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An Extension of Ortiz' Recursive Formulation of the Tau Method to Certain Linear Systems of Ordinary Differential Equations

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Abstract. Ortiz' step-by-step recursive formulation of the Lanczos tau method is extended to the numerical solution of linear systems of differential equations with polynomial coefficients. Numerical comparisons are made with Gear's and Enright's methods.

1. Introduction. This paper concerns the extension of Ortiz' [13], [17] step-by-step recursive formulation of Lanczos' tau method [9]–[11] to the numerical integration of linear systems of differential equations with polynomial coefficients.

Let us consider the differential problem:

$$\begin{cases} A(x)y'(x) + B(x)y(x) + F(x) = 0, \quad x \in [x_0, x_{\text{fin}}], & (1.1) \\ y(x_0) = y_0, & (1.2) \end{cases}$$

where $y(x) = [y_1(x) \cdots y_\nu(x)]^T$ is the vector of the ν unknown functions, $A(x) = (a_{ij}(x)\delta_{ij})$, $B(x) = (b_{ij}(x))$ and $F(x) = [f_1(x) \cdots f_\nu(x)]^T$ are two matrices and a vector of order ν whose elements are respectively:

$$a_{ij}(x) = \sum_{k=0}^{r_{ij}} a_{ij}^k x^k, \qquad b_{ij}(x) = \sum_{k=0}^{s_{ij}} b_{ij}^k x^k, \tag{1.3}$$

$$f_i(x) = \sum_{k=0}^{t_i} f_i^k x^k. \tag{1.4}$$

Thereafter the system (1.1) will be synthetically written as:

$$Dy(x) + F(x) = 0, \qquad x \in [x_0, x_{\text{fin}}],$$

having introduced the differential operator D defined by:

$$D = \begin{pmatrix} a_{11}(x)\dfrac{d}{dx} + b_{11}(x) & b_{12}(x) \cdots b_{1\nu}(x) \\ b_{21}(x) \quad a_{22}(x)\dfrac{d}{dx} + b_{22}(x) & \cdots b_{2\nu}(x) \\ \cdots\cdots\cdots\cdots & \cdots\cdots\cdots \\ b_{\nu 1}(x) \quad b_{\nu 2}(x) \cdots & a_{\nu\nu}(x)\dfrac{d}{dx} + b_{\nu\nu}(x) \end{pmatrix}.$$

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Following Lanczos' idea [9]–[11], the solution of (1.1)–(1.2) is approximated by a polynomial vector $y^*(x)$, of degree p, which is the exact solution of a perturbed system, obtained by adding to the right side of (1.1) a polynomial perturbation term.

The polynomial $y^*(x)$, which is called the τ-solution of (1.1)–(1.2), satisfies, then, the differential problem:

$$\begin{cases} Dy^*(x) + F(x) = H_m(x), & (1.5) \\ y^*(x_0) = y_0. & (1.6) \end{cases}$$

The perturbation term $H_m(x)$ is constructed in such a way that (1.5) has a polynomial solution of degree p, and a norm of $H_m(x)$ satisfies an extremal condition on $[x_0, x_{\text{fin}}]$.

Generally $H_m(x)$, following Lanczos, is taken as a linear combination of powers of x multiplied by Chebyshev polynomials.

As Ortiz [18] pointed out, the above method is of order p, in the sense that if the exact solution of (1.1), (1.2) is itself a polynomial of degree less or equal to p, the method will reproduce it.

Ortiz [17] has developed a step-by-step approach to the tau method along the following lines: let us divide the integration range $[x_0, x_{\text{fin}}]$ into subintervals $[x_n, x_{n+1}]$. The value in x_{n+1} of the solution of the given differential problem (1.1), (1.2) is approximated by the value in x_{n+1} of the τ-solution obtained applying the method above described in the subinterval $[x_n, x_{n+1}]$, taking as the initial condition the value in x_n of the solution constructed in the previous subinterval $[x_{n-1}, x_n]$.

Therefore, denoting with y_n the approximate value of $y(x)$ in x_n, the differential problem:

$$\begin{cases} Dy^*(x) + F(x) = H_m(x), \quad x \in [x_n, x_{n+1}], & (1.7) \\ y^*(x_n) = y_n. & (1.8) \end{cases}$$

has to be solved for each interval $[x_n, x_{n+1}]$, in order to give $y_{n+1} = y^*(x_{n+1})$. $H_m(x)$ is the polynomial vector:

$$H_m(x) = \begin{pmatrix} T_{m-\alpha_1}(x) \sum_{k=0}^{\alpha_1} \tau_1^k x^k \\ T_{m-\alpha_2}(x) \sum_{k=0}^{\alpha_2} \tau_2^k x^k \\ \cdots\cdots\cdots\cdots \\ T_{m-\alpha_\nu}(x) \sum_{k=0}^{\alpha_\nu} \tau_\nu^k x^k \end{pmatrix}, \tag{1.9}$$

where τ_j^k and α_j are parameters to be determined, and $T_{m-\alpha_j}(x)$ are Chebyshev polynomials defined in $[x_n, x_{n+1}]$.

The methods under consideration have been proved to be A-stable, for every order p, in [3].

In order to facilitate the construction of the solution, it is convenient to introduce the canonical polynomials, defined as follows: The ith canonical polynomial of order m associated with D is the polynomial vector $Q_i^m(x)$ such that

$$DQ_i^m(x) = x^m e_i, \tag{1.10}$$

where $e_i = (e_i^j), j = 1,\dots,\nu, e_i^j = \delta_{ij}$.

