Numerical Solution of Differential-Algebraic Equations by Block Methods

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Abstract. In this paper some class of nonlinear differential-algebraic equations of high index is considered. For the numerical solution of this problem the family of multistep, multistage difference schemes of high order is proposed. In some cases this difference schemes are Runge-Kutta methods. The estimate of error is found.

In the paper a family of high-order precision difference schemes which are intended for numerical solution of high-index differential algebraic equations (DAEs) is proposed and investigated. The condition of collocation forms the basis for constructing such schemes. The paper is a continuation of the author's works [1], [2], [3], [4].

Consider the following problem

$$f(x^{'}(t), x(t), t) = 0,\ t \in [0, 1], \tag{1}$$

$$x(0) = a. \tag{2}$$

Definition 1 ([5], p. 16). *Let J be an open subinterval of R, D a connected open subset of R^{2n+1}, and f a differentiable function from D to R^n. Then the DAE (1) is solvable on J in D if there is a k-dimensional family of solutions $y(t,c)$ defined on a connected open set $J \times D_1, D_1 \subset R^k$, such that:*

1. y(t,c) is defined on all of J for each $c \in D_1$

2. $(y^{'}(t,c), y(t,c), t) \in D$ for $(t,c) \in J \times D_1$

3. If $z(t)$ is any other solution with $(z^{'}(t), z(t), t) \in D$, then $z(t) = y(t,c)$ for some $c \in D_1$

4. The graph of y as a function of (t,c) is a $k+1$-dimensional manifold.

Let the following mesh be given on the segment $[0; 1]$

$$\Delta_h = \{t_i :\ t_i = ih,\ i = 1, ..., M,\ h = 1/M\}.$$

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For the purpose of numerical solving of the problem (1)–(2) it is advisable to construct s-stage, m-step difference schemes of the form

$$\begin{cases} f(h^{-1}\sum\limits_{j=0}^{m} k_j^1 x_{i+s-j},\ \sum\limits_{j=0}^{m} l_j^1 x_{i+s-j}, \bar{t}_{i+1}) = 0, \\ f(h^{-1}\sum\limits_{j=0}^{m} k_j^2 x_{i+s-j},\ \sum\limits_{j=0}^{m} l_j^2 x_{i+s-j}, \bar{t}_{i+2}) = 0, \\ \dots \\ f(h^{-1}\sum\limits_{j=0}^{m} k_j^s x_{i+s-j},\ \sum\limits_{j=0}^{m} l_j^s x_{i+s-j}, \bar{t}_{i+s}) = 0. \end{cases} \tag{3}$$

Here $f(h^{-1}\sum\limits_{j=0}^{m} k_j^q x_{i+s-j},\ \sum\limits_{j=0}^{m} l_j^q x_{i+s-j}, \bar{t}_{i+q}) = 0$ is an approximation of the initial problem. We assume that initial values of $x_1, x_2, ..., x_{m-s-1}$ have been computed earlier ($x_0 = a$).

Consider a particular case of schemes (3), say, the interpolation variant. Let an interpolation m-power manifold be passed through the points $x_{i+s}, x_{i+s-1}, ...,$ x_{i+s-m}. Then the scheme (3) writes

$$\begin{cases} f(h^{-1}\sum\limits_{j=0}^{m} k_j^1 x_{i+s-j},\ x_{i+1}, t_{i+1}) = 0, \\ f(h^{-1}\sum\limits_{j=0}^{m} k_j^2 x_{i+s-j},\ x_{i+2}, t_{i+2}) = 0, \\ \dots \\ f(h^{-1}\sum\limits_{j=0}^{m} k_j^s x_{i+s-j},\ x_{i+s}, t_{i+s}) = 0. \end{cases} \tag{4}$$

where $h^{-1}\sum\limits_{j=0}^{m} k_j^q x_{i+s-j}$ is an approximation $x^{'}(t_{i+q})$ of the order $h^m,\ q = 1, ..., s$.

