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Journal of Computational and Applied Mathematics 176 (2005) 59–76

JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS

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High-order finite difference schemes for the solution of second-order BVPs☆

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Received 14 July 2003; received in revised form 4 June 2004

Abstract

We introduce new methods in the class of boundary value methods (BVMs) to solve boundary value problems (BVPs) for a second-order ODE. These formulae correspond to the high-order generalizations of classical finite difference schemes for the first and second derivatives. In this research, we carry out the analysis of the conditioning and of the time-reversal symmetry of the discrete solution for a linear convection–diffusion ODE problem. We present numerical examples emphasizing the good convergence behavior of the new schemes. Finally, we show how these methods can be applied in several space dimensions on a uniform mesh.

MSC: 65L10; 65L12; 65L20

Keywords: Finite difference schemes; Boundary value methods; Two-point boundary value problems; Conditioning analysis

1. Introduction

Let us consider the following two-point boundary value problem (BVP) for a scalar ordinary differential equation (ODE) with separated boundary conditions

$$\begin{cases} f(x, y, y', y'') = 0 \quad x \in [x_0, x_f], \\ y(x_0) = y_0, \quad y(x_f) = y_f, \end{cases} \tag{1}$$

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☆ Work supported by GNCS and MIUR (60% Project).

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doi:10.1016/j.cam.2004.07.008

where f is a sufficiently smooth function and it is assumed that a unique smooth solution exists. This general formulation includes, for example, convection–diffusion problems corresponding to the one-dimensional version of PDE models occurring in many applications (computational fluid-dynamics, electromagnetism, electrochemistry, nonlinear elasticity, etc.).

In this paper, we propose to solve (1) by stable finite difference schemes of high order on a uniform meshgrid. We reckon that the same analysis can be applied when more general boundary conditions are considered, but for the sake of simplicity we prefer not to present this treatment here.

The traditional discretization schemes for BVPs that use finite differences (see e.g. [4,10]) replace the derivatives in (1) with difference quotients and look for a global approximation of the solution by solving a system of algebraic equations. In this approach the simplest approximation involves central differences for both the first and second derivatives. The overall scheme has order two and for linear BVPs implies the solution of a tridiagonal linear system. In the literature, in order to have well-conditioned discrete problems, the diagonal dominance of the coefficient matrix is imposed and this leads to a restriction in the choice of the stepsize discretization [4,10]. An improvement in this direction can be obtained by imposing a less restrictive algebraic diagonal dominance [15]. The most used alternative to this method, known as the *upwind method*, involves forward or backward differences for the first derivative. In this case, no restriction on the stepsize is required but only first-order accuracy is achieved. Despite their low accuracy, it is worth to note that all the above-mentioned schemes are still used nowadays for discretizations along one-space dimension, especially in the PDE context.

Historically, as outlined in [4], to avoid the drawback related to the low order of accuracy, two types of extensions are essentially considered. The first one devises families of methods to solve the system of first-order ODEs equivalent to the second-order equation. The relevant literature is very rich. For example, in the context of one-step schemes, we can mention a class of implicit Runge–Kutta methods used in the code MIRKDC [8]. Similarly, in the class of multistep formulae, we can cite the BVMs [5] used in the Matlab code TOM [13] (see also [14]). On the other hand, acceleration techniques based on extrapolation or deferred corrections have been applied to a basic scheme in order to obtain faster convergence. For example, the code TWPBVP is based on deferred corrections of the trapezoidal rule [6,7]. A different strategy seeks a high-order approximation for the BVP in the original form (even when derivatives of order greater than two are present). For this goal, the *collocation methods*, that are a class of Runge–Kutta methods, compute a continuous piecewise polynomial representation of the solution. The Matlab code BVP4c [18] and the code COLNEW [4] are based on this technique.

In line with the idea of approximating the BVP in the original form and in the framework of boundary value methods (BVMs) [5], we construct high-order extensions of the classical central, forward and backward schemes on a uniform mesh. To this aim, in Section 2 we give a general result to define a difference scheme of order p to approximate the vth derivative $y^{(v)}$, for all $v \leqslant p$. Particular attention is devoted to the treatment of the boundary additional values required by finite difference schemes of order greater than two. Hence, we define three new classes of methods of even order to solve (1). It is worth to note that the obtained results can be also applied to systems of ODE–BVP. In Section 3, we carry out the conditioning analysis of the new schemes when they are applied to a linear homogeneous scalar BVP with separated boundary conditions. Moreover, we consider the concept of time-reversal symmetry for a second-order ODE–BVP, and we find the conditions that a numerical method must satisfy in order to yield an isotropic discrete solution. The convergence behavior of the new techniques is discussed in Section 4 for both a linear and a nonlinear example. Moreover, the numerical results are compared with those given by the symmetric BVMs (ETRs and TOMs in [5]) applied to the equivalent first-order ODE–BVP

system. Eventually, in Section 5 we explain how the proposed schemes can be used along each space dimension and then easily combined to solve an elliptic PDE on a uniform mesh.

2. Numerical approximation

Let us consider the discretization of the interval $[x_0, x_f]$ in (1) by means of a constant stepsize $h=(x_f - x_0)/(n+1)$ such that $x_i = x_0 + ih$, for $i = 0, \ldots, n+1$, and $x_{n+1} \equiv x_f$. Moreover, let $y_0, \ldots, y_{n+1}$ be the numerical solutions in $x_0, \ldots, x_{n+1}$. We set the values $k_1, k_2, k_3, k_4 \geqslant 1$ and approximate simultaneously the derivatives in the nonlinear two-point BVP (1) through the following finite difference schemes:

$$y''(x_i) \approx \frac{1}{h^2} \sum_{j=-k_1}^{k_2} \alpha_{k_1+j} y_{i+j} \tag{2}$$

for $i = k_1, \ldots, n - k_2 + 1$, and

$$y'(x_i) \approx \frac{1}{h} \sum_{j=-k_3}^{k_4} \beta_{k_3+j} y_{i+j} \tag{3}$$

for $i = k_3, \ldots, n - k_4 + 1$, where the coefficients α_j and β_j have to be computed in order to obtain formulae of order $k_1 + k_2$ and $k_3 + k_4$, respectively.