As Ortiz points out in [13], the advantages of the introduction of the canonical polynomials are manifold: the solution $y^*(x)$ can be easily expressed as a linear combination of $Q_i^m(x)$, and they are independent of the integration range and the initial condition.

However, there are some problems connected with the $Q_i^m(x)$ and their construction; it is possible that some $Q_i^m(x)$ do not exist and the definition (1.10) does not hold but has to be generalized and more precisely stated. Besides, it is possible that some operators D have multiple canonical polynomials. These questions have been discussed by Ortiz [13] for the one-dimensional case. We extend them and his recursive technique for the generation of the canonical polynomials in Section 2. The class of integration methods is developed in Section 3, and for clarification the resulting algorithm is applied to an example in Section 4.

Finally numerical results are reported in Section 5, where the method is compared with Gear's [6], and Enright's [4], [1] methods. From the comparison carried out on both stiff and nonstiff standard test problems, it follows that the proposed method compares very favorably with the other two with respect to efficiency and reliability.

2. Canonical Polynomials. This section is concerned with the extension of Ortiz' theorems [13] to questions related to existence, uniqueness and construction of the canonical polynomials. We follow his approach; proofs can be extended without essential modifications.

Definition 2.1. The jth generating polynomial of order k associated with D is the polynomial vector:

$$P_j^k(x) = Dx^k e_j, \qquad j = 1,\dots,\nu. \tag{2.1}$$

Obviously $P_j^k(x)$ is a vector whose ith component is a polynomial of degree at most equal to $k + h_i$, where h_i is given by

$$h_i = \max\left\{r_{ii}, \max_{1\leq j\leq\nu}\{s_{ij}\}\right\}, \tag{2.2}$$

with the further convention that the degree of a polynomial identically equal to zero is -1.

Let Ω be the set of finite linear combinations of generating polynomials

$$\Omega = \left\{\sum_{j=1}^{\nu}\sum_{n\in\Gamma_j}\eta_j^n P_j^n(x)\right\}, \tag{2.3}$$

where Γ_j is a finite subset of N_0.

Now the set S_i of the indices m such that $Q_i^m(x)$ does not exist can be characterized:

Definition 2.2. S_i is the set of indices v such that there is no polynomial in Ω whose ith component has degree v and whose jth component, for every $j \neq i$, has degree less than $v - h_i + h_j$.

The nonexistence of some $Q_i^m(x)$ causes the definition (1.10) to be generalized, in such a way as to allow for the so-called residuals. For this purpose we extend to systems Ortiz' [13] definition of the residual subspace.

Definition 2.3. The subspace of residuals of D is the subspace R_S spanned by the vectors

$$R_i^s = x^s e_i, \qquad s \in S_i, i = 1,\dots,\nu.$$

This being stated, the canonical polynomials can be exactly defined.

Definition 2.4. The ith canonical polynomial of order m associated with D is the polynomial vector $Q_i^m(x)$ such that

$$DQ_i^m(x) = x^m e_i + R_i^m(x), \qquad i = 1,\dots,\nu;\ m \in N_0 - S_i, \tag{2.4}$$

where $R_i^m(x) \in R_S$ is the ith residual polynomial of $Q_i^m(x)$.

For every m, $Q_i^m(x)$ can be multiple. In this regard, let U_D be the subspace spanned by the eventual polynomial solutions $V_i(x)$ of the homogeneous system $Dy(x) = 0$. The following result extends Ortiz' theorem 3.1:

THEOREM 2.1. *For every $i \in \{1,\dots,\nu\}$, the multiple canonical polynomials $Q_i^m(x)$, $m \in N_0 - S_i$, differ by an element of U_D.*

Proof. The proof is by contradiction. Let $Q_i^{m_1}(x)$, $Q_i^{m_2}(x)$ be two ith canonical polynomials of order $m \in N_0 - S_i$, and $Q_i^{m_1}(x) - Q_i^{m_2}(x) \notin U_D$. Then $D[Q_i^{m_1}(x) - Q_i^{m_2}(x)]$ is a linear combination of generating polynomials. But it contradicts the definition (2.4), from which it follows that

$$D\big[Q_i^{m_1}(x) - Q_i^{m_2}(x)\big] = R_i^{m_1}(x) - R_i^{m_2}(x) \in R_S.$$

Therefore, it is suitable to introduce the equivalence relation E_i defined in $\{Q_i^m(x)\}$ such that

$$Q_i^{m_k}(x) E_i Q_i^{m_j}(x) \Leftrightarrow (Q_i^{m_k}(x) - Q_i^{m_j}(x)) \in U_D \tag{2.5}$$

and to consider the quotient set L_i

$$L_i = \{\mathfrak{L}_i^m(x)\} = \{Q_i^{m_k}(x)\}/E_i, \qquad i = 1,\dots,\nu, m \in N_0 - S_i, \tag{2.6}$$

instead of the set $Q_i = \{Q_i^{m_k}(x)\}$. Ortiz [13] called the set $L = \{L_i\}$ the Lanczos class of equivalence associated with the operator D.

Obviously, if the operator D has no polynomial solutions, $\mathfrak{L}_i^m(x)$ coincides with the canonical polynomial $Q_i^m(x)$.

Now the effective construction of the $\mathfrak{L}_i^m(x)$ has to be discussed.