If $s = m, \bar{h} = sh$, and $x_{i+1}, x_{i+2}, ..., x_{i+s-1}$ are considered as intermediate results, then schemes (4) can be interpreted as Runge-Kutta methods with abscissas $c = (1/s, 2/s, ..., 1)$, the weights $b = (1, 0, ..., 0)$ and with the matrix $\mathcal{A}$, determined from the conditions

$$V\mathcal{A}^\top = \mathcal{C},$$

where

$$C = \begin{pmatrix} 1/s & 1/(s-1) & \dots 1 \\ 1/(2s^2) & 1/(2(s-1)^2) & \dots 1/2 \\ . & . & \dots. \\ . & . & \dots. \\ . & . & \dots. \\ 1/(s^{s+1}) & 1/(s(s-1)^{s-1}) & \dots 1/s \end{pmatrix},$$

and V is the Vandermonde matrix:

$$V = \begin{pmatrix} 1 & 1 & \dots 1 \\ 1/s & 2/s & \dots 1 \\ . & . & \dots . \\ . & . & \dots . \\ . & . & \dots . \\ (1/s)^{s-1} & (2/s)^{s-1} & \dots 1 \end{pmatrix}.$$

Similar methods for ODEs have probably for the first time been proposed in [6]. In this paper, the abscissas were chosen as follows $c = (0, 1/s, ..., (s-1)/s)$.

Note that presently the theory of methods of difference coefficients for DAEs, which have the index not higher than 3 and the Hessenberg form [5], [7], [8], have been developed rather completely.

Consider a few schemes for the case when $m > s$.

For $s = 1$ we obtain the BDF methods.

For $s = 2, m = 3$ we have

$$\begin{cases} f((2x_{i+2} + 3x_{i+1} - 6x_i + x_{i-1})/6h, x_{i+1}, t_{i+1}) = 0, \\ f((11x_{i+2} - 18x_i + 9x_i - 2x_{i-1})/6h, x_{i+2}, t_{i+2}) = 0, \end{cases}$$

while assuming x_1 to be known and $x_0 = a$.

For $s = 2, m = 4$ we obtain

$$\begin{cases} f((3x_{i+2} + 10x_{i+1} - 18x_i + 6x_{i-1} - x_{i-2})/12h, x_{i+1}, t_{i+1}) = 0, \\ f((25x_{i+2} - 48x_i + 36x_i - 16x_{i-1} + 3x_{i-2})/12h, x_{i+2}, t_{i+2}) = 0, \end{cases}$$

while assuming x_1, x_2 known, $x_0 = a$.

Consider a particular case of problem (1)

$$x(t) + \xi(x'(t), t) = 0, \tag{5}$$

where $\partial\xi(x', t)/\partial x'$ is an upper-triangular matrix with the zero diagonal, furthermore, the number of zero square blocks on the diagonal is r.

It can readily be noted that our system (5) has a unique solution for a sufficiently smooth $\xi(x', t)$. Indeed, when rewriting (5) in the explicit form

$$\begin{cases} x_1 + \xi_1(x'_2, x'_3, ..., x'_r, t) = 0, \\ x_2 + \xi_2(x'_3, x'_4, ..., x'_r, t) = 0, \\ . \quad . \quad . \\ x_r + \xi_r(t) = 0, \end{cases}$$

where $x_1, x_2, ..., x_r$ correspond to zero blocks of the matrix $\partial\xi(x', t)/\partial x'$, we obtain that $x_r = -\xi_r(t), x_{r-1} = -\xi_{r-1}(-\xi'_r(t), t)$ and so on.

Lemma 1 ([4]). *Let $\partial F(x)/\partial x$ be an upper-triangular matrix with the zero diagonal, furthermore, $(\partial F(x)/\partial x)^r = 0$ corresponds to the zero matrix. Hence the system of nonlinear equations*

$$x = F(x), \tag{6}$$

has a unique solution, and the method of simple iteration

$$x^{i+1} = F(x^i), \tag{7}$$

gives a precision solution for the system (6) in r steps for any initial approximation x^0.

Lemma 2. *For the system of nonlinear equations $x = F(x)$, which satisfy the condition of Lemma 1, the Newton's method*

$$x^{i+1} = x^i - (E - \partial F(x)/\partial x|_{x=x^i})^{-1} F(x^i), \tag{8}$$

gives a precision solution of the system (6) in r steps for any initial approximation x^0.

Proving of this result can be conducted likewise in Lemma 2, and so, it is omitted.

Corollary 1. *Let for the system (6) the matrix $\partial F(x)/\partial x$ have the following block form*

$$\partial F(x)/\partial x = \begin{pmatrix} F_{11} & F_{12} & \dots & F_{1k} \\ F_{21} & F_{22} & \dots & F_{2k} \\ . & . & \dots & . \\ F_{k1} & F_{k2} & \dots & F_{kk} \end{pmatrix},$$

where F_{ij} are upper-triangular $(s \times s)-$matrices with the zero diagonal, furthermore, the maximum number of zero blocks on the diagonals F_{ij} is r. Hence this systems has a unique solution. The simple iteration method

$$x^{i+1} = F(x^i)$$

and the Newton's method

$$x^{i+1} = x^i - (E - \partial F(x)/\partial x|_{x=x^i})^{-1} F(x^i),$$

give a precision solution of this system in r steps for any initial approximation x^0.