If $k_r = 1$ for $r = 1, \ldots, 4$, we have the classical central differences for the second and the first derivatives. It is well known that the overall scheme has order 2 and it is the simplest one to solve problem (1) (see e.g. [4, 9,16]). Either $k_1 + k_2 > 2$ or $k_3 + k_4 > 2$, then $m = \max(k_1 + k_2 - 2, k_3 + k_4 - 2)$ additional values of the solution are needed, that are not given by the boundary conditions of the continuous problem. We decide to use $k_1 + k_2 - 2$ extra formulae of the same order as (2) to approximate the second derivative and $k_3 + k_4 - 2$ formulae of the same order as (3) for the first derivative. These additional schemes are different from those used in [9,11,17,19], which require less steps and could have lower order, thus reducing the global order of approximation. They are, instead, strictly connected to the theory of BVMs (see [5]), and are defined by the following schemes:

$$\begin{aligned} y''(x_i) &\approx \frac{1}{h^2} \sum_{j=0}^{k_1+k_2} \alpha_j^{(i)} y_j, \quad i = 1, \ldots, k_1 - 1, \\ y''(x_i) &\approx \frac{1}{h^2} \sum_{j=0}^{k_1+k_2} \alpha_j^{(i-m_1)} y_{j+m_1}, \quad i = n - k_2 + 2, \ldots, n \end{aligned} \tag{4}$$

($m_1 = n + 1 - k_1 - k_2$), and

$$\begin{aligned} y'(x_i) &\approx \frac{1}{h} \sum_{j=0}^{k_3+k_4} \beta_j^{(i)} y_j, \quad i = 1, \ldots, k_3 - 1, \\ y'(x_i) &\approx \frac{1}{h} \sum_{j=0}^{k_3+k_4} \beta_j^{(i-m_3)} y_{j+m_3}, \quad i = n - k_4 + 2, \ldots, n \end{aligned} \tag{5}$$

($m_3 = n + 1 - k_3 - k_4$), where the coefficients $\alpha_j^{(i)}$ and $\beta_j^{(i)}$ have to be computed to devise schemes with the same order as the main schemes (2) and (3), respectively. In this way, by using all the previous schemes to compute $y_i' \approx y'(x_i)$ and $y_i'' \approx y''(x_i)$, the discretization of the BVP (1) yields the system of equations

$$f(x_i, y_i, y_i', y_i'') = 0 \quad \text{for } i = 1, \ldots, n, \tag{6}$$

in the unknowns $y_1, \ldots, y_n$.

In vector form, if $Y = [y_1, y_2, \ldots, y_n]^{\mathrm{T}}$ represents the unknown solution vector, we define the following BVMs for the approximation of the derivatives

$$Y''(x) \approx \frac{1}{h^2}\tilde{A}\tilde{Y}, \quad Y'(x) \approx \frac{1}{h}\tilde{B}\tilde{Y},$$

where $\tilde{Y} = [y_0, Y^{\mathrm{T}}, y_f]^{\mathrm{T}}$, and $\tilde{A}$ and $\tilde{B}$ are the $n \times (n+2)$ matrices containing the coefficients of the schemes (2)–(4) and (3)–(5), respectively.

If the same order is selected for both the derivatives, that is $p = k_1 + k_2 = k_3 + k_4$, the entries of $\tilde{A}$ and $\tilde{B}$ can be determined by solving appropriate linear systems with the same $(p+1) \times (p+1)$ Vandermonde coefficient matrix

$$V = \begin{pmatrix} 1 & 1 & 1 & \ldots & 1 \\ 0 & 1 & 2 & \ldots & p \\ 0 & 1 & 4 & \ldots & p^2 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 1 & 2^p & \ldots & p^p \end{pmatrix}. \tag{7}$$

The right-hand side in each of these systems depends on the order of the derivative we want to approximate and on the number of initial conditions required by the scheme. The following general result holds true:

Propostion 2.1. *For all $\nu \leqslant p$, the coefficients of the formula of order p*

$$y^{(\nu)}(x_{i+l}) \approx \frac{1}{h^\nu} \sum_{j=0}^{p} c_j^{(l)} y_{i+j} \tag{8}$$

required to approximate the νth derivative of $y(x)$ in x_{i+l}, for $l = 0, \ldots, p$, are the entries of the $(l+1)$th column of the $(p+1) \times (p+1)$ matrix

$$C^{(\nu)} = V^{-1} K^\nu V, \tag{9}$$

where V is the Vandermonde matrix in (7) *and*

$$K = \begin{pmatrix} 0 & & & & \\ 1 & 0 & & & \\ & 2 & \ddots & & \\ & & \ddots & \ddots & \\ & & & p & 0 \end{pmatrix}.$$

Proof. For the first derivative ($v = 1$), see [1]. In general, the unknown coefficients $c_j^{(l)}$ have to be determined such that the approximation (8) has maximum order p. The usual Taylor expansion yields the following conditions to be satisfied:

$$\sum_{j=0}^{p} j^s c_j^{(l)} = 0, \quad 0 \leqslant s \leqslant v-1,$$
$$\sum_{j=0}^{p} j^s c_j^{(l)} = \frac{s!}{(s-v)!} l^{s-v}, \quad v \leqslant s \leqslant p.$$

The assertion easily follows by representing these relations in vector form for each $l = 0, \ldots, p$. In fact, the above conditions mean that the coefficients $c_0^{(l)}, \ldots, c_p^{(l)}$ have to be computed by solving the linear system

$$Vc = (K^v V)e_{l+1},$$

where e_l is the lth unit vector of $\mathbb{R}^{p+1}$. Hence, the $(l+1)$th column of the matrix $C^{(v)}$ in (9) contains the coefficients of a scheme of order p with l initial conditions. □

We observe that, if $C^{(1)} = C$, then $C^{(v)} = C^v$, for all $v \leqslant p$. Consequently, since $J_p C J_p = -C$ (see [1]), where J_p is the $(p+1) \times (p+1)$ permutation matrix

$$J_p = \begin{pmatrix} & & & 1 \\ & & 1 & \\ & \cdot & & \\ \cdot & & & \\ 1 & & & \end{pmatrix}, \tag{10}$$

one has that $C^{(v)}$ satisfies

$$J_p C^{(v)} J_p = (-1)^v C^{(v)}. \tag{11}$$

Property (11) implies that $C^{(v)}$ is a centro-symmetric matrix for even derivatives and a skew-centro-symmetric matrix for odd derivatives. Therefore, the coefficients of the jth column are the same as those of the $(p+2-j)$th column, but in reverse order (and also changed in sign for the approximation of odd derivatives). For example, for $p = 4$ and $v = 1, 2$, we have

$$C^{(1)} = \begin{pmatrix} -\frac{25}{12} & -\frac{1}{4} & \frac{1}{12} & -\frac{1}{12} & \frac{1}{4} \\ 4 & -\frac{5}{6} & -\frac{2}{3} & \frac{1}{2} & -\frac{4}{3} \\ -3 & \frac{3}{2} & 0 & -\frac{3}{2} & 3 \\ \frac{4}{3} & -\frac{1}{2} & \frac{2}{3} & \frac{5}{6} & -4 \\ -\frac{1}{4} & \frac{1}{12} & -\frac{1}{12} & \frac{1}{4} & \frac{25}{12} \end{pmatrix}, \quad C^{(2)} = \begin{pmatrix} \frac{35}{12} & \frac{11}{12} & -\frac{1}{12} & -\frac{1}{12} & \frac{11}{12} \\ -\frac{26}{3} & -\frac{5}{3} & \frac{4}{3} & \frac{1}{3} & -\frac{14}{3} \\ \frac{19}{2} & \frac{1}{2} & -\frac{5}{2} & \frac{1}{2} & \frac{19}{2} \\ -\frac{14}{3} & \frac{1}{3} & \frac{4}{3} & -\frac{5}{3} & -\frac{26}{3} \\ \frac{11}{12} & -\frac{1}{12} & -\frac{1}{12} & \frac{11}{12} & \frac{35}{12} \end{pmatrix}.$$

Since the BVP (1) has one initial and one final condition, we do not use the first and the last column of each matrix $C^{(v)}$, since the first one does not require initial conditions and the last one does not require

final conditions. The remaining $p-1$ formulae identify several BVMs for the approximation of the νth derivative. A peculiar BVM is characterized by the choice of the main scheme (which must be used $n-p+2$ times) and, hence, by the number of initial conditions that it requires.

