, 3, 3+p, 4, \dots, N$, we have

$$\begin{aligned} f\big(x_i, z(x_i), z'(x_i)\big) - f(x_i, z_i, z'_i) &= \big(z(x_i) - z_i\big)\frac{\partial f}{\partial z}(\xi_i) + \big(z'(x_i) - z'_i\big)\frac{\partial f}{\partial z'}(\xi_i), \\ g\big(x_i, z(x_i), z'(x_i)\big) - g(x_i, z_i, z'_i) &= \big(z(x_i) - z_i\big)\frac{\partial g}{\partial z}(\eta_i) + \big(z'(x_i) - z'_i\big)\frac{\partial g}{\partial z'}(\eta_i). \end{aligned} \tag{3.6}$$

Here, ξ_i and η_i refer to the intermediate points on the segment joining $(x_i, z(x_i), z'(x_i))$ and (x_i, z_i, z'_i). The representations (3.6) give

$$\mathscr{F} - \bar{\mathscr{F}} = J_{(4N+6)\times(4N+4)}\mathscr{E}_{4N+4}, \tag{3.7}$$

where J is a matrix of partial derivatives of f, g with respect to z, z', evaluated at the intermediate points. Note that we used known boundary conditions, so that $E_0 = z(x_0) - z_0 = 0$ and $E_N = z(x_N) - z_N = 0$. It follows from the Eqs. (3.5) and (3.7) that

$$D_{(4N+4)\times(4N+4)}\mathscr{E}_{4N+4} + hX_{(4N+4)\times(4N+6)}J_{(4N+6)\times(4N+4)}\mathscr{E}_{4N+4} = \mathscr{L}(h)_{4N+4}. \tag{3.8}$$

The matrix $\mathscr{M}_{(4N+4)\times(4N+4)} = D_{(4N+4)\times(4N+4)} + hX_{(4N+4)\times(4N+6)}J_{(4N+6)\times(4N+4)}$ is invertible for all sufficiently small h. Moreover, it is singular only for a few h. Indeed, taking into account the sparsity of D, one can use the cofactor expansion along a row or a column to show that $\det(D_{(4N+4)\times(4N+4)}) = -Nh$, so that D is invertible as soon as $h > 0$. Writing matrix $\mathscr{M}$ in the form

$$\mathscr{M} = D + hXJ = (Id - B)D$$

with the identity matrix Id of order $4N+4$ and $B = -hXJD^{-1}$, we have

$$\det \mathscr{M} = \det(Id - B)\, \det D.$$

Let $\bar{\lambda}_i$ denote an eigenvalue of XJD^{-1}. Considering the characteristic polynomial

$$\det(\lambda Id - B) = \prod_{i=1}^{4N+4} (\lambda - \lambda_i)$$

of B, we note that for $\lambda = 1$, the determinant of $Id - B$ does not vanish if $1 + h\bar{\lambda}_i \neq 0$, $i = 1, \dots, N+4$. Therefore, we can write

$$\mathscr{E}_{4N+4} = \mathscr{M}^{-1}_{(4N+4)\times(4N+4)}\mathscr{L}(h)_{4N+4}. \tag{3.9}$$

Consider the maximum norm $\|\mathscr{E}\| = \max_i |E_i|$ in $\mathbb{R}^{4N+4}$ and the induced matrix norm in $\mathbb{R}^{(4N+4)\times(4N+4)}$. Expanding each term of $\mathscr{M}^{-1}_{(4N+4)\times(4N+4)}$ in a series in powers of h one can show that $\|\mathcal{M}^{-1}_{(4N+4)\times(4N+4)}\| = \mathcal{O}(h^{-1})$. The proof relies on the special structure of matrix $\mathcal{M}$. More exactly, if $N = 2j+1, j \geq 1, j \in \mathbb{N}$, the matrix $\mathcal{M}$ can written as

$$\mathcal{M} = \begin{pmatrix} \mathcal{M}_{11} & \mathcal{M}_{12} \\ \mathcal{M}_{21} & \mathcal{M}_{22} \end{pmatrix},$$

where the $(2N+2)\times(2N+1)$ submatrices $\mathcal{M}_{i1}, i = 1,2$ and the $(2N+2)\times(2N+3)$ submatrices $\mathcal{M}_{i2}, i = 1,2$ have the form