Now let us turn back to problem (5). For the purpose of numerical solving this problem let us consider the difference schemes (4), which with respect to it have the form

$$\begin{cases} x_{i+1} = \xi(h^{-1} \sum\limits_{j=0}^{m} k_j^1 x_{i+s-j}, t_{i+1}), \\ x_{i+2} = \xi(h^{-1} \sum\limits_{j=0}^{m} k_j^2 x_{i+s-j}, t_{i+2}), \\ . \quad . \quad . \\ x_{i+s} = \xi(h^{-1} \sum\limits_{j=0}^{m} k_j^s x_{i+s-j}, t_{i+s}), \end{cases} \tag{9}$$

where $h^{-1} \sum\limits_{j=0}^{m} k_j^q x_{i+s-j}$ is an approximation of $x^{'}(t_{i+q})$, furthermore,

$$h^{-1}\sum_{j=0}^{m} k_j^q x_{i+s-j} - x^{'}(t_{i+q}) = \sigma_{i+q}/h,$$

$$\sigma_{i+q}/h = h^{m+1}x^{(m+1)}(t_{i+q})/(m+1) + O(h^{m+2}). \tag{10}$$

On account of the corollary of the lemmas, the system (9) has a unique solution, and the method of simple iteration (or the Newton's method) in r steps suggests a precision solution of the given system.

Let us reduce the result concerning the convergence of schemes (9) to the precision solution of problem (5).

Theorem 1. *Let the vector function $\xi(x^{'},t)$ in the problem (5) be sufficiently smooth with respect to the set of arguments, and let*

$$\| x_j - x(t_j) \| = O(h^{m+1}),\ j = 0,1,...,m-s.$$

Then

$$\| x_i - x(t_i) \| = O(h^{m+2-r}),\ i = m+1, m+2, ..., M.$$

Proof. Having substituted the precision value of $x(t)$ into the system (9), we have

$$\begin{cases} x_{i+1} + \varepsilon_{i+1} = \xi(h^{-1}\sum\limits_{j=0}^{m} k_j^1 \varepsilon_{i+s-j} + x^{'}(t_{i+1}) + \sigma_{i+1}/h, t_{i+1}), \\ x_{i+2} + \varepsilon_{i+2} = \xi(h^{-1}\sum\limits_{j=0}^{m} k_j^2 \varepsilon_{i+s-j} + x^{'}(t_{i+2}) + \sigma_{i+2}/h, t_{i+2}), \\ . \qquad . \ . \\ x_{i+s} + \varepsilon_{i+s} = \xi(h^{-1}\sum\limits_{j=0}^{m} k_j^s \varepsilon_{i+s-j} + x^{'}(t_{i+s}) + \sigma_{i+s}/h, t_{i+s}). \end{cases}$$

From the last formula and the initial system (5) we obtain the following result for the solution error:

$$\begin{cases} \varepsilon_{i+1} = A_{i+1}h^{-1}\sum\limits_{j=0}^{m} k_j^1 \varepsilon_{i+s-j} + A_{i+1}\sigma_{i+1}/h, \\ \varepsilon_{i+2} = A_{i+2}h^{-1}\sum\limits_{j=0}^{m} k_j^2 \varepsilon_{i+s-j} + A_{i+2}\sigma_{i+2}/h, \\ . \qquad . \ . \\ \varepsilon_{i+s} = A_{i+s}h^{-1}\sum\limits_{j=0}^{m} k_j^s \varepsilon_{i+s-j} + A_{i+s}\sigma_{i+s}/h, \end{cases} \tag{11}$$

where $A_j = \partial\xi/\partial x^{'}$.

For the purpose of simplicity of our reasoning assume s to be $m-$fold (one can always obtain this by increasing m artificially up to the minimum value m_1, which is multiple to s, and assuming $k_l^p = 0,\ l = m+1, m+2, ..., m_1$).

