Rendiconti di Matematica, Serie VII
Volume 24, Roma (2004), 239-260

A method for global approximation of the solution of second order IVPs

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ABSTRACT: *For the numerical solution of the second order initial value problem, a family of global methods is derived by finding Galerkin approximations on a given interval. For each $n \geq 1$ a method is defined that uses a particular inner product in the Galerkin equation. The methods are symmetric collocation on the zeros of Chebyshev polynomials of the second kind and are related to implicit Runge-Kutta-Nyström methods. Order, stability and error analysis are here studied. Numerical examples provide favorable comparisons with other existing methods.*

1 – Introduction

In this paper we will consider the initial value problem in ordinary differential equations

$$(1) \qquad \begin{cases} y''(x) = f(x, y(x)) & x \in [x_0, b] \\ y(x_0) = y_0 \\ y'(x_0) = y'_0 \,. \end{cases}$$

We suppose that $f(x, y(x))$ is a real function defined and continuous on the strip $S = [x_0, b] \times \mathbb{R}$ and a constant L exists so that the inequality

$$|f(x, y_1) - f(x, y_2)| \leq L |y_1 - y_2|$$

KEY WORDS AND PHRASES: *Initial value problem – Chebyshev series.*
A.M.S. CLASSIFICATION: 65L05 – 65L60

holds over the strip S. Under these hypotheses the problem (1) has a unique solution $y(x)$.

Problems of this kind arise in a variety of physical contexts such as molecular-dynamics calculations for liquid and gases, stellar mechanics, atomic and nuclear scattering problems.

We assume that (1) represents a single scalar equation, but nearly all of the numerical and theoretical considerations in this paper carry over systems of second order equations, where (1) could be treated in vector form.

For higher order differential equations, one may solve them numerically by first reducing them to systems of first order equations. However, for an equation of the form (1), it is simpler to attack it directly and it is well known that several advantages (substantial gain in efficiency, lower storage requirements, etc.) are realized when the equations are treated in their original second-order form.

We develop a family of direct methods which produce smooth, global approximations to $y(x)$ in the form of polynomial functions. The basic idea is to approximate $y''(x)$ on $[-1,1]$ by a linear combination of Chebyshev polynomials of second kind and then to require that it provides Galerkin approximation (Section 2).

In Section 3 we show that these methods (GCM) are also collocation methods; we study the global approximation error in Section 4; then we propose two algorithms to compute the numerical solution of (1) in the nodal points and present some numerical examples in comparison with Dormand-Prince methods.

In Section 6 we illustrate the corresponding implicit Runge-Kutta-Nyström form, we observe that these methods have even order and we compare them with other Runge-Kutta-Nyström methods.

In Section 7 the study of stability of the method for $n = 3$ shows that it compares quite favorably with other fourth-order methods.

Finally (Section 8), we show that GCM may be formulated as symmetric hybrid two-step methods.

2 – Some polynomial Galerkin-type methods

We may approximate y'' on $[-1,1]$ by an $(n-1)$-th degree polynomial

$$y_n''(x) = \sum_{k=1}^{n} c_{k-1} U_{k-1}(x) , \qquad x \in [-1,1] \tag{2}$$

where $U_k(x)$ is the k-th degree Chebyshev polynomial of second kind, which satisfies:

$$U_{k-1}(x) = \frac{\sin kt}{\sin t} \tag{3}$$

with $x = \cos t$.

The coefficients c_k, $k = 0, \ldots, n-1$, are determined by a polynomial Galerkin-type method: we require the residual function $y_n'' - f$ to be orthogonal to all polynomials U_{j-1}, that is what this relation holds:

$$(y_n'' - f(x, y_n), U_{j-1}) = 0$$

$j = 1, \ldots, n$, or equivalently

$$(y_n'', U_{j-1}) = (f(x, y_n), U_{j-1}) \tag{4}$$

$j = 1, \ldots, n$.
By defining the discrete inner product [10]

$$(u, v) = \sum_{i=1}^{n} u\left(\pi - \frac{\pi i}{n+1}\right) v\left(\pi - \frac{\pi i}{n+1}\right),$$

we have

$$\left(\sin^2 t\, U_{k-1}, U_{j-1}\right) = \sum_{i=1}^{n} \sin\frac{k\pi i}{n+1} \sin\frac{j\pi i}{n+1} = \begin{cases} 0 & j \neq k \\ \dfrac{n+1}{2} & j = k \end{cases}$$

and

$$\sin^2 t\,(y_n'', U_{j-1}) = \frac{n+1}{2} c_{j-1}\,. \tag{5}$$

By multiplying the right term of (4) by $\sin^2 t$, it becomes:

$$\left(\sin^2 t\, f(x, y_n), U_{j-1}\right) = \sum_{i=1}^{n} f(x_i, y_n(x_i)) \sin\frac{\pi i}{n+1} \sin\frac{j\pi(n+1-i)}{n+1} \tag{6}$$

with

$$x_i = \cos\left(\pi - \frac{\pi i}{n+1}\right) = -\cos\frac{\pi i}{n+1} \qquad i = 1, \ldots, n\,. \tag{7}$$