$$\mathcal{M}_{11} = \begin{pmatrix} \bar{\mathcal{M}}_{11} & \bar{\mathcal{M}}_{12} & & & & \\ & \bar{\mathcal{M}}_{22} & \bar{\mathcal{M}}_{23} & & & \\ & & \bar{\mathcal{M}}_{33} & & & \\ & & & \ddots & & \\ & & & & \bar{\mathcal{M}}_{k-1\,k-1} & \bar{\mathcal{M}}_{k-1\,k} \\ & & & & & \bar{\mathcal{M}}_{k\,k} \end{pmatrix}, \quad k = \frac{N+1}{2},$$

$$\bar{\mathcal{M}}_{11} = \begin{pmatrix} P(h^2) \end{pmatrix}_{4\times 3}, \quad \bar{\mathcal{M}}_{ii} = \begin{pmatrix} p(h^3) & \\ p(h^3) & \\ p(h^3) & P(h^2) \\ p(h^3) & \end{pmatrix}_{4\times 4}, \quad i = 2, \ldots, k,$$

$$\bar{\mathcal{M}}_{12} = \begin{pmatrix} p(h^2) & \\ p(h^2) & \\ p(h^2) & \mathbf{0} \\ 1 & \end{pmatrix}_{4\times 4}, \quad \bar{\mathcal{M}}_{i\,i+1} = \begin{pmatrix} p(h^3) & \\ p(h^3) & \\ p(h^3) & \mathbf{0} \\ p(h^2) & \end{pmatrix}_{4\times 4}, \quad i = 2, \ldots, k-1,$$

$$\mathcal{M}_{12} = \begin{pmatrix} \hat{\mathcal{M}}_{11} & \hat{\mathcal{M}}_{12} & & & & \\ & \hat{\mathcal{M}}_{22} & \hat{\mathcal{M}}_{23} & & & \\ & & \hat{\mathcal{M}}_{33} & & & \\ & & & \ddots & & \\ & & & & \hat{\mathcal{M}}_{k-1\,k-1} & \hat{\mathcal{M}}_{k-1\,k} \\ & & & & & \hat{\mathcal{M}}_{k\,k} \end{pmatrix}, \quad k = \frac{N+1}{2},$$

$$\hat{\mathcal{M}}_{11} = \begin{pmatrix} p(h) & \\ p(h) & \\ p(h) & P(h^2) \\ p(h) & \end{pmatrix}_{4\times 4}, \quad \hat{\mathcal{M}}_{ii} = \begin{pmatrix} p(h^3) & \\ p(h^3) & \\ p(h^3) & P(h^2) \\ p(h^3) & \end{pmatrix}_{4\times 4}, \quad i = 2, \ldots, k-1,$$

$$\hat{\mathcal{M}}_{12} = \begin{pmatrix} p(h^2) & \\ p(h^2) & \\ p(h^2) & \mathbf{0} \\ 0 & \end{pmatrix}_{4\times 4}, \quad \hat{\mathcal{M}}_{i\,i+1} = \begin{pmatrix} p(h^3) & \\ p(h^3) & \\ p(h^3) & \mathbf{0} \\ p(h^2) & \end{pmatrix}_{4\times 4}, \quad i = 2, \ldots, k-2,$$

$$\hat{\mathcal{M}}_{k-1\,k} = \begin{pmatrix} p(h^3) & \\ p(h^3) & \\ p(h^3) & \mathbf{0} \\ p(h^2) & \end{pmatrix}_{4\times 5}, \quad \hat{\mathcal{M}}_{k\,k} = \begin{pmatrix} p(h^3) & & p(h^3) \\ p(h^3) & P(h^2) & p(h^3) \\ p(h^3) & & p(h^3) \\ p(h^3) & & p(h^3) \end{pmatrix}_{4\times 5},$$

$$\mathscr{M}_{21} = \begin{pmatrix} \tilde{\mathscr{M}}_{11} & \tilde{\mathscr{M}}_{12} & & & & \\ & \tilde{\mathscr{M}}_{22} & \tilde{\mathscr{M}}_{23} & & & \\ & & \tilde{\mathscr{M}}_{33} & & & \\ & & & \ddots & & \\ & & & & \tilde{\mathscr{M}}_{k-1\,k-1} & \tilde{\mathscr{M}}_{k-1\,k} \\ & & & & & \tilde{\mathscr{M}}_{k\,k} \end{pmatrix}, \quad k = \frac{N+1}{2},$$