Since the second derivative represents the symmetric part of the convection–diffusion operator associated with the ODE–BVP (1), we discard the odd-order schemes. In fact, for this choice, the number of initial methods would be different from the number of the final ones and then a global symmetry would be lost. Moreover, for even-order $p=2k$ we choose as main scheme the BVM with k initial conditions, that is the $(k+1)$th column of $C^{(2)}$, since the centro-symmetry of $C^{(2)}$ implies the symmetry of this formula ($\alpha_i=\alpha_{2k-i}$). In this case we have $k_1=k_2=k$ and the $k-1$ initial and the $k-1$ final schemes fulfill the following property:

$$\alpha_i^{(j)}=\alpha_{2k-i}^{(2k-j)},\quad i=0,\dots,2k,\quad j=1,\dots,k-1.$$

We remark that the overall method is an even-order generalization of the *central difference scheme* which has been already introduced in [3] for the solution of Hamiltonian problems. In the following, we refer to these formulae as $D2$.

An explicit representation and some properties of the coefficients for the approximation of the first derivative are given in [1]. In our context, these formulae have different features since we use them in the solution of BVPs and coupled with those of the same order for the second derivative. Due to the definition of the D2 schemes, we prefer to consider BVMs of even order $p=2k$. Hence, we propose three classes of methods according to the choice of the main scheme.

The first one, introduced in [5] as a generalization of the midpoint formula for IVPs, is defined for $k_3=k_4=k$ and corresponds to choosing the $(k+1)$th column of $C^{(1)}$ as main BVM scheme. In this case, $k-1$ initial and $k-1$ final schemes are considered. The skew-centro-symmetry of $C^{(1)}$ implies that, in the main scheme, we have $\beta_i=-\beta_{2k-i}$ and, for the additional schemes, we have

$$\beta_i^{(j)}=-\beta_{2k-i}^{(2k-j)},\quad i=0,\dots,2k,\quad j=1,\dots,k-1.$$

The overall method leads to a high (even)-order extension of the classical *central difference scheme* [9] for the first derivative. For this reason, we define the formulae in this class as *extended central difference formulae* (ECDFs).

The second class of methods is defined for $k_3=k_4+2=k+1$ and corresponds to choosing the $(k+2)$th column of $C^{(1)}$ as main BVM scheme. In this case there are k initial and $k-2$ final schemes. We remark that the first $k-1$ initial schemes are the same of the ECDF and the kth is the main scheme of the ECDF. Note that any kind of symmetry is lost. These schemes can be considered an even-order extension of the classical first-order *backward difference scheme* and correspond to the *generalized backward differentiation formulae* (GBDFs) of even order (see [5]).

The third class of formulae is defined for $k_4=k_3+2=k+1$ and corresponds to choosing the kth column of $C^{(1)}$ as main BVM scheme. In this case, there are $k-2$ initial and k final formulae. These schemes can be considered as an even-order extension of the classical first-order *forward difference scheme*. For this reason, we define them as *generalized forward differentiation formulae* (GFDFs). Also in this case any kind of symmetry is lost.

In the following sections, the combination of these three classes of BVMs with the $D2$ scheme of the same order will be called D2ECDF, D2GBDF and D2GFDF, respectively. In Tables 1 and 2, we report the coefficients of all the formulae used for approximating the second and the first derivatives of even

Table 1
Coefficients α_i $(i = 0, \ldots, p)$ of the schemes of order p with j initial conditions $(j = 1, \ldots, p/2)$ for the approximation of the second derivative

p	j	α_0	α_1	α_2	α_3	α_4	α_5	α_6	α_7	α_8
2	**1**	1	−2	1						
4	1	$\frac{11}{12}$	$-\frac{5}{3}$	$\frac{1}{2}$	$\frac{1}{3}$	$-\frac{1}{12}$				
4	**2**	$-\frac{1}{12}$	$\frac{4}{3}$	$-\frac{5}{2}$	$\frac{4}{3}$	$-\frac{1}{12}$				
6	1	$\frac{137}{180}$	$-\frac{49}{60}$	$-\frac{17}{12}$	$\frac{47}{18}$	$-\frac{19}{12}$	$\frac{31}{60}$	$-\frac{13}{180}$		
6	2	$-\frac{13}{180}$	$\frac{19}{15}$	$-\frac{7}{3}$	$\frac{10}{9}$	$\frac{1}{12}$	$-\frac{1}{15}$	$\frac{1}{90}$		
6	**3**	$\frac{1}{90}$	$-\frac{3}{20}$	$\frac{3}{2}$	$-\frac{49}{18}$	$\frac{3}{2}$	$-\frac{3}{20}$	$\frac{1}{90}$		
8	1	$\frac{363}{560}$	$\frac{8}{315}$	$-\frac{83}{20}$	$\frac{153}{20}$	$-\frac{529}{72}$	$\frac{47}{10}$	$-\frac{39}{20}$	$\frac{599}{1260}$	$-\frac{29}{560}$
8	2	$-\frac{29}{560}$	$\frac{39}{35}$	$-\frac{331}{180}$	$\frac{1}{5}$	$\frac{9}{8}$	$-\frac{37}{45}$	$\frac{7}{20}$	$-\frac{3}{35}$	$\frac{47}{5040}$
8	3	$\frac{47}{5040}$	$-\frac{19}{140}$	$\frac{29}{20}$	$-\frac{118}{45}$	$\frac{11}{8}$	$-\frac{1}{20}$	$-\frac{7}{180}$	$\frac{1}{70}$	$-\frac{1}{560}$
8	**4**	$-\frac{1}{560}$	$\frac{8}{315}$	$-\frac{1}{5}$	$\frac{8}{5}$	$-\frac{205}{72}$	$\frac{8}{5}$	$-\frac{1}{5}$	$\frac{8}{315}$	$-\frac{1}{560}$

orders $p = 2k$ up to 8. For the second derivative, the main BVM schemes are typed bold for emphasis. Because of the symmetry, the formulae of order p with $p - j$ initial conditions $(j = 1, \ldots, p/2 - 1)$ are omitted.