By equaling (5) and (6) we have:

$$c_{j-1} = \frac{2}{n+1} \sum_{i=1}^{n} \sin\frac{\pi i}{n+1} \sin\frac{j\pi(n+1-i)}{n+1} f(x_i, y_n(x_i))\,.$$

Using the identity

$$kU_{k-1}(x) = T_k'(x)\,, \qquad k \geq 1\,, \tag{8}$$

and integrating (2) between -1 and x we have

$$y'_n(x) = y'_0 + \sum_{i=1}^{n} {}^n\gamma_i(x)\, f(x_i, y_n(x_i)) \tag{9}$$

where

$${}^n\gamma_i(t) = \frac{2}{n+1}\sin\frac{\pi i}{n+1}\sum_{k=1}^{n}\frac{p_k(t)}{k}\sin\frac{\pi k(n+1-i)}{n+1}$$

with

$$p_k(x) = T_k(x) - (-1)^k$$

and $T_k(x)$ are the Chebyshev polynomials of first kind of degree k.

If $f(x, y(x))$ does not depend on $y(x)$, the (9)

$$\int_{-1}^{x} f(t)dt = \sum_{i=1}^{n} {}^n\gamma_i(x)\, f(x_i) \tag{10}$$

coincides with the modified Filippi Clenshaw-Curtis quadrature formula [10]. Hence, for $x \in [-1, 1]$, (10) is a positive quadrature procedure which converges for every $f \in C^0[-1, 1]$.

Integration of (9) gives

$$y_n(x) = y_0 + (x+1)\, y'_0 + \sum_{i=1}^{n} {}^n\beta_i(x)\, f(x_i, y_n(x_i)) \tag{11}$$

where

$${}^n\beta_i(x) = \frac{1}{n+1}\sin\frac{\pi i}{n+1}\left\{\sin\frac{\pi i}{n+1}(x+1)^2 + \right.$$
$$\left. + \sum_{k=2}^{n}\frac{1}{k}\sin\frac{k\pi(n+1-i)}{n+1}\left[\frac{T_{k+1}(x)}{k+1} - \frac{T_{k-1}(x)}{k-1} - 2\left(x + \frac{k^2}{k^2-1}\right)(-1)^k\right]\right\}.$$

Thus we obtain:

$$\begin{cases} y(x) \approx y_n(x) = y_0 + (x+1)y'_0 + \sum_{i=1}^{n} {}^n\beta_i(x) f(x_i, y_n(x_i)) \\ \\ y'(x) \approx y'_n(x) = y(x_0) = y'_0 + \sum_{i=1}^{n} {}^n\gamma_i(x) f(x_i, y_n(x_i)). \end{cases}$$

3 – Chebyshev-Galerkin methods as collocation methods

THEOREM 1. *Let us consider the initial value problem* (1) *with* $x_0 = -1$, $[x_0, b] = [-1, 1]$. *If* x_i, $i = 1, \ldots, n$ *are defined as* (7), *then the polynomial* (11) *of degree* $n+1$ *satisfies the relations*

$$\begin{aligned} & y_n(-1) = y_0 \\ & y_n'(-1) = y_0' \\ & y_n''(x_j) = f(x_j, y_n(x_j)), \quad j = 1, \ldots, n \end{aligned} \tag{12}$$

i.e. it is a collocation polynomial for (1) [11].

PROOF.

$$ {}^n\beta_i(x) = \int_{-1}^{x} {}^n\gamma_i(t)\, dt. $$

Hence, $\forall i, n \in \mathbb{N}$, we have

$$ {}^n\beta_i(-1) = 0 $$

and

$$ {}^n\beta_i'(x) = {}^n\gamma_i(x) \quad \Longrightarrow \quad {}^n\beta_i'(-1) = 0. $$

It follows that

$$ y_n(-1) = y_0\,; $$

$$ y_n'(-1) = y_0' + \sum_{i=1}^{n} {}^n\beta_i'(-1)\, y_n''(x_i) = y_0'. $$

Moreover, for the polynomial ${}^n\gamma_i(x)$, we get

$$ {}^n\gamma_i'(x) = \frac{2}{n+1} \sin\frac{\pi i}{n+1} \sum_{k=1}^{n} \frac{T_k'(x)}{k} \sin\frac{\pi k(n+1-i)}{n+1}. $$

Putting $x = \cos t$, we have

$$ {}^n\gamma_i'(\cos t) = \frac{2}{n+1} \sin\frac{\pi i}{n+1} \sum_{k=1}^{n} \frac{\sin kt}{\sin t} \sin\frac{k\pi(n+1-i)}{n+1} $$

and for $t = t_j = \arccos x_j$, from the orthogonality of the system of functions $\sin mt$ ([10]), it follows that

$$ {}^n\gamma_i'(x_j) = {}^n\gamma_i'(\cos t_j) = \delta_{ij}. $$

for $j = 1, \ldots, n$. Hence we have

$$ y_n''(x_j) = \sum_{i=1}^{n} {}^n\beta_i''(x_j)\, f(x_i, y_n(x_i)) = f(x_i, y_n(x_i)). $$

□

From Theorem 1 we give the following definition

DEFINITION 1. The polynomial (11) is a global approximation method for the solution of (1) in $[-1,1]$. It is a symmetric collocation method.