$$\tilde{\mathscr{M}}_{11} = \begin{pmatrix} \\ P(h) \\ \\ \end{pmatrix}_{4\times 3}, \quad \tilde{\mathscr{M}}_{ii} = \begin{pmatrix} p(h^2) & \\ p(h^2) & \\ p(h^2) & P(h) \\ p(h^2) & \end{pmatrix}_{4\times 4}, \quad i = 2,\dots,k,$$

$$\tilde{\mathscr{M}}_{12} = \begin{pmatrix} p(h) & \\ p(h) & \\ p(h) & \mathbf{0} \\ p(h) & \end{pmatrix}_{4\times 4}, \quad \tilde{\mathscr{M}}_{i\,i+1} = \begin{pmatrix} p(h^2) & \\ p(h^2) & \\ p(h^2) & \mathbf{0} \\ p(h^2) & \end{pmatrix}_{4\times 4}, \quad i = 2,\dots,k-1,$$

$$\mathscr{M}_{22} = \begin{pmatrix} \breve{\mathscr{M}}_{11} & \breve{\mathscr{M}}_{12} & & & & \\ & \breve{\mathscr{M}}_{22} & \breve{\mathscr{M}}_{23} & & & \\ & & \breve{\mathscr{M}}_{33} & & & \\ & & & \ddots & & \\ & & & & \breve{\mathscr{M}}_{k-1\,k-1} & \breve{\mathscr{M}}_{k-1\,k} \\ & & & & & \breve{\mathscr{M}}_{k\,k} \end{pmatrix}, \quad k = \frac{N+1}{2},$$

$$\breve{\mathscr{M}}_{11} = \begin{pmatrix} -1 & \\ -1 & \\ -1 & P(h) \\ -1 & \end{pmatrix}_{4\times 4}, \quad \breve{\mathscr{M}}_{ii} = \begin{pmatrix} p(h^2) & \\ p(h^2) & \\ p(h^2) & P(h) \\ p(h^2) & \end{pmatrix}_{4\times 4}, \quad i = 2,\dots,k-1,$$

$$\breve{\mathscr{M}}_{12} = \begin{pmatrix} p(h) & \\ p(h) & \\ p(h) & \mathbf{0} \\ p(h) & \end{pmatrix}_{4\times 4}, \quad \breve{\mathscr{M}}_{i\,i+1} = \begin{pmatrix} p(h^2) & \\ p(h^2) & \\ p(h^2) & \mathbf{0} \\ p(h^2) & \end{pmatrix}_{4\times 4}, \quad i = 2,\dots,k-2,$$

$$\breve{\mathscr{M}}_{k-1\,k} = \begin{pmatrix} p(h^2) & \\ p(h^2) & \\ p(h^2) & \mathbf{0} \\ p(h^2) & \end{pmatrix}_{4\times 5}, \quad \breve{\mathscr{M}}_{k\,k} = \begin{pmatrix} p(h^2) & & p(h^2) \\ p(h^2) & & p(h^2) \\ p(h^2) & P(h) & p(h^2) \\ p(h^2) & & p(h^2) \end{pmatrix}_{4\times 5}.$$

The notation $p(h^m)$ means a polynomial in h of the degree at most m, while $P(h^m)$ and $\mathbf{0}$ are submatrices all entries of which are polynomials in h of the degree m and zeros, respectively. The not explicitly written entries are zeros.

To construct the inverse we use cofactors and determinant. The determinant of $\mathscr{M}$ has cumbersome representation $\det(\mathscr{M}) = hQ_r(h)$, where $Q_r(h) = a_0 + a_1 h + \cdots + a_r h^r$ is a polynomial of degree r. The cofactors are also polynomials $R_s(h) = b_0 + b_1 h + \cdots + b_s h^s$ with $r \le s$. Thus the entries of $\mathscr{M}^{-1}$ with the lower order approximation have the form

$$\frac{b_0 + b_1 h + \cdots + b_s h^s}{h(a_0 + a_1 h + \cdots + a_r h^r)} = \mathcal{O}\big(h^{-1}\big).$$

Finally, using the Eq. (3.9) and assuming that $z(x)$ has bounded derivatives up to order nine, we get

$$\|\mathcal{E}_{4N+4}\| \le \left\|\mathcal{M}^{-1}_{(4N+4)\times(4N+4)}\right\| \left\|\mathcal{L}(h)_{4N+4}\right\|.$$

We are interested in the components $E_j, j = 1, 2, \ldots, N-1$, of $\mathcal{E}$ corresponding to the grid points, not the intermediate ones, and thus we have

$$\left\|(E_1, E_2, \ldots, E_{N-1})^T\right\| \le \left|\mathcal{O}\big(h^{-1}\big)\right| \left|\mathcal{O}\big(h^8\big)\right| \le K h^7.$$

This completes the proof. □

4. Implementation Details

In this section, we discuss how to implement the block global method for solving the SBVP (1.1) with the boundary conditions (1.2). The algorithm could be written as follows.