For this purpose it is suitable to introduce the following notations:

$$d_i = \max\{s_{ii}, r_{ii} - 1\}, \qquad i = 1,\dots,\nu, \tag{2.7}$$

$$\Delta_j = \min\left\{\min_{\substack{1 \le i \le \nu \\ i \ne j}} \{h_i - s_{ij}\}, (h_j - d_j)\right\}, \qquad j = 1,\dots,\nu, \tag{2.8}$$

and to consider, as in [13], the generating polynomials

$$P_j^{n+\Delta_j}(x), \qquad j = 1,\dots,\nu.$$

The quantities Δ_j have been defined so that, for every j, $P_j^{n+\Delta_j}(x)$ has at least one component, say ith, whose effective degree is $n + h_i$. From the definition (1.10) it follows formally that D^{-1} applied to $P_j^{n+\Delta_j}(x)$ defines $x^{n+\Delta_j}e_j$ as a linear combination of the $Q_i^m(x)$, $m = 0, 1, \ldots, n + h_i$. These can be regarded as recurrence relations for $Q_i^{n+h_i}(x)$ in terms of $x^{n+\Delta_i}e_i$ and $Q_j^k(x), j = 1, \ldots, \nu, k = 0, 1, \ldots, n + h_i - 1$.

However, in the most general case, the nonexistence of some $Q_i^m(x)$ requires a more precise discussion.

Let $W_n(x) = (w_{ij}^n(x))$ be the matrix whose columns are the vectors $P_j^{n+\Delta_j}(x)$. There is in the ith row of $W_n(x)$ at least one polynomial of effective degree $n + h_i$, and so $W_n(x)$ can be written:

$$W_n(x) = \begin{pmatrix} \sum_{k=0}^{n+h_1} p_{11}^k x^k & \sum_{k=0}^{n+h_1} p_{12}^k x^k & \cdots & \sum_{k=0}^{n+h_1} p_{1\nu}^k x^k \\ \cdots & \cdots & \cdots & \cdots \\ \sum_{k=0}^{n+h_\nu} p_{\nu 1}^k x^k & \sum_{k=0}^{n+h_\nu} p_{\nu 2}^k x^k & \cdots & \sum_{k=0}^{n+h_\nu} p_{\nu\nu}^k x^k \end{pmatrix}. \tag{2.9}$$

Obviously $p_{ij}^k = 0$ for k greater than the effective degree of $w_{ij}^n(x)$.

Let P_n be the matrix

$$P_n = \begin{pmatrix} p_{11}^{n+h_1} & p_{12}^{n+h_1} & \cdots & p_{1\nu}^{n+h_1} \\ p_{21}^{n+h_2} & p_{22}^{n+h_2} & \cdots & p_{2\nu}^{n+h_2} \\ \cdots & \cdots & \cdots & \cdots \\ p_{\nu 1}^{n+h_\nu} & p_{\nu 2}^{n+h_\nu} & \cdots & p_{\nu\nu}^{n+h_\nu} \end{pmatrix}. \tag{2.10}$$

Since at most the diagonal elements contain a factor n, $\det(P_n)$ is a polynomial in n of degree less than or equal to ν; therefore, if $\det(P_n)$ is not identically zero, the set

$$\Psi = \{n \colon \det(P_n) = 0, n \in N_0\} \tag{2.11}$$

is finite and $\operatorname{card}(\Psi) \leqslant \nu$.

Now a recursive relation for the elements $\mathfrak{L}_i^m(x)$, $i = 1, \ldots, \nu$, can be stated. In this regard, the following result extends Ortiz' theorem 3.3 [13].

THEOREM 2.2. *For every $i \in \{1, \ldots, \nu\}$ the elements of L_i are connected by the following recursive relations*:

$$\mathfrak{L}_i^{m+h_i}(x) = \sum_{r=1}^{\nu} d_{ir} \left(x^{m+\Delta_r} e_r - \sum_{j=1}^{\nu} \sum_{\substack{k=0 \\ k \notin S_j}}^{m+h_j-1} p_{jr}^k \mathfrak{L}_j^k(x) \right), \qquad m \in N_0 - \Psi, \tag{2.12}$$

where

$$(d_{ir}) = \left(P_n^T\right)^{-1}$$

and p_{jr}^k are the coefficients of the elements of (2.9) *for $n = m$.*

Proof. Let $\chi_i^{m+h_i}$ be the class of equivalence modulo E_i, $i \in \{1, \ldots, \nu\}$, of the polynomial

$$\Lambda_i^{m+h_i}(x) = \sum_{r=1}^{\nu} d_{ir} \left[x^{m+\Delta_r} e_r - \sum_{j=1}^{\nu} \sum_{\substack{k=0 \\ k \notin S_j}}^{m+h_j-1} p_{jr}^k Q_j^k(x) \right], \qquad m \in N_0 - \Psi. \tag{2.13}$$

The application of D to χ_i^m, using (2.4), after some algebraic manipulation, yields

$$D\chi_i^{m+h_i}(x) = \sum_{j=1}^{\nu} x^{m+h_j} \sum_{r=1}^{\nu} d_{ir} p_{jr}^{m+h_j} e_j + R_i^{m+h_i}(x). \tag{2.14}$$

As it is

$$\sum_{r=1}^{\nu} d_{ir} p_{jr}^{m+h_i} = \delta_{ij}.$$

(2.14) can be written as

$$D\chi_i^{m+h_i}(x) = x^{m+h_i} e_i + R_i^{m+h_i}(x).$$

Hence $\chi_i^{m+h_i}$ can be identified with $\mathfrak{L}_i^{m+h_i}(x)$.