3. Time-reversal symmetry and conditioning analysis

In this section, we show some properties of the new methods when applied to the linear and homogeneous scalar problem

$$y'' - 2\gamma y' + \mu y = 0, \tag{12}$$

with constant real coefficients γ and μ and with separated boundary conditions $y(x_0) = y_0$ and $y(x_f) = y_f$. By assuming that $\delta = \gamma^2 - \mu > 0$, the exact solution of (12) is given by

$$y(x) = c_1 e^{\lambda_1 x} + c_2 e^{\lambda_2 x},$$

where $\lambda_1 = \gamma + \sqrt{\delta}$ and $\lambda_2 = \gamma - \sqrt{\delta}$. The coefficients c_1 and c_2 depend on the boundary conditions and are given by

$$c_1 = \frac{y_0 e^{\lambda_2 x_f} - y_f}{e^{\lambda_2 x_f} - e^{\lambda_1 x_f}}, \quad c_2 = \frac{y_f - y_0 e^{\lambda_1 x_f}}{e^{\lambda_2 x_f} - e^{\lambda_1 x_f}}.$$

Table 2
Coefficients β_i $(i = 0, \ldots, p)$ of the schemes of order p with j initial conditions $(j = 1, \ldots, p/2)$ for the approximation of the first derivative

p	j	β_0	β_1	β_2	β_3	β_4	β_5	β_6	β_7	β_8
2	1	$-\frac{1}{2}$	0	$\frac{1}{2}$						
4	1	$-\frac{1}{4}$	$-\frac{5}{6}$	$\frac{3}{2}$	$-\frac{1}{2}$	$\frac{1}{12}$				
4	2	$\frac{1}{12}$	$-\frac{2}{3}$	0	$\frac{2}{3}$	$-\frac{1}{12}$				
6	1	$-\frac{1}{6}$	$-\frac{77}{60}$	$\frac{5}{2}$	$-\frac{5}{3}$	$\frac{5}{6}$	$-\frac{1}{4}$	$\frac{1}{30}$		
6	2	$\frac{1}{30}$	$-\frac{2}{5}$	$-\frac{7}{12}$	$\frac{4}{3}$	$-\frac{1}{2}$	$\frac{2}{15}$	$-\frac{1}{60}$		
6	3	$-\frac{1}{60}$	$\frac{3}{20}$	$-\frac{3}{4}$	0	$\frac{3}{4}$	$-\frac{3}{20}$	$\frac{1}{60}$		
8	1	$-\frac{1}{8}$	$-\frac{223}{140}$	$\frac{7}{2}$	$-\frac{7}{2}$	$\frac{35}{12}$	$-\frac{7}{4}$	$\frac{7}{10}$	$-\frac{1}{6}$	$\frac{1}{56}$
8	2	$\frac{1}{56}$	$-\frac{2}{7}$	$-\frac{19}{20}$	2	$-\frac{5}{4}$	$\frac{2}{3}$	$-\frac{1}{4}$	$\frac{2}{35}$	$-\frac{1}{168}$
8	3	$-\frac{1}{168}$	$\frac{1}{14}$	$-\frac{1}{2}$	$-\frac{9}{20}$	$\frac{5}{4}$	$-\frac{1}{2}$	$\frac{1}{6}$	$-\frac{1}{28}$	$\frac{1}{280}$
8	4	$\frac{1}{280}$	$-\frac{4}{105}$	$\frac{1}{5}$	$-\frac{4}{5}$	0	$\frac{4}{5}$	$-\frac{1}{5}$	$\frac{4}{105}$	$-\frac{1}{280}$

By means of the change of variable $\tau = x_0 + x_f - x$, from (12) we obtain

$$u'' + 2\gamma u' + \mu u = 0, \quad \tau \in [x_0, x_f], \tag{13}$$

where $u = u(\tau)$ and the derivatives are calculated with respect to τ. If we set the boundary conditions $u(x_0) = u_0 \equiv y_f$ and $u(x_f) = u_f \equiv y_0$, the two parametric curves $C_\tau : \{(\tau, u(\tau)), \tau \in [x_0, x_f]\}$ and $C_x : \{(x, y(x)), x \in [x_0, x_f]\}$ coincide. Moreover, a point that is moving forth on C_x, is running back on C_τ and viceversa. This property of the solution $y(x)$ of the BVP (12) is called *time isotropy* or *time-reversal symmetry* (see [5, p. 218]). It would be important to design a method yielding a numerical solution with this kind of invariance. For this reason, we derive a set of conditions that the coefficients of the BVMs introduced in this paper must satisfy in order to preserve the time isotropy also in the discrete case.

The numerical approximation of (12) is

$$(\tilde{A} - 2\gamma h\tilde{B} + \mu h^2 \tilde{I}_n)\tilde{Y} = 0, \tag{14}$$

where $\tilde{I}_n = [0_n, I_n, 0_n]$, 0_n is a null vector of length n, I_n is the $n \times n$ identity matrix, $\tilde{A}$, $\tilde{B}$ and $\tilde{Y}$ are defined in the previous section. Similarly, the numerical approximation of (13) with the same method on the same grid is

$$(\tilde{A} + 2\gamma h\tilde{B} + \mu h^2 \tilde{I}_n)\tilde{U} = 0, \tag{15}$$

where $\tilde{U} = [u_0, U^{\mathrm{T}}, u_f]^{\mathrm{T}} = [u_0, u_1, \ldots, u_n, u_f]^{\mathrm{T}}$ and $u_i \approx u(\tau_i)$ for $i = 1, \ldots, n$. The time reversal symmetry of the discrete solution corresponds to imposing that

$$\tilde{Y} = J_{n+2}\tilde{U},$$

where J_{n+2} is defined in (10). From (14) and (15), it is straightforward to obtain that the above property is fulfilled if

$$\tilde{A} = J_n \tilde{A} J_{n+2}, \quad \tilde{B} = -J_n \tilde{B} J_{n+2}. \tag{16}$$

These relations mean that the numerical method is isotropic when the coefficients of the matrices $\tilde{A}$ and $\tilde{B}$ satisfy, for all $i = 1, \ldots, n$ and $j = 1, \ldots, n+2$:

$$\tilde{a}_{ij} = \tilde{a}_{n+1-i,n+3-j} \quad \text{and} \quad \tilde{b}_{ij} = -\tilde{b}_{n+1-i,n+3-j},$$

that is: (i) the main scheme is symmetric for the approximation of the y'' and skew-symmetric for the y'; (ii) the same number of initial and final schemes is used, and (iii) the coefficients of the ith additional initial method are those of the $(n+1-i)$th final method in reverse order (and also changed in sign for the approximation of y').

We observe that only the D2ECDFs satisfy property (16). As a consequence, it is worth noting that the midpoint rule, belonging to this class for $p = 2$, is isotropic when applied to second-order BVPs even if it is not isotropic when applied to first-order BVPs, as outlined in [5].

In order to analyze the conditioning of the discrete problem associated to the proposed numerical methods, we rewrite problem (12) as the equivalent first-order ODE system

$$\begin{pmatrix} y' \\ z' \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\mu & 2\gamma \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix},$$

whose coefficient matrix has eigenvalues given by λ_1 and λ_2. Since $\lambda_1\lambda_2 = \mu$, the problem is well conditioned if and only if $\mu < 0$ (see Fig. 1). In fact, in this case the eigenvalues have different signs and the dichotomy holds in the space of solutions of the problem [4]. If $\mu = 0$ (along the vertical axis) the problem is said to be moderately conditioned (see [5]). On the other hand, if $\mu > 0$ (and $\delta > 0$) the problem is ill- conditioned (the case $\delta < 0$ corresponds to an oscillating solution and will not be considered in the following analysis). For this reason, we are looking for methods which yield a well-conditioned discrete problem for $\mu < 0$.