Step 1. Consider the ad hoc formulas (2.8).

Step 2. Consider the main formulas (2.5)-(2.6) for $n = 1(2)N-2$.

Step 3. Combining all equations in Steps 1 and 2 with two BCs (1.2) leads to the system of $4N+6$ equations in $4N+6$ unknowns

$$\begin{aligned}&\left\{z_0, z_r, z_s, z_t, z_1, z_{1+p}, z_2, z_{1+q}, z_3, z_{3+p}, z_4, \ldots, z_N\right\},\\ &\left\{z'_0, z'_r, z'_s, z'_t, z'_1, z'_{1+p}, z'_2, z'_{1+q}, z'_3, z'_{3+p}, z'_4, \ldots, z'_N\right\}.\end{aligned}$$

For the system of equations obtained in Step 3, we shall consider the following possibilities:

(i) If the resulting system is linear, one can use the existing linear system solvers.

(ii) If the system is nonlinear, one can use Newton-Raphson's-type or other nonlinear system solvers. For details on Newton-Raphson method and other methods the reader is referred to [3, 29].

Remark 4.1. Applying an iterative method to nonlinear systems, one needs a good starting point. To solve a given SBVP (1.1) with any two BCs in (2.1) by the global hybrid block method, we have to solve a system of $4N+6$ equations with $4N+6$ unknowns. It is reduced to a system of $4N+4$ equations with $4N+4$ unknowns for Dirichlet or Neumann boundary conditions. The resulting system can be solved by any corresponding system solver. For nonlinear systems, a Newton-Raphson's-type iterative algorithm can be used. In order to implement Newton-Raphson's-type iterative algorithms, a good starting approximation is required. For this, we consider the following criteria.

(i) For Dirichlet-type BC $z_0 = z_a, z_N = z_b$, the resulting system of equations is further reduced to $4N+4$ equations in $4N+4$ unknowns. The following criterion could be used for appropriate initial starting values

$$z_i^{(0)} = z_0 + \frac{z_N - z_0}{b-a} ih, \quad i = r,s,t,1,1+p,2,1+q,\dots,N-2+q,$$
$$z_i'^{(0)} = \frac{z_N - z_0}{b-a}, \qquad i = 0,r,s,t,1,1+p,2,1+q,\dots,N-2+q,N.$$

(ii) For Neumann BC, we can follow the strategy presented in [32], viz. consider a class of nonlinear BVPs called $\Theta_j, j = 0(1)c$ such that for $j=0$, initially we have a problem Θ_0, which has only trivial solution $z(x) = 0$. If we take $j = c$ we recover the original problem. Thus, one has a set of BVPs given by

$$\Theta_j = \begin{cases} z'' = f(x,z,z') - f(x,0,0) + \dfrac{j}{c} f(x,0,0), \\ g_1\big(z(a), z'(a)\big) = \dfrac{j}{c} v_a, \\ g_2\big(z(b), z'(b)\big) = \dfrac{j}{c} v_b \end{cases}$$

for j=0(1)c.

Each of the above problems $\Theta_j, j = 1(1)c$ can be solved by the proposed method with starting values derived from the problem Θ_{j-1}. Setting $j = c$, we have that the resulting nonlinear system corresponds to the original SBVP (1.1).

Other criteria for finding appropriate initial approximations can be also used. In some cases, the zero initial approximations can be used (that may be accomplished with $c = 1$). For more details the reader can consult [32] and references therein.

5. Numerical Experiments

In this section, some numerical experiments are carried out for different problems. Some notations used in the following tables are: N is the number of sub-intervals of the interval of interest $[a,b]$ with $N \geq 3$ must be odd; we have taken $M = N-1$, and thus the first step is to apply the ad hoc formulas while the rest of subintervals are an even number, as it must be for a two-step block scheme. MAE_h is the designation of maximum absolute errors along the grid points on the interval of interest, considering a step size h. We have included the estimation of the numerical order of convergence with the proposed method in the tables presented. This estimation has been obtained with the usual formula

$$ROC \simeq \log_2\left(\frac{MAE_{2h}}{MAE_h}\right)$$

and the execution time in seconds is denoted by CPU.