From this and from Theorem 2.1 an extension to systems of Ortiz' Corollary 3.3 [13] follows:

COROLLARY 2.3. *For every $i \in \{1, 2, \ldots, \nu\}$ the canonical polynomials $Q_i^m(x)$, $m \in N_0 - \Psi$, are connected by the following recursive relations*:

$$Q_i^{m+h_i}(x) = \sum_{r=1}^{\nu} d_{ir} \left(x^{m+\Delta_r} e_r - \sum_{j=1}^{\nu} \sum_{\substack{k=0 \\ k \notin S_j}}^{m+h_j-1} p_{jr}^k Q_j^k(x) \right) \tag{2.15}$$

plus an arbitrary linear combination of elements of U_D.

3. Development of the Integration Formulas. As stated in the introduction, in order to derive the integration formulas, the differential problem (1.7), (1.8) has to be solved, and the solution $y^*(x)$ has to be computed in x_{n+1}.

From the results of the previous section, it follows that $y^*(x)$ can be expressed as a linear combination of canonical polynomials, of the form

$$y^*(x) = \sum_{j=1}^{\nu} \sum_{\substack{i=0 \\ i \notin S_j}}^{M_j} d_j^i Q_j^i(x) + \sum_{j=1}^{q} g_j V_j(x), \tag{3.1}$$

where the following position has been made:

$$d_j^i = \sum_{k=0}^{\alpha_j} \tau_j^k c_{m-\alpha_j}^{i-k} - f_j^i. \tag{3.2}$$

In the above $M_j = \max\{m, t_j\}$, q is the number of the polynomial solution $V_j(x)$ of the homogeneous system $Dy(x) = 0$, α_j are integer numbers given by

$$\alpha_j = \begin{cases} \bar{s}_j - 1, & 1 \leqslant j \leqslant q, \\ \bar{s}_j, & q < j \leqslant \nu, \end{cases} \tag{3.3}$$

$$\bar{s}_j = \operatorname{card}\big(\{s\colon s \in S_j, s \leqslant m\}\big).$$

$c_{m-\alpha_j}^k$ is the coefficient of x^k in the Chebyshev polynomial $T_{m-\alpha_j}(x)$ defined in $[x_n, x_{n+1}]$, t_j, f_j^k are, respectively, the degree and the coefficients of the polynomial (1.4). τ_j^i, g_j are parameters to be determined by imposing $y^*(x)$ to be the solution of (1.7), (1.8).

So, combining (3.1) with (1.7), from the linearity of the operator D and the canonical polynomial definition, it follows that

$$(3.4)\qquad Dy^*(x) + F(x) = \sum_{j=1}^{\nu}\left(\sum_{\substack{i=0\\ i\notin S_j}}^{M_j} d_j^i\left(x^i e_j + R_j^i(x)\right) + \sum_{i=0}^{t_j} f_j^i x^i e_j\right)$$

$$= \sum_{j=1}^{\nu}\sum_{i=0}^{m} x^i \sum_{k=0}^{\alpha_j} c_{m-\alpha_j}^{i-k}\tau_j^k e_j .$$

To satisfy this equation the coefficients of the same powers x^k must be equal. For every $j = 1,\dots,\nu$, the resulting equations for the coefficients of x^k are identically satisfied when $k \in N_0 - S_j$, while, when $k \in S_j$, they yield $\bar{s}_j$ scalar equations. Denoting by $[u]_j^k$ the coefficient of x^k in the jth component of a polynomial vector u, these equations can be written

$$(3.5)\qquad \sum_{p=1}^{\nu}\sum_{\substack{i=0\\ i\notin S_p}}^{M_p} d_p^i\left[R_p^i(x)\right]_j^k - d_j^k = 0, \qquad k \in S_j, j = 1,\dots,\nu.$$

Further equations are obtained by making (3.1) satisfy the initial condition (1.8). Denoting by $[w]_j$ the jth component of a vector w, these equations can be written

$$(3.6)\qquad \sum_{p=1}^{\nu}\sum_{\substack{i=0\\ i\notin S_p}}^{M_p} d_p^i\left[Q_p^i(x_n)\right]_j + \sum_{i=1}^{q} g_i\left[V_i(x_n)\right]_j = [y_n]_j, \qquad j = 1,\dots,\nu.$$

From the above discussion, it follows that the linear system (3.5), (3.6) consists of $\nu + \sum_{j=1}^{\nu}\bar{s}_j$ scalar equations.

Therefore, to make, in this system, the number of the unknowns τ_j^i, g_j equal to the number of the equations, as the number q of the g_j is determined by the differential operator, the number α_j of the τ_j^i must satisfy

$$(3.7)\qquad \sum_{j=1}^{\nu}\alpha_j = \nu + \sum_{i=1}^{\nu}\bar{s}_i - q.$$

Moreover, from (3.5) α_j must satisfy also

$$(3.8)\qquad \alpha_j \geqslant \bar{s}_j, \qquad j = 1,\dots,\nu.$$

α_j are not uniquely determined by (3.7) and (3.8), therefore they can be suitably chosen as in (3.3).

Finally, the following class of one-step methods is obtained from (3.1), (3.2), (3.5), (3.6),

$$(3.9)\qquad y_{n+1} = \sum_{j=1}^{\nu}\sum_{i=0}^{M_j} d_j^i Q_j^i(x_{n+1}) + \sum_{j=1}^{q} g_j V_j(x_{n+1}),$$

$$(3.10)\qquad d_j^i = \sum_{k=0}^{\alpha_j}\tau_j^k c_{m-\alpha_j}^{i-k} - f_j^i,$$

$$(3.11)\qquad \sum_{p=1}^{\nu}\sum_{\substack{i=0\\ i\notin S_p}}^{M_p} d_p^i\left[R_p^i(x)\right]_j^k - d_j^k = 0, \qquad k \in S_j, j = 1,\dots,\nu,$$

$$(3.12)\qquad \sum_{p=1}^{\nu}\sum_{\substack{\iota=0\\ \iota\notin S_p}}^{M_p} d_p^{\iota}\big[Q_p^{\iota}(x_n)\big]_j+\sum_{\iota=1}^{q} g_\iota\big[V_\iota(x_n)\big]_j=[y_n]_j,\qquad j=1,\dots,\nu.$$

Remark. If the first-order differential system is originated by a differential equation of order ν, choosing the following perturbation term

$$(3.13)\qquad H_m(x)\begin{pmatrix}0\\ \vdots\\ 0\\ T_{m-\alpha_\nu}(x)\displaystyle\sum_{k=0}^{\alpha_\nu}\tau_\nu^k x^k\end{pmatrix},$$

we recover Ortiz' form [13] of the Lanczos tau approximant for a differential equation of order ν.