From Eq. (14) the following linear system arises:

$$(A - 2\gamma h B + \mu h^2 I)Y = d, \tag{17}$$

where d is the vector involving the known boundary conditions and A and B are quasi-Toeplitz matrices obtained by considering the columns from the second to the $(n+1)$th one of $\tilde{A}$ and $\tilde{B}$. For n large enough, the contribution of the initial and final methods on the condition number is in general negligible with respect to that of the main formula (see, for example, [12] for an analysis of the matrices arising from GBDFs applied to first-order problems and Problem 4 in the next Section 4). Moreover, the conditioning of finite dimension Toeplitz band matrices derives from the analysis of the corresponding infinite matrices [2]. For this reason, a simple way to study the well conditioning of the discrete problem, is to analyze the roots of the characteristic polynomial associated to the main method (see [5]) which is given by

$$\pi(z, \mu h^2, \gamma h) = \alpha(z) - 2\gamma h \beta(z) + \mu h^2 z^s, \tag{18}$$

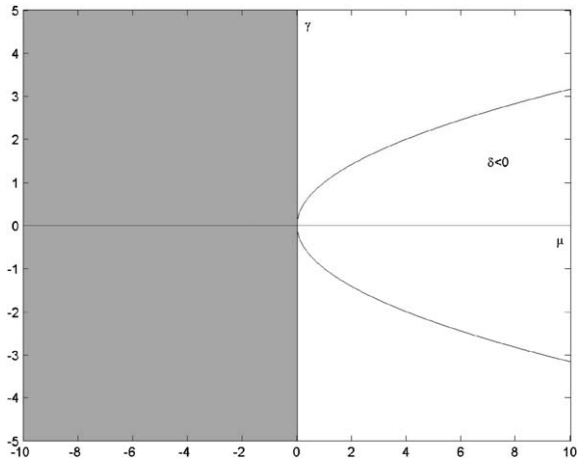

Fig. 1. (μ, γ)-region for the well conditioning of the continuous problem.

where $s = \max(k_1, k_3)$ and

$$\alpha(z) = \sum_{j=-k_1}^{k_2} \alpha_{k_1+j} z^{s+j}, \quad \beta(z) = \sum_{j=-k_3}^{k_4} \beta_{k_3+j} z^{s+j}.$$

Hence, (18) is a real polynomial of degree $s + r$, with $r = \max(k_2, k_4)$. Note that s corresponds to the number of lower diagonals of the coefficient matrix in (17) while r is the number of upper diagonals. If $\xi_i = \xi_i(\mu h^2, \gamma h)$ are the roots of (18) ordered by increasing modulus, the coefficient matrix in (17) is well conditioned if s roots are inside the unit circle and the remaining r roots are outside, that is $|\xi_i| < 1$, for $i = 1, \ldots, s$, and $|\xi_i| > 1$ otherwise. The roots ξ_s and ξ_{s+1} are said *principal roots* of the polynomial (18) since they essentially generate the numerical solution (the other ones give a negligible contribution). For $h \to 0$, they approximate the double root equal to 1 of the polynomial $\alpha(z)$.

To yield the counterpart of Fig. 1 in the discrete case, we can find a $(\mu h^2, \gamma h)$-region of well conditioning of the discrete problem. For this reason, we solve for $|\hat{z}|=1$ the equation $\pi(\hat{z}, \gamma h, \mu h^2)=0$ in order to obtain the boundaries separating the regions of well conditioning from those of ill conditioning. Therefore, since the polynomial (18) is linear with respect to γh and μh^2, the boundaries are indeed straight lines and they can be identified by the analysis of the following three cases:

- $z=1$: since the consistence of the schemes implies $\alpha(1)=\beta(1)=0$, the line $\mu h^2=0$ must be considered;
- $z = -1$: the equation to be analyzed is

$$\mu h^2 - 2\hat{\beta}\gamma h + \hat{\alpha} = 0, \tag{19}$$

where $\hat{\alpha} = \alpha(-1)/(-1)^s$ and $\hat{\beta} = \beta(-1)/(-1)^s$. By simple calculations, we have that $\hat{\alpha} < 0$ for all the methods of any order. Moreover, the value of $\hat{\beta}$ is positive for the D2GBDFs and negative for the D2GFDFs. The intersection of line (19) with the μh^2-axis is given by $-\hat{\alpha} > 0$. For the D2ECDFs, we have $\hat{\beta} = 0$ and then this line is parallel to the vertical axis and it is given by $\mu h^2 = |\hat{\alpha}|$. For the D2GBDFs and D2GFDFs, we have $\hat{\beta} \neq 0$ and then this line intercepts the vertical axis in $q = \hat{\alpha}/(2\hat{\beta})$.

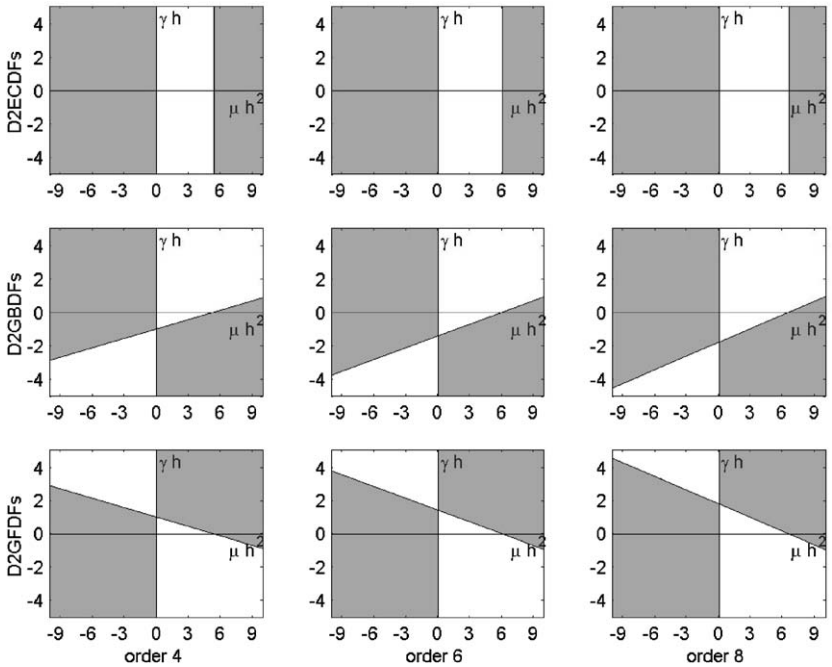

Fig. 2. $(\mu h^2, \gamma h)$-regions for the well conditioning of the D2ECDFs, D2GBDFs, D2GFDFs of orders 4, 6 and 8.