All the experiments have been carried out by using Mathematica 11.3 on a personal computer with configuration i7-7500U, 1.80 GHz, using double precision arithmetic in the numerical computations.

5.1. Equilibrium of isothermal gas sphere problem

Consider the following nonlinear SBVP related with the equilibrium of the isothermal gas sphere

$$\left(x^2 z'(x)\right)' = -x^2 z(x)^5,$$
$$z'(0) = 0, \quad z(1) = \frac{\sqrt{3}}{2}.$$

The true solution of this problem is $z(x) = \sqrt{3/(3+x^2)}$. The problem has been solved by various methods, which are referred here to as Scheme-1, Scheme-2, Scheme-3 and Scheme-4, cf. [17, 20, 22, 38] and New Scheme. Numerical results presented in Tables 1 and 2, show a good performance of the method.

Table 1: MAEs for Example 5.1.

M	New Scheme	Scheme-1	Scheme-2
8	3.032×10^{-11} ROC:– CPU: 0.06	5.336×10^{-8}	–
16	6.959×10^{-14} ROC: 8.76 CPU: 0.86	1.594×10^{-9}	2.439×10^{-7}
32	2.053×10^{-16} ROC: 8.40 CPU: 1.07	2.673×10^{-11}	2.598×10^{-8}
64	6.948×10^{-19} ROC: 8.20 CPU: 2.29	4.320×10^{-13}	1.803×10^{-9}
128	2.524×10^{-21} ROC: 8.10 CPU: 16.29	6.804×10^{-15}	1.154×10^{-10}

Table 2: MAEs for Example 5.1.

M	New Scheme	Scheme-1	Scheme-3	Scheme-4
50	3.7820×10^{-18} ROC: – CPU: 1.28	1.8688×10^{-12}	2.2341×10^{-6}	7.6178×10^{-10}
100	1.5817×10^{-20} ROC: 7.90 CPU: 7.46	2.9696×10^{-14}	5.5832×10^{-7}	4.7553×10^{-11}

5.2. Thermal explosion problem

Consider a nonlinear singular boundary value problem that arises in the theory of thermal explosion [12,38], viz.

$$\begin{aligned} &\big(x\, z'(x)\big)' = x\, e^{z(x)}, \\ &z'(0) = 0, \quad z(1) = 0. \end{aligned}$$

The true solution of this problem is $z(x) = 2\log((d+1)/(d\,x^2+1))$, where $d = -5 + 2\sqrt{6}$. The numerical results obtained by New Scheme, Scheme-1 [38] and Scheme-2 [12] demonstrate a good performance of the new method — cf. Table 3.

Table 3: MAEs for Example 5.2.

M	New Scheme	Scheme-1	Scheme-2
8	3.378×10^{-11} ROC: - CPU: 0.06	3.592×10^{-9}	-
16	3.459×10^{-13} ROC: 6.60 CPU: 0.10	5.465×10^{-11}	2.520×10^{-3}
32	4.429×10^{-15} ROC: 6.28 CPU:0.34	7.175×10^{-13}	1.833×10^{-4}
64	6.283×10^{-17} ROC: 6.13 CPU: 1.64	1.134×10^{-14}	1.280×10^{-5}

5.3. Lane-Emden type problem

Consider the nonlinear Lane-Emden type problem studied in [19,40], i.e.

$$z''(x) + \left(1 + \frac{r}{x}\right) z'(x) = \frac{5x^3(5x^5 e^{z(x)} - x - r - 4)}{4 + x^5}, \tag{5.1}$$

$$z'(0) = 0, \quad z(1) + 5z'(1) = \log\left(\frac{1}{5}\right) - 5. \tag{5.2}$$

The true solution of this problem is $z(x) = -\log(4 + x^5)$. Here the problem is solved for $r = 0.25$ and $r = 1$ as in [19]. Numerical results obtained by the new method and by Scheme-1 and Scheme-2 [19,40] and presented in Tables 4 and 5 show a good behaviour of the proposed method.

Table 4: MAEs for Example 5.3 when $r = 0.25$.