OBSERVATION. Now an alternative representation for the ${}^n\beta_i(x), i=1,\dots,n$ can be derived by observing from (12) that, since $y_n''(x)$ interpolates $f\left(x,y(x)\right)$ at x_i, using Lagrangian interpolation we have

$$w_n''(x)=\sum_{k=1}^{n} l_k(t) f\left(x_k, y_n\left(x_k\right)\right). \tag{13}$$

After two integrations and comparing with (11), we obtain

$${}^n\beta_i(x)=\int_{-1}^{x}\left(\int_{-1}^{s} l_i(t)dt\right)ds=\int_{-1}^{x}(x-t)l_i(t)dt \tag{14}$$

where $l_i(t)$ is a polynomial of Lagrange interpolation on the set of points $\{x_i\}$:

$$l_i(t)=\prod_{k=1\ k\neq i}^{n}\frac{t-x_k}{x_i-x_k}.$$

4 – Global error

For the global error

$$L_n\left(y,x\right)=y\left(x\right)-y_n\left(x\right).$$

the following theorem holds:

THEOREM 2. *For all fixed* $x\in[-1,1]$

$$y(x)-y_n(x)=\frac{1}{n!}\left[\int_{-1}^{x}(x-t)^{n+1}y^{(n+2)}(t)dt+\right.$$
$$\left.-n\sum_{k=1}^{n}{}^n\beta_k(x)\int_{x_k}^{x}(x_k-t)^{n+1}y^{(n+2)}(t)dt\right].$$

PROOF. We observe that for all fixed $x \in [-1,1]$

$$L_n(y,x) = \int_{-1}^{x} \left(\int_{-1}^{s} y''(l)dl \right) ds - \sum_{k=1}^{n} {}^n\beta_k(x)\, y''(x_k)$$

is a linear functional vanishing if $y(t)$ is a polynomial of degree less than or equal to $n+1$. In fact, if $y(t)$ is a polynomial, it can be written in the Lagrange form:

$$y_n''(x) = \sum_{k=1}^{n} l_k(t) y_n''(x_k),$$

and from (14)

$$L_n(y,x) = \int_{-1}^{x} \left(\int_{-1}^{s} y''(l)dl \right) ds - \sum_{k=1}^{n} \int_{-1}^{x} \left(\int_{-1}^{s} l_k(t)dt \right) ds\, y''(x_k) = 0.$$

Hence from Peano's Lemma [8],

$$y(x) - y_n(x) = \int_{-1}^{x} K(t,x)\, y^{(n+2)}(t)\, dt$$

where

$$K(t,x) = \frac{1}{(n-1)!} \left[\int_{-1}^{x} \left(\int_{-1}^{s} (l-t)_+^{n-1} dl \right) ds - \sum_{k=1}^{n} {}^n\beta_k(x)\, (x_k - t)_+^{n-1} \right].$$

The thesis follows after some calculations.

OBSERVATION. If $y^{(n+2)}(t)$ is continuous in $[-1,1]$, then there exist η_0, η_k, $k = 1, \ldots, n$ in $[-1,1]$ such that

$$y(x) - y_n(x) = \frac{1}{n!(n+2)} \Bigg[(x-1)^{n+2} y^{(n+2)}(\eta_0) + \\ + n \sum_{k=1}^{n} {}^n\beta_k(x)(x_k - x)^{n+2} y^{(n+2)}(\eta_k) \Bigg].$$

5 – Algorithms and numerical examples

In order to calculate the approximate solution of the initial value problem by (11) at $x \in [-1,1]$ we need the values $y_n(x_i)$, $i = 1,\dots,n$. For this aim we propose two algorithms:

A1. Solve the system

$$y_n(x_i) = y_0 + (x_i+1)y_0' + \sum_{k=1}^{n} {}^n\beta_k(x_i)\, f(x_k, y_n(x_k)) \quad i = 1,...,n.$$

by iterative methods, particularly a modified Newton-type method for general non linear case. For linear problems the computational cost is considerably lower.

A2. An alternative way to calculate $y_n(x_j)$ is the iterative algorithm

$$\begin{cases} G_{n,j}^0 = y_0 + (x_j+1)\, y_0' + (x_j+1)^2 f(-1, y_0)/2 \\ G_{n,j}^\nu = y_0 + (x_j+1)y_0' + \sum\limits_{k=1}^{n} a_{kj} f\left(x_k, G_{n,k}^{\nu-1}\right) \quad \nu = 1,2,... \end{cases}$$

$j = 1,\dots,n$, $a_{kj} = {}^n\beta_k(x_j)$ and $G_{n,j}^\nu = G_{n,j}^\nu(x_j)$ where $G_{n,j}^0$ are the first three terms of Taylor approximation of $y_n(x_j)$ used to initialize the iterations.

We apply A1 to find numerical approximations of the solutions of some test problems. Similar results are obtained by algorithm A2.

Results are compared with the ones obtained by applying the Matlab ODE solver based on Dormand-Prince formula. We consider the following problems:

$$i) \quad \begin{cases} y'' = y + 2e^x \\ y(-1) = 0 \\ y'(-1) = \dfrac{1}{e} \end{cases}$$

with solution $y(x) = (x+1)e^x$

$$ii) \quad \begin{cases} y'' = -y + 2\cos x \\ y(-1) = -\sin(-1) \\ y'(-1) = \sin(-1) - \cos(-1) \end{cases}$$

with solution $y(x) = x\sin(x)$.