- z (and its conjugate) is a complex root such that $|z| = 1$: it is possible to show that $\alpha(\overline{z}) - \overline{z}^s \alpha(z)/z^s = 0$. The polynomial $\pi(z, \gamma h, \mu h^2) = 0$ reduces to $\mu h^2 - \alpha(z)/z^s$ that covers the segment between the points (0,0) and $(0, |\hat{\alpha}|)$.

The shaded regions in Fig. 2 represent the values of $(\mu h^2, \gamma h)$ such that the coefficient matrices are well conditioned for D2ECDFs, D2GBDFs and D2GFDFs of orders 4, 6 and 8.

The D2ECDFs always yield well-conditioned matrices for $\mu < 0$. Therefore, generalizations of the midpoint rule are unstable for initial value problems (see [5]) and BVPs of first order, but they are stable if applied to BVPs of second order. On the other hand, the discrete problem associated to the D2GBDFs and the D2GFDFs could be ill-conditioned for some values of $(\mu h^2, \gamma h)$ with $\mu < 0$. In fact, a restriction on the stepsize h can arise by solving the Eq. (19). If $\hat{\delta} = (\gamma\hat{\beta})^2 - \hat{\alpha}\mu$, the two roots of (19) are

$$h_1 = \frac{\gamma\hat{\beta} + \sqrt{\hat{\delta}}}{\mu}, \quad h_2 = \frac{\gamma\hat{\beta} - \sqrt{\hat{\delta}}}{\mu}.$$

Since $\hat{\alpha}\mu > 0$, no restriction on the stepsize arises when $\hat{\delta} < 0$ or $\gamma\hat{\beta} \geqslant 0$. The D2ECDFs have $\hat{\beta} = 0$ and this justifies the above well conditioning result independently from the value of γ. On the other hand, real positive values of h_1 and h_2 $(h_1 < h_2)$ exist for the D2GBDFs and D2GFDFs if and only if $\hat{\delta} > 0$ and $\gamma\hat{\beta} < 0$. Under this hypothesis the stepsize restriction $h \leqslant h_1$ arises for

Table 3
Maximum value of $|\gamma|h$ required to obtain well-conditioned matrices from D2GBDFs ($\gamma < 0$) and D2GFDFs ($\gamma > 0$)

Order	4	6	8	10
$\|q\|$	1	$\frac{17}{12}$	$\frac{16}{9}$	$\frac{21}{10}$

D2GBDFs when $\gamma < 0$ and for D2GFDFs when $\gamma > 0$. Moreover, if $\hat{\alpha}\mu$ is much smaller than $(\gamma\hat{\beta})^2$, then the previous restriction may be simplified as follows:

$$h \leqslant \frac{\hat{\alpha}}{2\gamma\hat{\beta}} \equiv \frac{q}{\gamma}.$$

This condition is sufficient to have well-conditioned matrices associated to the two methods. In Table 3, we report the values of q that give a measure of this restriction which only depends on the order p of the method. Note that the value of q increases when the order increases, that is the well-conditioning regions tend to become wider.

The above result on the conditioning is not entirely surprising because the D2GBDF can be seen as a high-order extension of the well-known backward finite differences that are used only when the coefficient γ of the first derivative (velocity) in (12) is positive. Conversely, the D2GFDF can be seen as a high-order extension of the forward finite differences that are used when $\gamma < 0$. We remark that the D2GBDFs and D2GFDFs could be combined to yield a well-conditioned method without stepsize restrictions that corresponds to a high (even)-order extension of the *upwind method*. In fact, the upwind scheme (of first-order) uses the forward differences when $\gamma < 0$ and the backward differences when $\gamma > 0$ (see e.g. [10], p. 153ff and [4], p. 434ff). A more detailed study of this method will be the subject of future research.

4. Numerical examples

The main goal of this section is to compare the convergence behavior of the proposed schemes for two test problems given in the "BVP software page" [6] of J. Cash. To this aim, we use a constant stepsize and we consider only mildly stiff examples. The first linear problem allows us to emphasize the restrictions required on the stepsize when the first derivative is approximated by the GBDFs. A similar result could be shown for the D2GFDFs by considering an analogous BVP with the coefficient of the first derivative of opposite sign. The second nonlinear problem is useful to underline some connections between the linear and the nonlinear case. Since the analytic solution is known for both tests, all tables and figures in this section report the absolute error (in the infinity norm). The continuous lines in the Figs. 3 and 5 represent the theoretical convergence orders. All tests were performed with Matlab 6.5.

4.1. Test problem 4 by Cash

Let us consider the linear problem

$$\varepsilon y'' + y' - (1+\varepsilon)y = 0,$$

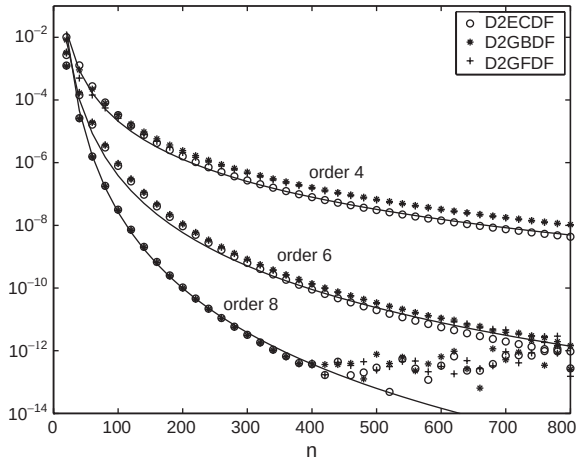

Fig. 3. Problem 4 for $\varepsilon = 0.1$: convergence behavior of D2ECDFs, D2GBDFs and D2GFDFs on a uniform meshgrid.

in $[-1, 1]$ with known boundary conditions. The exact solution

$$y_e(x) = \exp(x - 1) + \exp(-(1 + \varepsilon)(1 + x)/\varepsilon)$$

has a boundary layer in $x = -1$. We solve this problem for $\varepsilon = 0.1$ and $\varepsilon = 0.01$.

For $\varepsilon = 0.1$, the absolute errors of the three methods are plotted in Fig. 3. All the methods exhibit a behavior in line with the corresponding expected order. In particular, we observe that the D2ECDFs of orders 4 and 6 have an error smaller than the other formulae when equal order and equal number of meshpoints are considered. Moreover, all the methods are unable to attain accuracy up to the machine precision because of the conditioning of the corresponding discrete problem.

For $\varepsilon = 0.01$, we report the absolute errors given by the three methods in Table 4. For large values of n the error of each method decreases according to the theoretically predicted order. For small values of n the obtained results lead to some interesting considerations.