M	New Scheme	Scheme-1	Scheme-2
16	9.626×10^{-13} ROC: – CPU: 0.23	1.231×10^{-9}	5.010×10^{-9}
32	7.940×10^{-16} ROC: 10.24 CPU: 0.56	1.906×10^{-11}	7.32×10^{-9}
64	6.772×10^{-19} ROC: 10.19 CPU: 2.42	2.967×10^{-13}	4.77×10^{-10}
128	6.000×10^{-22} ROC: 10.14 CPU: 16.32	2.665×10^{-15}	5.21×10^{-11}

Table 5: MAEs for Example 5.3 when $r = 1$.

M	New Scheme	Scheme-1	Scheme-2
16	1.134×10^{-12} ROC: - CPU: 0.17	1.761×10^{-9}	3.15×10^{-8}
32	9.122×10^{-16} ROC: 10.27 CPU: 0.57	2.682×10^{-11}	4.22×10^{-10}
64	7.762×10^{-19} ROC: 10.19 CPU: 2.45	4.183×10^{-13}	2.09×10^{-10}
128	7.016×10^{-22} ROC: 10.11 CPU: 15.89	9.769×10^{-15}	4.17×10^{-11}
256	6.578×10^{-25} ROC: 10.05 CPU: 134.01	1.332×10^{-15}	1.76×10^{-13}

5.4. SBVP with Dirichlet type BC

Consider the following two-point BVP [2] given by

$$z''(x) + \frac{2}{x}z'(x) - \frac{2}{(x-2)^2}z(x) = -\frac{3}{(x-2)^2(x+1)^2},$$
$$z(0) = -0.5, \quad z(1.5) = \frac{-4}{3}\log(2.5).$$

The true solution of the problem is $z(x) = \log(1+x)/x(x-2)$. We compare our method with a highly accurate scheme in [2]. The numerical results presented in Table 6 show a good performance of the proposed method.

Table 6: MAEs for Example 5.4.

M	New Scheme	Scheme in [44]
20	3.133×10^{-8} ROC: – CPU: 0.09	7.079×10^{-6}
40	1.081×10^{-10} ROC: 8.17 CPU: 0.29	1.269×10^{-7}
80	2.758×10^{-13} ROC: 8.61 CPU: 1.25	1.427×10^{-9}

5.5. SBVP with Dirichlet type BC

Finally, consider the nonlinear two-point SBVP with Dirichlet type BC [44]

$$
\begin{aligned}
&z''(x) + \frac{0.5}{x} z'(x) = 0.5e^{z(x)} - e^{2z(x)}, \\
&z(0) = \log(2), \quad z(1) = 0.
\end{aligned}
$$

The true solution of the problem is $z(x) = \log(2/(x^2+1))$. For this problem, we have plotted CPU time versus maximum absolute errors (MAEs) along the integration interval for different number of steps. Fig. 1 indicates that the method proposed very accurately solves the problem with a low CPU time.

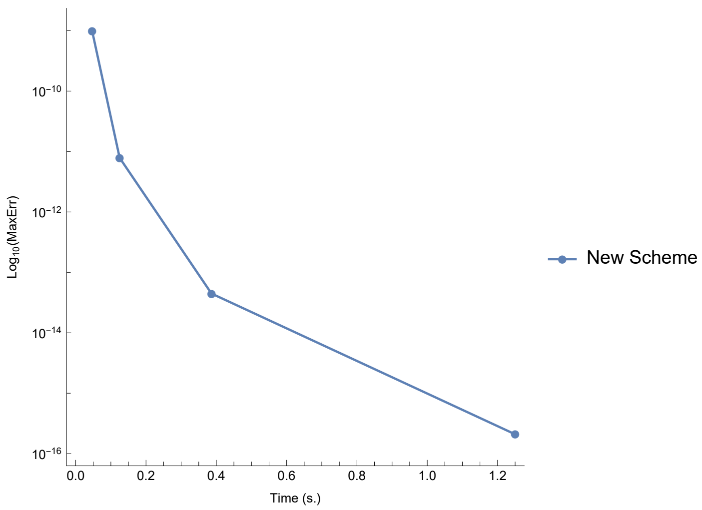

Figure 1: CPU times versus MAEs.

6. Conclusion

We developed an optimised global hybrid block method for second order SBVPs with two boundary conditions. It is a combination of main and an ad hoc formulas with optimised intra-step points. The ad hoc procedure is used just to pass the singularity and the main formulas are applied for other discrete points of interest. A theoretical analysis shows the method convergence order. Numerical experiments demonstrate that the method presents a good alternative for the problems considered.

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