The figures (Fig. 1) and (Fig. 2) present the error function in the interval $[-1,1]$ in the case of Dormand-Prince approximation (dotted line) and in the case of approximation by GCM (solid line), algorithm A1.

In the first case (ode45) 85 function evaluations are needed for problem 1 and 67 for problem 2, while A1 requires 32 function evaluations if we use a modified

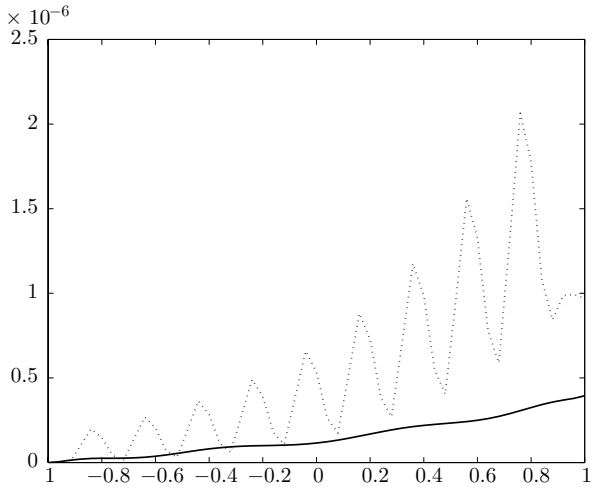

Fig. 1: Problem *i*.

Newton-type method and only 16 evaluations of functions of one variable if we use a direct method.

We can observe the smoothness of the error function in the case of approximation by A1.

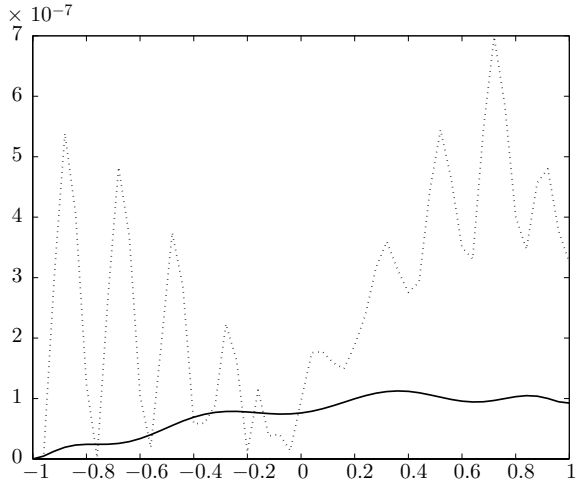

Fig. 2: Problem *ii*.

Moreover, with no additional cost, we have the approximation of the first derivative (Fig. 3 and 4).

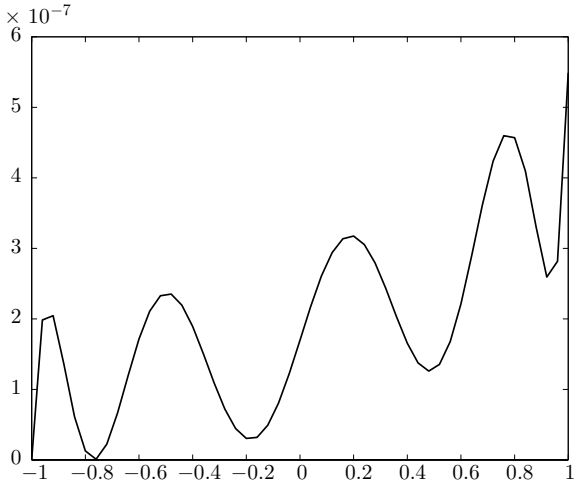

Fig. 3: Error function $|y'(x) - y'_n(x)|$ of problem i.

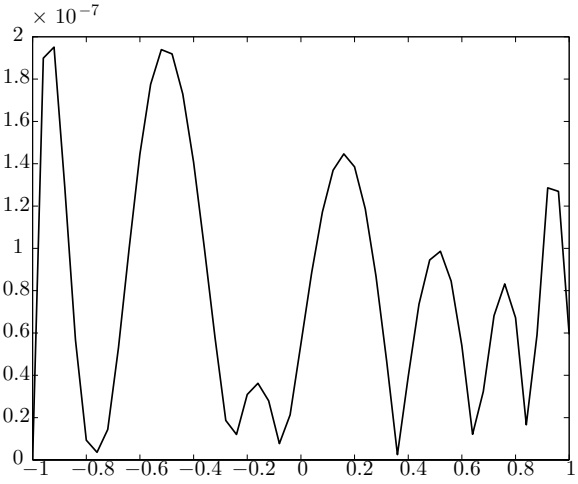

Fig. 4: Error function $|y'(x) - y'_n(x)|$ of problem ii.