4. An Example. The methods derived above are, in this section, exemplified on a simple differential problem, in order to better clarify the use of the resulting algorithm.

For this purpose, the following problem is considered:

$$(4.1)\qquad \begin{cases}(x^2+1)y_1'(x)+y_2(x)=0, & y_1(0)=1,\\ y_2'(x)+xy_1(x)+y_2(x)=0, & y_2(0)=0.\end{cases}$$

The canonical polynomials will be, now, constructed as developed in Section 2.

The generating polynomials are

$$P_1^n(x)=\begin{pmatrix}nx^{n+1}+nx^{n-1}\\ x^{n+1}\end{pmatrix},\qquad P_2^n(x)=\begin{pmatrix}x^n\\ x^n+nx^{n-1}\end{pmatrix},$$

and, applying (2.2), (2.7), (2.8), it follows that

$$h_1=1,\quad h_2=0,$$
$$\Delta_1=0,\quad \Delta_2=1.$$

Therefore the matrix $W_n(x)$ is

$$W_n(x)=\begin{pmatrix}nx^{n+1}+nx^{n-1} & x^{n+1}\\ x^{n+1} & x^{n+1}+(n+1)x^n\end{pmatrix},$$

and accordingly P_n is

$$P_n=\begin{pmatrix}n & 1\\ 1 & 1\end{pmatrix}.$$

Applying Theorem 2.2 with elementary algebraic passages, as D has no polynomial solutions, the following recursive relations for the canonical polynomials are determined:

$$(4.2)\qquad \begin{cases}Q_1^n(x)=\dfrac{1}{n-2}\big(x^{n-1}e_1-x^ne_2-(n-1)Q_1^{n-2}(x)+nQ_2^{n-1}(x)\big),\\[2mm] Q_2^n(x)=\dfrac{1}{n-2}\big(-x^{n-1}e_1+(n-1)x^ne_2\\ \qquad\qquad +(n-1)Q_1^{n-2}(x)-n(n-1)Q_2^{n-1}(x)\big),\\ \hfill n\in N_0-\{0,2\}.\end{cases}$$

Therefore it is sufficient, in order to determine S_i, to verify if 0 and 2 belong to S_1 and/or S_2.

From the definition (2.2) it follows that neither 0 nor 2 belong to S_2, because

$$P_0^2(x) = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \text{and} \quad P_2^2(x) = \begin{pmatrix} x^2 \\ x^2 + 2x \end{pmatrix}$$

belong to Ω. Analogously $0 \notin S_1$, since $2P_1^0 + P_1^1 + P_2^2 = \binom{1}{0}$ belongs to Ω.

Therefore

$$S_1 = \{2\}, \qquad S_2 = \varnothing .$$

Now the canonical polynomials and the associated residuals can be constructed. $Q_0^1(x)$, $Q_0^2(x)$, $Q_2^2(x)$ are derived from the definition (2.4), the others by (4.2). It follows that

$$Q_1^0(x) = \begin{pmatrix} x+2 \\ -x^2 \end{pmatrix}, \qquad R_1^0(x) = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

$$Q_2^0(x) = \begin{pmatrix} -x-2 \\ x^2+1 \end{pmatrix}, \qquad R_2^0(x) = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

$$Q_1^1(x) = \begin{pmatrix} x+1 \\ -x^2+x-1 \end{pmatrix}, \qquad R_1^1(x) = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

$$Q_2^1(x) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad R_2^1(x) = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

$$Q_1^2(x), \qquad R_1^2(x) \text{ do not exist},$$

$$Q_2^2(x) = \begin{pmatrix} -2 \\ x^2 \end{pmatrix}, \qquad R_2^2(x) = \begin{pmatrix} x^2 \\ 0 \end{pmatrix},$$

$$Q_1^3(x) = \begin{pmatrix} x^2-2x-8 \\ -x^3+5x^2-2x+2 \end{pmatrix}, \qquad R_1^3(x) = \begin{pmatrix} 3x^2 \\ 0 \end{pmatrix},$$

$$Q_2^3(x) = \begin{pmatrix} -x^2+2x+14 \\ 2x^3-8x^2+2x-2 \end{pmatrix}, \qquad R_2^3(x) = \begin{pmatrix} -6x^2 \\ 0 \end{pmatrix},$$

$$Q_1^4(x) = \begin{pmatrix} \dfrac{x^3}{2} - 2x^2 + 4x + 28 \\ -\dfrac{1}{2}x^4 + 4x^3 - 16x^2 + 4x - 4 \end{pmatrix}, \qquad R_4^1(x) = \begin{pmatrix} -\dfrac{21}{2}x^2 \\ 0 \end{pmatrix},$$

$$Q_2^4(x) = \begin{pmatrix} -\dfrac{x^3}{2} + 6x^2 - 12x - 48 \\ \dfrac{3}{2}x^4 - 12x^3 + 48x^2 - 12x + 12 \end{pmatrix}, \qquad R_4^2(x) = \begin{pmatrix} \dfrac{69}{2}x^2 \\ 0 \end{pmatrix}.$$

. . . .