Introduce the denotations:

$$m_2 = m/s, \quad n_1 = (M-m+s)/s,$$

$$\bar{\varepsilon}_i = (\varepsilon^\top_{m-s+1+is}, \varepsilon^\top_{m-s+2+is}, ..., \varepsilon^\top_{m+is})^\top,$$

$$\bar{\sigma}_i = ((A_{m-s+1+is}\sigma_{m-s+1+is})^\top, ..., (A_{m+is}\sigma_{m+is})^\top)^\top.$$

On account of these denotations the recurrent relation (11) may be rewritten in the form of a block m_2-diagonal system of linear algebraic equations

$$(\mathcal{N} + \mathcal{E})\Upsilon = \Sigma, \tag{12}$$

where $\mathcal{N} + \mathcal{E} =$

$$\begin{pmatrix} hE+N_{11} & 0 & 0\,0\,0 & . & . \, . \, 0\,0 \\ N_{21} & hE+N_{22} & 0\,0\,0 & . & . \, . \, 0\,0 \\ . & . & . \; . \; . & . & . \; . \; . \; . \\ N_{m_2 1} & . & . \; . \; hE+N_{m_2 m_2} & 0 & . \; . \; . \; 0 \\ . & . & . \; . \; . & . & . \; . \; . \; . \\ 0 & 0 & . \; . \; . & N_{n_1 n_1 - m_2} & . \; . \; . \; hE+N_{n_1 n_1} \end{pmatrix},$$

$$\Upsilon = \begin{pmatrix} \bar{\varepsilon}_1 \\ \bar{\varepsilon}_2 \\ . \\ . \\ . \\ \bar{\varepsilon}_{n_1} \end{pmatrix}, \quad \Sigma = -\begin{pmatrix} \bar{\sigma}_1 \\ \bar{\sigma}_2 \\ . \\ . \\ . \\ \bar{\sigma}_{n_1} \end{pmatrix},$$

and

$$N_{ii} = \begin{pmatrix} k^1_{m-s+1}A_{m-s+is+1} & k^1_{m-s}A_{m-s+is+1} & . \; . \; . \; k^1_0 A_{m-s+is+1} \\ k^2_{m-s+1}A_{m-s+is+2} & k^2_{m-s}A_{m-s+is+2} & . \; . \; . \; k^2_0 A_{m-s+is+2} \\ . & . & . \; . \; . \; . \\ k^s_{m-s+1}A_{m+is} & k^s_{m-s}A_{m+is} & . \; . \; . \; k^s_0 A_{m+is} \end{pmatrix},$$

$$N_{i-j\; i} = \begin{pmatrix} k^1_{m-s+1}A_{m-s+is+1} & k^1_{m-s}A_{m-s+is+1} & . \; . \; . \; k^1_0 A_{m-s+is+1} \\ k^2_{m-s+1}A_{m-s+is+2} & k^2_{m-s}A_{m-s+is+2} & . \; . \; . \; k^2_0 A_{m-s+is+2} \\ . & . & . \; . \; . \; . \\ k^s_{m-s+1}A_{m+is} & k^s_{m-s}A_{m+is} & . \; . \; . \; k^s_0 A_{m+is} \end{pmatrix}.$$

From the system (12) we have:

$$\| \Upsilon \| = \| (\mathcal{N} + \mathcal{E})^{-1}\Sigma \| . \tag{13}$$

Due to the theorem's condition, A_j are upper-triangular matrices with zero quadratic blocks on the diagonal, whose number is r. It can easily be shown that

$$(\mathcal{N} + \mathcal{E})^{-1} = h^{-1}\mathcal{E} - h^{-2}\mathcal{N} + ... + (-h)^{-r}\mathcal{N}^{r-1}. \tag{14}$$

Each of the addends of the right-hand side of the identity (14) $\mathcal{N}^l$, $l = 1, 2, ...r-1$ is a block matrix, and each of its blocks contains a multiplication of l upper-triangular matrices of the form A_j. Having restored in the memory that

$$\bar{\sigma}_i = ((A_{m-s+1+is}\sigma_{m-s+1+is})^\top, ..., (A_{m+is}\sigma_{m+is})^\top)^\top,$$

we obtain that

$$\mathcal{N}^{r-1}\Sigma = 0.$$

By employing the formula (14), the estimate (10) and the latter identity in (13), we have

$$\| \Upsilon \| = \| (\mathcal{N} + \mathcal{E})^{-1}\Sigma \| = \| h^{-1}\mathcal{E}\Sigma - h^{-2}\mathcal{N}\Sigma + ... + (-h)^{-r}\mathcal{N}^{r-1}\Sigma \| =$$

$$= \| h^{-1}\Sigma - h^{-2}\mathcal{N}\Sigma + ... + (-h)^{1-r}\mathcal{N}^{r-2}\Sigma \| \leq$$

$$\leq K_1 h^{m+1} + K_2 h^m + ... + K_{r-1} h^{m+2-r} = O(h^{m+2-r}).$$

□

In conclusion, we would like to note that multistep, multistage methods of numerical solving of ODEs are presently under intensive development (see, for example [9]). Although their form is different with respect to that of (3).

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