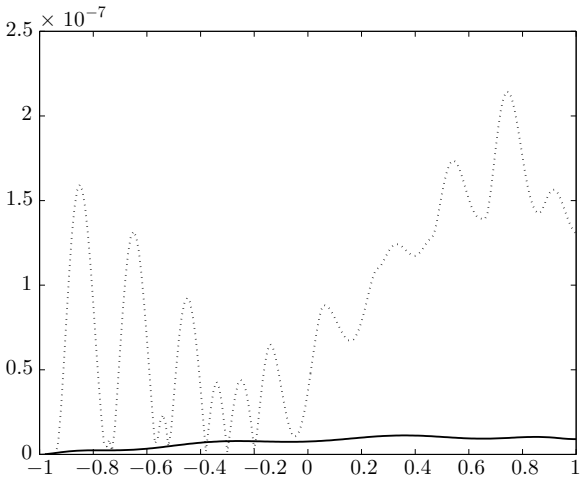

Fig. 5: Problem *iii*.

Now we consider the following non-linear problem:

$$iii) \quad \begin{cases} y'' = -\left(1 + 0.01y^2\right) y + 0.01\cos^3 x \\ y\,(-1) = \cos(-1) \\ y'(-1) = -\sin(-1). \end{cases}$$

The differential non-linear equation is a particular case of the undamped Duffing's equation, with a forcing term chosen so that the exact solution is $y\,(x) = \cos x$. Figure 5 show the error function in $[-1, 1]$ when we use ode45 (dotted line) and when we approximate by algorithm A1 (solid line).
The approximation by ode45 requires 67 function evaluations, algorithm A1 64.
Figure 6 presents the approximation of the first derivative using algorithm A1.

6 – Chebyshev-Galerkin methods as implicit Runge-Kutta-Nyström methods

Any one-step collocation method is equivalent to some implicit Runge-Kutta methods, where of course "equivalent" here means "matches the discrete values". Let $\chi : t_k = t_0 + kh$ be a uniform mesh with $t_0 = x_0$. On each subinterval we apply GCM (11), so that we have a collocation method on the points $t_{k+c_j} = t_k + c_j h$, $j = 1, \ldots, n$, with $c_j = \frac{1}{2}(x_j + 1)$, which are the images of the x_j under

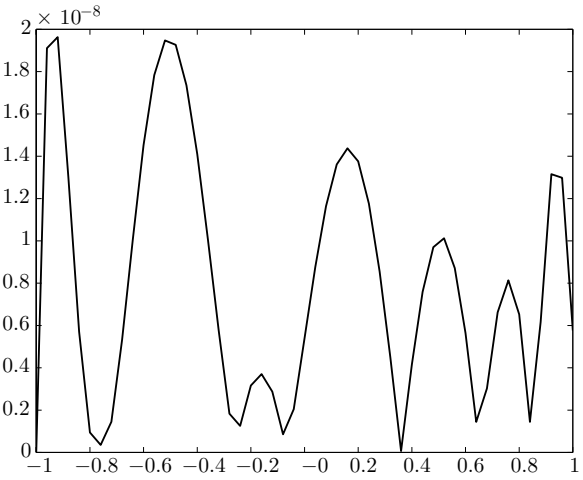

Fig. 6: Error function $|y'(x) - y'_n(x)|$ of problem *iii*.

a linear transform mapping $[-1, 1]$ onto $[0, 1]$:

$$y(t_{i+1}) = y(t_i) + hy'(t_i) + h^2 \sum_{j=1}^{n} b_j f\left(t_{i+c_j}, y\left(t_{i+c_j}\right)\right)$$

where $b_j = \frac{1}{4}\beta_j(1)$. Putting

$$k_j = f\left(t_i + c_j h, y_i + c_j h y'_i + h^2 \sum_{m=1}^{n} b_{jm} k_m\right), \tag{15}$$

with $b_{jm} = \frac{1}{4}\beta_m(x_j)$,we have:

$$y_{i+1} = y_i + hy'_i + h^2 \sum_{j=1}^{n} b_j k_j \tag{16}$$

and from (9)

$$y'_{i+1} = y'_i + h \sum_{j=1}^{n} a_j k_j \tag{17}$$

with $a_j = \frac{1}{2}\gamma_j(1)$. Equations (15), (16) and (17) gives rise to an n-stage implicit Runge-Kutta-Nyström method (CRK) with

$$\sum_{j=1}^{n} b_j = \frac{1}{2} \qquad \sum_{j=1}^{n} a_j = 1.$$

Using Butcher's notation ([1]), the first three of these methods are presented in Tables 1,2 and 3.

Table 1.

$\frac{1}{2}$	$\frac{1}{4}$
	$\frac{1}{2}$
	1

Table 2.

$\frac{1}{4}$	$\frac{1}{24}$	$-\frac{1}{96}$
$\frac{3}{4}$	$\frac{9}{32}$	0
	$\frac{5}{12}$	$\frac{1}{12}$
	$\frac{1}{2}$	$\frac{1}{2}$

Table 3.