From (1.9), (3.3) the perturbation term is

$$H_m(x) = \begin{pmatrix} (\tau_1^0 + \tau_1^1 x)\cdot T_{m-1}(x) \\ \tau_2^0 T_m(x) \end{pmatrix}.$$

From (3.1), (3.2), with elementary algebraic passages, the solution $y^*(x)$ of the perturbed system can be written

$$(4.3) \quad y^*(x) = \tau_1^0 \sum_{\substack{i=0 \\ i\neq 2}}^{m-1} c_{m-1}^i Q_1^i(x) + \tau_1^1 \sum_{\substack{i=0 \\ i\neq 1}}^{m-1} c_{m-1}^i Q_1^{i+1}(x) + \tau_2^0 \sum_{i=0}^{m} c_m^i Q_2^i(x).$$

The (4.3) has to be evaluated at every discretization point, and the τ parameters are determined at every step by solving the linear system (3.11), (3.12).

In particular, setting $m = 3$, the integration formula is

$$y_{n+1} = \tau_1^0 \sum_{i=0}^{1} c_2^i Q_1^i(x_{n+1}) + \tau_1^1 \sum_{\substack{i=0 \\ i \neq 1}}^{2} c_2^i Q_1^{i+1}(x_{n+1}) + \tau_2^0 \sum_{i=0}^{3} c_3^i Q_2^i(x_{n+1}),$$

with the τ parameters being solutions of the following system, whose first equation is obtained by setting the expression of the residuals in (3.11)

$$\begin{cases} -c_2^2\tau_1^0 + \left(3c_2^2 - c_2^1\right)\tau_1^1 - 6c_3^3\tau_2^0 = 0, \\ \tau_1^0 \displaystyle\sum_{i=0}^{1} c_2^i\left[Q_1^i(x_n)\right]_j + \tau_1^1 \sum_{\substack{i=0 \\ i \neq 1}}^{2} c_2^i\left[Q_1^{i+1}(x_n)\right]_j + \\ +\tau_2^0 \displaystyle\sum_{i=0}^{3} c_3^i\left[Q_2^i(x_n)\right]_j = \left[y_n\right]_j, \qquad j = 1,2. \end{cases}$$

5. Numerical Results. Numerical experiments have been carried out in order to test the performance of the methods (3.9)–(3.12). For this purpose, the above methods have been implemented into a fixed-order, variable-step algorithm, taking as error estimate the difference between the values obtained by two methods of successive orders. As the methods have been proved to be A-stable [3], they have been evaluated on problems both stiff and nonstiff. They have been compared with Gear's methods and with Enright's second derivative multistep methods, using, respectively, the routines EPISODE [2] and SECDER [1]. The comparison has been carried out on some significant test problems picked out from those proposed by Hull [5], [7] and Krogh [8]. These problems, listed in the Appendix, have been classified in the following classes:

(A) *Stiff problems with real eigenvalues.* These are three systems, of varying size, with stiffness ratio: 200, 10^5, 10^5.

(B) *Stiff problems with complex eigenvalues.* These are four systems with real eigenvalues –0.1, –0.5, –1, –4, and two complex eigenvalues $-10 \pm i\alpha$, where α takes the values 3, 8, 25, 100, so that it is possible to see the behavior of a method as the eigenvalues approach the imaginary axis.

(C) *No stiff problems.* These are three systems; the first has solutions asymptotically tending to 1, the second has oscillating solutions, the third has an inherent instability.

In order to test the performance for different ranges of accuracy, each system has been solved for four tolerances, namely TOL $= 10^{-2}, 10^{-4}, 10^{-6}, 10^{-8}$.

The method (3.9)–(3.12) utilized (and implemented into the routine TAU) is that of order three for TOL $= 10^{-2}$, four for TOL $= 10^{-4}$, five for TOL $= 10^{-6}, 10^{-8}$. Also EPISODE uses these orders in most of the cases, whereas SECDER generally uses orders higher than these.

All the calculations have been carried out in double precision floating-point arithmetic with a 60 bit mantissa (approximately 18 decimals) on the Univac 1100/80 computer of the University of Naples.