First of all, we note that the solution computed with $n = 49$ ($h = \frac{2}{50}$) by using the D2GBDF of any order is completely different from the theoretical one. This result agrees with the conditioning analysis of the previous section. In fact, from (12) we have $\mu = -(1 + \varepsilon)/\varepsilon < 0$ and $\gamma = -1/(2\varepsilon) < 0$. This means that we expect an ill-conditioned discrete problem when we use D2GBDF with the stepsizes $h > 2.02\text{e-}2$ ($n < 99$) for the order 4, $h > 2.87\text{e-}2$ ($n < 69$) for the order 6 and $h > 3.63\text{e-}2$ ($n < 55$) for the order 8. Note that these bounds for h essentially correspond to those in Table 3. Actually, as reported in Fig. 4, the condition number of the coefficient matrices associated to the D2GBDFs seems to grow quadratically when n is less then the previous critical values and linearly for larger ones (in Fig. 4 the continuous lines are used to connect the condition numbers computed for the D2GBDFs). Therefore, the theoretical results concerning the conditioning analysis of Section 3 are indeed supported by the numerical ones.

As shown in Table 4, the drawback associated to the D2GBDFs is avoided when the D2GFDFs are used even if, as for D2ECDFs, from $n = 49$ to 99 the error does not decrease according to the expected rate. This bad behavior is due to the small number of points in the boundary layer. In particular, the D2ECDFs exhibit a solution with small oscillations. These oscillations have been observed in correspondence of centered schemes of order two by several authors (see, for example, [16]). They arise when the principal

Table 4
Problem 4 for $\varepsilon = 0.01$: convergence behavior of D2ECDFs, D2GBDFs and D2GFDFs on a uniform meshgrid

		D2ECDF		D2GBDF		D2GFDF	
p	n	Error	Rate	Error	Rate	Error	Rate
4	49	5.06e-02		9.51e+00		5.40e-02	
	99	3.10e-02	0.70	4.29e-02	7.79	1.48e-02	1.87
	199	8.79e-03	1.82	8.23e-03	2.38	3.44e-03	2.10
	399	9.81e-04	3.16	8.55e-04	3.27	4.91e-04	2.81
	799	6.30e-05	3.96	6.99e-05	3.61	5.09e-05	3.27
	1599	3.20e-06	4.30	4.94e-06	3.82	4.18e-06	3.61
6	49	1.07e-02		7.38e+00		1.47e-02	
	99	9.67e-03	0.15	1.50e-02	8.94	1.50e-02	−0.03
	199	1.89e-03	2.36	2.48e-03	2.60	2.56e-03	2.55
	399	8.88e-05	4.41	1.11e-04	4.48	1.15e-04	4.48
	799	1.78e-06	5.64	2.20e-06	5.66	2.25e-06	5.67
	1599	2.26e-08	6.30	2.78e-08	6.31	2.81e-08	6.32
8	49	1.02e-02		1.04e+00		7.17e-03	
	99	8.86e-03	0.20	7.96e-03	7.03	8.18e-03	−0.19
	199	8.37e-04	3.40	7.73e-04	3.36	8.02e-04	3.35
	399	1.49e-05	5.82	1.39e-05	5.80	1.43e-05	5.81
	799	9.34e-08	7.31	8.81e-08	7.30	8.98e-08	7.32
	1599	3.33e-10	8.13	3.15e-10	8.13	3.19e-10	8.14

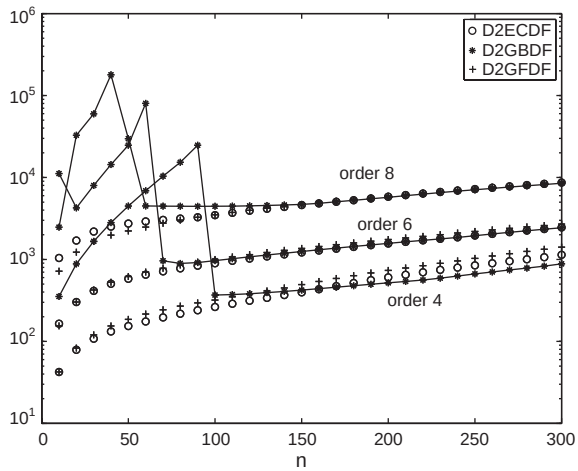

Fig. 4. Problem 4 for $\varepsilon = 0.01$: 2-norm condition number for the matrices associated to D2ECDFs, D2GBDFs and D2GFDFs.

Table 5
Problem 4 for $\varepsilon = 0.01$: convergence behavior of ETRs and TOM on a uniform meshgrid

	ETR4		TOM6		ETR8	
n	Error	Rate	Error	Rate	Error	Rate
49	1.21e-01		6.75e-02		4.28e-02	
99	3.28e-02	1.88	1.34e-02	2.34	6.32e-03	2.76
199	4.28e-03	2.94	9.15e-04	3.87	2.32e-04	4.77
399	3.10e-04	3.79	2.56e-05	5.16	2.53e-06	6.52
799	1.52e-05	4.35	3.97e-07	6.01	1.24e-08	7.67
1599	9.68e-07	3.98	4.42e-09	6.49	3.92e-11	8.31

roots of (18) have different sign, that is when $|\gamma h| \gg |\mu h^2| \gg 0$ and the polynomial (18) is approximated by $\beta(z)$, whose principal roots are equal to 1 and -1. Viceversa, if γh and μh^2 are small (n is large), the principal roots can be approximated by those of $\alpha(z)$, both equal to 1. For this reason, the oscillations are reduced when the number of meshpoints increases.

In order to complete our analysis, we apply the BVM schemes [5] to solve the first order system equivalent to the Problem 4. Here, we have used the ETRs of order 4 and 8 and the TOM of order 6 with GAMs as initial and final methods [5]. The computed errors reported in Table 5 show that, in general, these methods behave like the new formulae. We only observe that, due to a better conditioning of the discrete problem, a greater precision of these schemes holds when a large number of points is used. For example, in the case of order 8 on a mesh of 1599 points, the matrix associated to the ETR8 has both the size and the number of nonzero diagonals doubled with respect to D2ECDF8, but its condition number is $\kappa(\text{ETR8}) = 3.5\text{e}3$, while $\kappa(\text{D2ECDF8}) = 8.1\text{e}4$.

4.2. Test Problem 20 by Cash

The nonlinear BVP

$$\varepsilon y'' + (y')^2 = 1$$

in [0, 1] with exact solution

$$y_e(x) = 1 + \varepsilon \log\left(\cosh\left(\frac{x - 0.745}{\varepsilon}\right)\right),$$

is considered by Cash for $\varepsilon = 0.5$, 0.3 and 0.06. The solution has a corner layer in the point $x = 0.745$. We have solved Problem 20 for $\varepsilon = 0.1$ and 0.01. The obtained nonlinear system is solved by means of the Newton method with $tol = 1\text{e-}12$ as the stopping criterion on the residual and the Newton direction in the Euclidean norm.

For $\varepsilon = 0.1$, we have used the segment connecting the boundary conditions as starting approximation. In Fig. 5, we report the absolute error for the methods of orders 4, 6 and 8 in the three classes considered. We observe that for each order all methods have very similar error behaviors, attaining their expected rate of convergence. It is worth noting that, as in the linear example, the three methods are not able to give a solution with accuracy up to the machine precision, because of the conditioning of the corresponding discrete problem.