$\frac{2-\sqrt{2}}{4}$	$\frac{1}{64}$	$\frac{5-4\sqrt{2}}{96}$	$\frac{23-16\sqrt{2}}{192}$
$\frac{1}{2}$	$\frac{3+2\sqrt{2}}{48}$	0	$\frac{3-2\sqrt{2}}{48}$
$\frac{2+\sqrt{2}}{4}$	$\frac{23+16\sqrt{2}}{192}$	$\frac{5+4\sqrt{2}}{96}$	$\frac{1}{64}$
	$\frac{2+\sqrt{2}}{12}$	$\frac{1}{6}$	$\frac{2-\sqrt{2}}{12}$
	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$

Note that the c_j have the symmetry property

$$c_{n+1-j} = 1 - c_j, \qquad j = 1, \ldots, \left[\frac{n}{2}\right]. \tag{18}$$

A Runge-Kutta-Nyström method has order p [11] if for sufficiently smooth problems (1)

$$y\left(x_{i+1}\right) - y_{i+1} = O\left(h^{p+1}\right) \qquad y'\left(x_{i+1}\right) - y'_{i+1} = O\left(h^{p+1}\right).$$

Being the method (11) a collocation method, $\forall x \in [-1, 1]$ the following estimates hold [11]:

$$y(x) - y_n(x) = O\left(h^{n+2}\right), \qquad y'(x) - y'_n(x) = O\left(h^{n+1}\right).$$

So the method (11) has order at least n. We may prove that for odd n the order is $n + 1$. In fact, putting

$$M(t) = \prod_{i=1}^{n} \left(t - c_i\right),$$

if $n = 2k + 1$, we have

$$\int_0^1 M(t)dt = 0 \tag{19}$$

and this condition is equivalent to orthogonality to polynomials of degree $q = 0$, so the method has order [11] $p = n + q + 1 = n + 1$.

The (19) follows from the fact that $M(t) = (-1)^n M(-t)$, hence, if n is odd, $M(t)$ is an odd function.

Coleman and Booth in [5], starting from Panovsky-Richardson method [13], derived a class of Runge-Kutta-Nyström methods for differential equations of the form $y''(x) = f(x, y)$ which uses in each interval $[x_k, x_{k+1}]$ the set of $n + 1$ collocation points $\{x_k + c_j h, j = 0, \ldots, n\}$ where $c_j = \frac{1}{2}(x_j + 1)$ and x_j are the extrema of Chebyshev polynomials of first kind $T_k(x)$ of degree k.

In this context CRK method can be compared with other similar methods, among which the Coleman and Booth Runge-Kutta-Nyström one [5], which we indicate by CBRKN.

Thus we make a comparison between the forth order CBRKN, and the CRK method of order four derived in this section.

6.1 – Harmonic oscillator

Let's now solve the initial value problem

$$y'' = -y, \qquad y(0) = 1, \qquad y'(0) = 0 \tag{20}$$

using the forth order CBRKN and CRK methods. The results in Figures 7 and 8, produced by a MatLab code, show the absolute errors for the two methods (dotted line for the CBRKN) applied to problem (20) with steplengths respectively $h = 0.01$ and $h = 0.05$. Both methods have the same cost and are based upon the zeros of Chebyshev polynomials but of different degrees so their coefficients are different.

The maximum absolute errors on intervals $[0, x]$ with steplength $h = 0.01$ are displayed in Table 4.

Table 4.

x	CBRKN	CRK
1	$4.4 \cdot 10^{-12}$	$1.1 \cdot 10^{-12}$
2	$9.5 \cdot 10^{-12}$	$2.4 \cdot 10^{-12}$
5	$2.5 \cdot 10^{-11}$	$6.2 \cdot 10^{-12}$
10	$4.1 \cdot 10^{-11}$	$7.1 \cdot 10^{-12}$
20	$9.5 \cdot 10^{-11}$	$2.4 \cdot 10^{-11}$
50	$2.5 \cdot 10^{-10}$	$1.7 \cdot 10^{-11}$
100	$5.1 \cdot 10^{-10}$	$6.6 \cdot 10^{-11}$

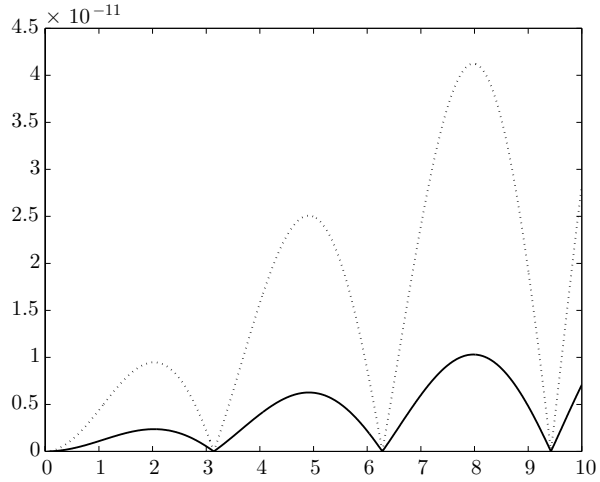

Fig. 7:

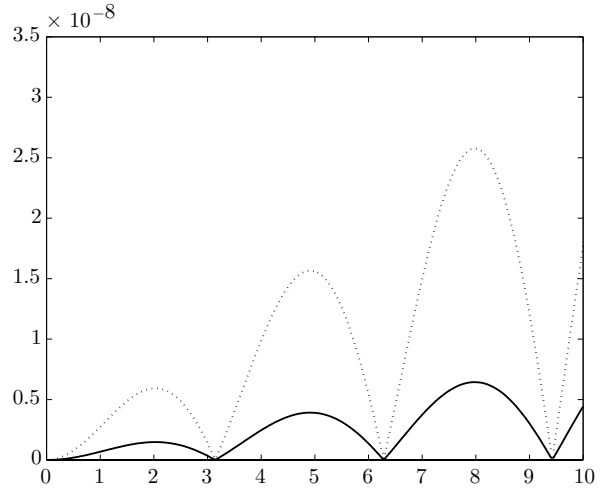

Fig. 8:

Table 5 illustrates the effects of different steplengths used over a given number of steps.