TABLE I

SYSTEM	TOL	TIME(1)			STEP			MAX LOCAL ERROR(2)			GLOBAL ERROR(2)		
		EPISODE	SECDER	TAU	EPISODE	SECDER	TAU	EPISODE	SECDER	TAU	EPISODE	SECDER	TAU
A1	10^{-2}	0.059	0.076	0.056	36	23	11	1.09	$0.80.10^{-1}$	0.16	0.12	$0.10.10^{-2}$	$0.66.10^{-3}$
	10^{-4}	0.144	0.151	0.078	78	45	15	2.26	0.25	0.19	0.42	$0.35.10^{-2}$	$0.19.10^{-2}$
	10^{-6}	0.256	0.264	0.131	135	77	19	3.34	0.27	0.31	0.10	$0.52.10^{-1}$	$0.15.10^{-2}$
	10^{-8}	0.480	0.376	0.219	264	110	32	7.63	0.31	0.78	1.43	$0.24.10^{-1}$	$0.10.10^{-1}$
A2	10^{-2}	0.235	0.501	0.145	57	42	17	1.81	$0.76.10^{-1}$	0.16	0.30	$0.16.10^{-2}$	$0.22.10^{-3}$
	10^{-4}	0.496	0.844	0.297	119	78	25	2.61	0.33	0.17	1.30	$0.11.10^{-1}$	$0.16.10^{-2}$
	10^{-6}	0.951	1.332	0.507	231	136	32	9.80	0.27	0.20	0.71	$0.31.10^{-2}$	$0.32.10^{-4}$
	10^{-8}	1.644	1.922	0.885	450	204	56	12.23	0.31	0.41	20.11	$0.32.10^{-2}$	$0.32.10^{-3}$
A3	10^{-2}	0.095	0.117	0.294	53	35	18	5.07	0.34	0.72	1.12	$0.50.10^{-2}$	0.72
	10^{-4}	0.228	0.235	0.487	121	70	23	2.28	0.49	0.29	$0.16.10^{-1}$	$0.62.10^{-2}$	$0.77.10^{-2}$
	10^{-6}	0.439	0.379	0.770	233	110	29	2.65	0.40	0.85	0.62	$0.17.10^{-3}$	$0.27.10^{-3}$
	10^{-8}	0.719	0.562	1.272	393	163	48	5.64	0.44	0.69	16.21	$0.68.10^{-1}$	$0.52.10^{-2}$

(1) In seconds on the Univac 1100/80
(2) In units of TOL

TABLE II

SYSTEM	TOL	TIME(1) EPISODE	TIME(1) SECDER	TIME(1) TAU	STEP EPISODE	STEP SECDER	STEP TAU	MAX LOCAL ERROR(2) EPISODE	MAX LOCAL ERROR(2) SECDER	MAX LOCAL ERROR(2) TAU	GLOBAL ERROR(2) EPISODE	GLOBAL ERROR(2) SECDER	GLOBAL ERROR(2) TAU
B1	10^{-2}	0.070	0.113	0.083	30	21	10	1.19	0.19	0.79	0.19	$0.12.10^{-2}$	$0.25.10^{-2}$
	10^{-4}	0.167	0.205	0.139	68	40	13	3.36	0.34	0.27	0.34	$0.16.10^{-1}$	$0.53.10^{-2}$
	10^{-6}	0.291	0.331	0.227	117	67	17	5.92	0.41	0.52	1.27	$0.67.10^{-2}$	$0.72.10^{-2}$
	10^{-8}	0.560	0.495	0.384	240	100	29	3.18	0.34	0.47	3.63	$0.42.10^{-1}$	$0.70.10^{-1}$
B2	10^{-2}	0.079	0.123	0.107	32	23	13	0.76	0.17	0.80	$0.73.10^{-1}$	$0.12.10^{-2}$	$0.76.10^{-3}$
	10^{-4}	0.181	0.215	0.160	74	43	15	1.40	0.35	0.26	0.27	$0.10.10^{-1}$	$0.17.10^{-2}$
	10^{-6}	0.329	0.365	0.253	138	73	19	5.00	0.41	0.70	0.89	$0.48.10^{-1}$	$0.13.10^{-2}$
	10^{-8}	0.602	0.525	0.423	263	109	32	4.57	0.43	0.47	1.58	$0.32.10^{-1}$	$0.10.10^{-1}$
B3	10^{-2}	0.121	0.163	0.147	55	32	18	1.13	0.29	0.63	0.46	$0.59.10^{-2}$	$0.61.10^{-2}$
	10^{-4}	0.270	0.307	0.223	114	63	21	2.40	0.37	0.43	0.89	$0.33.10^{-2}$	$0.21.10^{-2}$
	10^{-6}	0.635	0.520	0.384	268	110	29	4.87	0.35	0.45	0.15	$0.59.10^{-1}$	$0.12.10^{-2}$
	10^{-8}	1.183	0.774	0.672	517	165	51	4.73	0.34	0.57	1.62	$0.41.10^{-1}$	$0.10.10^{-1}$
B4	10^{-2}	4.868	0.342	0.357	2273	76	44	2.28	0.18	0.63	0.11	$0.80.10^{-2}$	$0.81.10^{-1}$
	10^{-4}	5.324	0.704	0.599	2323	161	57	5.67	0.28	0.70	7.36	$0.97.10^{-2}$	$0.41.10^{-1}$
	10^{-6}	5.593	1.245	1.053	2507	287	80	6.07	0.34	0.66	4.38	$0.39.10^{-1}$	$0.18.10^{-1}$
	10^{-8}	6.960	2.021	1.983	3132	465	151	5.67	0.38	0.68	9.28	$0.46.10^{-1}$	$0.62.10^{-2}$