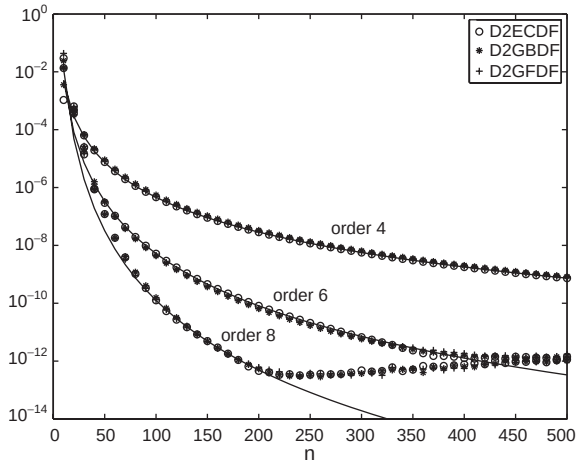

Fig. 5. Problem 20 for $\varepsilon = 0.1$: convergence behavior of D2ECDFs, D2GBDFs and D2GFDFs on a uniform meshgrid.

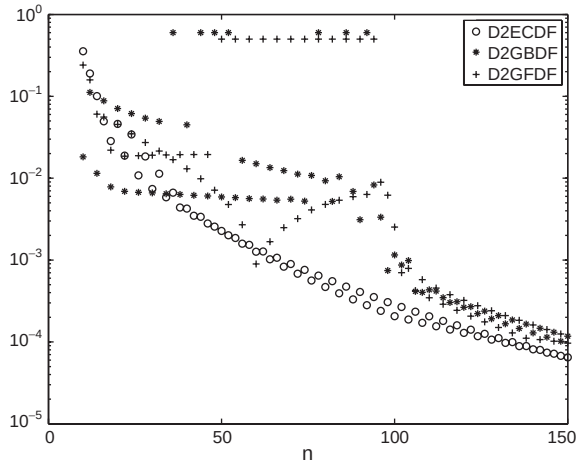

Fig. 6. Problem 20 for $\varepsilon = 0.01$: convergence behavior of D2ECDFs, D2GBDFs and D2GFDFs of order 4 on a uniform meshgrid.

In order to solve the problem for $\varepsilon = 0.01$, we need to identify a good starting guess for the convergence of the Newton method. For this reason, a continuation technique for $\varepsilon = 0.1$, 0.05 and 0.025 has been applied. Fig. 6 shows the absolute errors for all the methods of order 4, but similar behavior has been obtained also for orders 6 and 8. We observe that only the D2ECDFs exhibit their expected order for all the values of n. All the other methods converge with their predicted order only for values of n larger than a critical value n^* that decreases when the order increases. The worst case holds for the order 4 where $n^* \simeq 100$. Moreover, for some values of $n \leqslant n^*$ and for both the D2GBDFs and D2GFDFs the Newton method does not converge within the required precision in spite of the careful choice of the initial solution (these values of n are represented as the largest errors in Fig. 6). In these cases no convergence holds even if the exact solution or the one obtained by the D2ECDF of the same order is used as starting guess. We

can deduce that the iterative method, even if very efficient in the other cases, has a very small convergence domain.

We suppose that the bad behavior observed for $n < n^*$ is in some sense connected with the ill-conditioning of these formulae outlined by the linear analysis and by the results of Problem 4. In particular, since the ill-conditioning areas are reduced when the order increases, this link could explain why more accurate formulae have a smaller critical threshold n^*.

5. Application to elliptic PDEs

Let us consider the solution of a two-dimensional *elliptic PDE* formulated as:

$$\begin{aligned} &F(x, y, u, u_x, u_y, u_{xx}, u_{yy}, u_{xy}) = 0, \quad (x, y) \in \Omega, \\ &u(x, y) = g(x, y) \qquad\qquad\qquad\quad \text{on } \partial\Omega \end{aligned} \tag{20}$$

where $\Omega = [x_0, x_f] \times [y_0, y_f]$. In this section, we show how the new schemes can be applied along each space dimension and then combined to yield a high-order extension of classical second-order methods for elliptic PDEs based on central and upwind differences (see, for example, [10,16]). For this aim, also classical BVMs have been used in [17], but they show a high cost due to the double size of the discrete problem for each dimension and a loss of symmetry in the schemes.

The discretization of Ω by means of different stepsizes $h_x = (x_f - x_0)/(n+1)$ and $h_y = (y_f - y_0)/(m+1)$ yields the unknown vector

$$U = (U_1, U_2, \ldots, U_m)^{\mathrm{T}}, \quad U_j = (u_{1j}, \ldots, u_{nj}),$$

of the discrete solution $u_{ij} \approx u(x_i, y_j)$ in the internal points (x_i, y_j), for $j = 1, \ldots, m$, $i = 1, \ldots, n$. We introduce the following approximations for the derivatives in (20):

$$\begin{aligned} &U_x(x, y) \approx \frac{1}{h_x}(\tilde{I}_m \otimes \tilde{B}_n)\tilde{U}, \qquad U_y(x, y) \approx \frac{1}{h_y}(\tilde{B}_m \otimes \tilde{I}_n)\tilde{U}, \\ &U_{xx}(x, y) \approx \frac{1}{h_x^2}(\tilde{I}_m \otimes \tilde{A}_n)\tilde{U}, \quad U_{yy}(x, y) \approx \frac{1}{h_y^2}(\tilde{A}_m \otimes \tilde{I}_n)\tilde{U}, \\ &U_{xy}(x, y) \approx \frac{1}{h_x h_y}(\tilde{B}_m \otimes \tilde{B}_n)\tilde{U}, \end{aligned}$$

where $U_d(x, y)$, $d \in \{x, y, xx, yy, xy\}$ represents the exact derivatives in the internal points, $\tilde{I}_r = [0_r, I_r, 0_r]$ and 0_r is a vector of r zeros. $\tilde{A}_r$ and $\tilde{B}_r$ are the same matrices of dimension $r \times (r+2)$, defined in Section 2. $\tilde{U}$ also contains the boundary values and it is defined as

$$\tilde{U} = (\tilde{U}_0, \tilde{U}_1, \ldots, \tilde{U}_{m+1})^{\mathrm{T}}, \quad \tilde{U}_j = (u_{0j}, \ldots, u_{n+1,j}).$$

6. Conclusions

The formulae introduced in this paper seem to be promising to solve both BVPs for second-order ODEs and elliptic PDEs on a regular domain without doubling the number of unknowns and the size of the discrete problem. Numerical tests on uniform meshes exhibit good results also on nonlinear problems.

For n large enough, all the methods show essentially the same behavior. We note that, the D2GBDFs and D2GFDFs could require a restriction on the choice of the stepsize, for this reason the D2ECDFs could be preferable.

Future developments of this research concern the generalization of these schemes to a non uniform mesh and then a suitable strategy of mesh variation. Good insights in this direction can be given by [15], where the D2ECDF of order two have been applied with variable stepsize to second-order singular perturbation ODEs.

Acknowledgements

The authors gratefully acknowledge the anonymous referee whose comments were helpful to improve the initial version of the paper.

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