Table 5.

h	steps	CBRKN	CRK
0.1	500	$2.5 \cdot 10^{-6}$	$1.7 \cdot 10^{-7}$
0.1	1000	$5.1 \cdot 10^{-6}$	$6.6 \cdot 10^{-7}$
0.005	500	$5.9 \cdot 10^{-13}$	$1.2 \cdot 10^{-13}$
0.005	1000	$1.6 \cdot 10^{-12}$	$3.9 \cdot 10^{-13}$
0.002	500	$8.1 \cdot 10^{-15}$	$1.5 \cdot 10^{-15}$
0.002	1000	$1.5 \cdot 10^{-14}$	$3.5 \cdot 10^{-15}$
0.001	500	$1.9 \cdot 10^{-15}$	$2.0 \cdot 10^{-15}$
0.001	1000	$3.1 \cdot 10^{-15}$	$2.8 \cdot 10^{-15}$

Table 6 shows the maximum absolute errors on intervals $[0, x]$ for the same methods of order six applied to problem (20) with steplength $h = 0.01$:

Table 6.

x	CBRKN	CRK
1	$5.6 \cdot 10^{-16}$	$3.3 \cdot 10^{-16}$
2	$9.4 \cdot 10^{-16}$	$1.1 \cdot 10^{-16}$
5	$1.1 \cdot 10^{-15}$	$1.1 \cdot 10^{-16}$
10	$2.7 \cdot 10^{-15}$	$2.4 \cdot 10^{-15}$
20	$4.4 \cdot 10^{-15}$	$1.2 \cdot 10^{-15}$
50	$7.9 \cdot 10^{-15}$	$4.2 \cdot 10^{-15}$
70	$1.1 \cdot 10^{-14}$	$7.8 \cdot 10^{-16}$
100	$1.2 \cdot 10^{-14}$	$3.9 \cdot 10^{-14}$

Values of column 2 are the ones which appear in [5].
Figure 9 illustrates absolute errors when $h = 0.05$, in the case of order six.

6.2 – Two-body problem

A non-linear example frequently used to test numerical methods (see, e.g. [5]) is provided by the two-body problem:

$$\text{(21)} \qquad \begin{cases} y'' + \dfrac{y}{r^3} = 0, \quad y(0) = 1 - e, & y'(0) = 0 \\ z'' + \dfrac{z}{r^3} = 0, \quad z(0) = 0, & z'(0) = \sqrt{\dfrac{1+e}{1-e}} \end{cases}$$

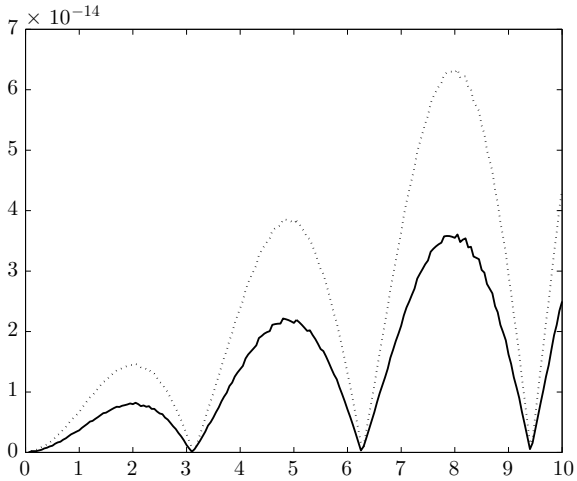

Fig. 9:

with $r^2 = y^2 + z^2$. The exact solution is

$$y = \cos E - e, \qquad z = \sqrt{1 - e^2}\sin E,$$

where e is the eccentricity of the orbit and E is implicitly defined as $x = E - e\sin E$.

In Table 7 we compare the maximum absolute errors on $[0, x]$ for the two fourth order methods, CRK and CBRKN, applied to (21) when $e = 0.1$ and steplength $h = 0.01$.

Table 7.

x	CBRKN	CRK
1	$2.9 \cdot 10^{-11}$	$7.4 \cdot 10^{-12}$
2	$4.0 \cdot 10^{-11}$	$9.9 \cdot 10^{-12}$
5	$1.2 \cdot 10^{-10}$	$2.9 \cdot 10^{-11}$
10	$2.8 \cdot 10^{-10}$	$7.1 \cdot 10^{-11}$
20	$8.4 \cdot 10^{-10}$	$2.1 \cdot 10^{-10}$
50	$2.1 \cdot 10^{-9}$	$5.4 \cdot 10^{-10}$
100	$4.2 \cdot 10^{-9}$	$1.0 \cdot 10^{-9}$

These results were produced by MatLab programs on a microcomputer and show that CRK method is favourably comparable to CBRKN one.

7 – Stability and periodicity

Now we investigate the numerical stability of method (11) for $n = 3$. Towards this aim we consider its equivalent implicit Runke-Kutta-Nyström form (CRK) and then we compare results with other forth-order methods.