(1) In seconds on the Univac 1100/80
(2) In units of TOL

TABLE III

SYSTEM	TOL	TIME(1)			STEP			MAX LOCAL ERROR(2)			GLOBAL ERROR(2)		
		EPISODE	SECDER	TAU	EPISODE	SECDER	TAU	EPISODE	SECDER	TAU	EPISODE	SECDER	TAU
C1	10^{-2}	0.033	0.034	0.076	22	16	13	0.20	$0.75.10^{-1}$	0.26	$0.73.10^{-2}$	$0.15.10^{-7}$	$0.33.10^{-3}$
	10^{-4}	0.091	0.081	0.102	49	30	14	2.17	0.17	0.29	$0.58.10^{-3}$	$0.10.10^{-2}$	$0.20.10^{-3}$
	10^{-6}	0.253	0.131	0.188	104	49	21	1.99	0.28	0.29	0.31	$0.22.10^{-2}$	$0.40.10^{-4}$
	10^{-8}	0.337	0.207	0.392	133	74	44	8.44	0.31	0.42	0.62	$0.69.10^{-2}$	$0.47.10^{-3}$
C2	10^{-2}	0.067	0.050	0.046	40	24	14	0.95	0.23	0.77	2.59	2.62	7.10
	10^{-4}	0.136	0.089	0.064	90	43	15	1.48	0.22	0.66	15.81	4.76	4.49
	10^{-6}	0.216	0.139	0.109	115	66	20	1.35	0.32	0.68	11.69	7.25	5.32
	10^{-8}	0.338	0.201	0.208	162	95	38	1.04	0.32	0.70	13.99	9.24	11.19
C3	10^{-2}	0.024	0.023	0.026	18	12	8	0.42	$0.75.10^{-1}$	0.86	$0.10.10^{-1}$	$0.21.10^{-6}$	$0.57.10^{-4}$
	10^{-4}	0.060	0.047	0.034	37	21	8	1.25	0.96	0.24	0.46	$0.27.10^{-4}$	$0.19.10^{-4}$
	10^{-6}	0.112	0.082	0.055	56	38	10	1.28	0.28	0.21	0.44	$0.20.10^{-2}$	$0.80.10^{-4}$
	10^{-8}	0.119	0.122	0.088	93	55	16	5.89	0.31	0.39	$0.37.10^{-1}$	$0.99.10^{-4}$	$0.76.10^{-3}$

(1) In seconds on the Univac 1100/80
(2) In units of TOL

The comparison criteria have been chosen in such a way as to reflect both the efficiency and the reliability of a method.

The measures of efficiency chosen are:

(1) TIME—the total computing time, measured in seconds. It includes also the time for calculating the exact local solution in each step.

(2) STEP—the number of integration steps, performed to cover the whole integration range.

The measures of reliability chosen are:

(1) MAX LOCAL ERROR—the largest local error committed in all steps taken; the error is measured in units of the tolerance and it is defined as the maximum norm of $y_n(x_{n+1}) - y_{n+1}$, where $y_n(x)$ is the true solution through the previously computed point (x_n, y_n).

(2) GLOBAL ERROR—The maximum norm of the absolute error at the end of the integration interval. It is measured in units of the tolerance.

Numerical results are presented in Tables I, II, III. They show that the proposed method compares very favorably with the other two methods. In fact, it is better than the other two as concerns the efficiency, and it is better than EPISODE and comparable to SECDER as concerns the reliability.

This behavior is observed for all tolerances and for almost every problem. At the present time high quality software, implementing the above methods in a variable-order, variable-step algorithm, is in progress. Users of this package will be requested to supply, for the differential system that is to be integrated, the degrees and the coefficients of the polynomials $a_{ij}(x)$ and $b_{ij}(x)$, as quoted in (1.3).

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Appendix

Class A—Stiff systems with real eigenvalues

A1[5]

$$\begin{cases} y_1' = -0.5y_1 & y_1(0) = 1 \\ y_2' = -y_2 & y_2(0) = 1 \\ y_3' = -100y_3 & y_3(0) = 1 \\ y_4' = -90y_4 & y_4(0) = 1 \end{cases}$$

$$x \in [0, 20]$$

Eigenvalues: –0.5, –1, –90, –100

A2[5]

$$y_i' = -i^5 y_i \quad y_i(0) = 1 \quad i = 1, \ldots, 10$$

$$x \in [0, 1]$$

Eigenvalues: –1, –32, –243, –1024, –3125, –7776, –16807, –32768, –59049, –100000

A3[5]

$$\begin{cases} y_1' = -10^4 y_1 + 100 y_2 - 10 y_3 + y_4 & y_1(0) = 1 \\ y_2' = -10^3 y_2 + 10 y_3 - 10 y_4 & y_2(0) = 1 \\ y_3' = -y_3 + 10 y_4 & y_3(0) = 1 \\ y_4' = -0.1 y_4 & y_4(0) = 1 \end{cases}$$

$x \in [0, 20]$

Eigenvalues: -0.1, -1, -1000, -10000

Class B—Stiff systems with complex eigenvalues [5]

$$\begin{cases} y_1' = -10 y_1 + \alpha y_2 & y_1(0) = 1 \\ y_2' = -\alpha y_1 - 10 y_2 & y_2(0) = 1 \\ y_3' = -4 y_3 & y_3(0) = 1 \\ y_4' = -y_4 & y_4(0) = 1 \\ y_5' = -.5 y_5 & y_5(0) = 1 \\ y_6' = -.1 y_6 & y_6(0) = 1 \end{cases}$$

$x \in [0, 20]$

Eigenvalues: -0.1, -0.5, -1, -4, $-10 \pm \alpha i$

B1 $\alpha = 3$
B2 $\alpha = 8$
B3 $\alpha = 25$
B4 $\alpha = 100$

Class C—No Stiff system

C1[7]

$$\begin{cases} y_1' = -y_1 + y_2 & y_1(0) = 2 \\ y_2' = y_1 - 2 y_2 + y_3 & y_2(0) = 0 \\ y_3' = y_2 - y_3 & y_3(0) = 1 \end{cases}$$

$x \in [0, 20]$

Eigenvalues: 0, -1, -3

C2[8]

$$\begin{cases} y_1' = y_2 & y_1(0) = 0 \\ y_2' = -y_1 & y_2(0) = 1 \end{cases}$$

$x \in [0, 20]$

Eigenvalues: i, $-i$

C3[8]

$$\begin{cases} y_1' = y_2 & y_1(0) = 1 \\ y_2' = y_1 & y_2(0) = -1 \end{cases}$$

$$x \in [0, 20]$$

Eigenvalues: 1, −1

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