We apply CRK to the test equation

$$y'' = -\alpha y$$

where α is a real number, and after some calculation we obtain:

$$(22) \quad \begin{cases} y_{i+1} = \dfrac{-B}{A}\left(36864 + 17280h^2\alpha + 968h^4\alpha^2 + 11h^6\alpha^3\right) y_i + \\ \qquad\qquad -\dfrac{hB}{A}\left(36864 + 4992h^2\alpha + 136h^4\alpha^2 + h^6\alpha^3\right) y_i' \\ y_{i+1}' = \dfrac{-h\alpha B}{A}\left(36864 + 4992h^2\alpha + 120h^4\alpha^2\ \right) y_i + \\ \qquad\qquad -\dfrac{B}{A}\left(36864 + 17280h^2\alpha + 968h^4\alpha^2 + 11h^6\alpha^3\right) y_i' \end{cases}$$

where

$$A = (17 + 12\sqrt{2})[4608 - 72h^2\alpha + (1 + 2\sqrt{2})h^4\alpha^2] \cdot \left(-36864 + 1152h^2\alpha - 8h^4\alpha^2 + h^6\alpha^3\right)$$

$$B = 4608\left(17 + 12\sqrt{2}\right) - 72\left(17 + 12\sqrt{2}\right)h^2\alpha + \left(65 + 46\sqrt{2}\right)h^4\alpha^2$$

The equations (22) written in matrix notation are

$$(23) \qquad u_{i+1} = Mu_i$$

in which $u_i = [y_i, y_i']^T$, $M = (m_{ij})$,

$$\begin{aligned} m_{11} &= -\frac{B}{A}\left(36864 + 17280h^2\alpha + 968h^4\alpha^2 + 11h^6\alpha^3\right) \\ m_{12} &= -\frac{hB}{A}\left(36864 + 4992h^2\alpha + 136h^4\alpha^2 + h^6\alpha^3\right) \\ m_{21} &= -\frac{h\alpha B}{A}\left(36864 + 4992h^2\alpha + 120h^4\alpha^2\ \right) \\ m_{22} &= m_{11} \end{aligned}$$

We treat the cases $\alpha = k^2$ and $\alpha = -k^2$.

In the following we set $H = hk$ and denote the eigenvalues of the matrix M by $\mu_{1,2}$.

In the first case we get oscillating solutions, so it is important to have eigenvalues of M on or inside the unit circle.

In general the eigenvalues of the amplification matrix M are the roots of the characteristic equation

$$\lambda^2 - 2R\left(H^2\right)\lambda + P\left(H^2\right) = 0$$

where $R\left(H^2\right) = \frac{1}{2}$ trace (M) and $P\left(H^2\right) = \det(M)$ are rational functions of H^2; numerator and denominator of R are polynomials of degree $\leq n$ in H^2. It is known that for polynomial collocation $P\left(H^2\right) = 1$ when the collocation nodes are symmetric [12]. In this case, $R\left(H^2\right)$ is a rational approximation for $\cos H$, called stability function of the method.

Stability means that the numerical solutions remain bounded moving further away from the starting point.

Definition 2. A method is weakly stable in an interval $(0, r)$ if, for each H in $(0, r)$, $|\mu_1| = |\mu_2| = 1$.

Weak stability prevents the numerical solution u_i to spiral into the origin. Every symmetric collocation method is weakly stable in an interval of the form $(0, r)$ [12].

We have that the eigenvalues $\mu_{1,2}$ are complex when $0 \leq H^2 < 9.6$ and $|\mu| = 1 \; \forall H$ in $(0, 9.6)$.

The stability of method CRK compares quite favorably with other one-step fourth-order methods, for example, Runge-Kutta, Runge-Kutta-Nyström methods [9] and Chang-Gnepp method [2]. The stability range of the Runge-Kutta method is $0 \leq H^2 \leq 7.756$, of the Runge-Kutta-Nyström method is $0 \leq H^2 \leq 6.690$ and of the Chang-Gnepp method is $0 \leq H \leq 8.0722$.

Definition 3. An interval $\left(0, H_p^2\right)$ is said to be an interval of periodicity for a method (23) if, for all $H^2 \in \left(0, H_p^2\right)$, $\mu_{1,2}$ are distinct, complex and of modulii one.

If conditions of definition 3 are satisfied for all $H^2 > 0$, the method is P-stable, but one-step polynomial collocation does not provide any P-stable methods [4].

For method CRK, $n = 3$, the interval of periodicity is $(0, 9.6)$. The interval of stability of the fifth-order Nyström method in [3] is $(0, 8.46)$.

Let's now consider the case $\alpha = -k^2$. In the previous case we have oscillating solutions, here the solutions are exponential. We'll study the relative error of method CRK for the equation under discussion, in the case of small h, that is a large number of integration intervals, following the idea of Rutishauser [14].

The maximum eigenvalue of matrix M is

$$\mu = 1 + hk + \frac{1}{2}h^2k^2 + \frac{1}{6}h^3k^3 + \frac{1}{24}h^4k^4 + \frac{13}{1536}h^5k^5 + O\left(h^6k^6\right)$$

Thus the relative error is

$$F \approx \frac{hk - \ln \mu}{h} = \frac{\ln\left(e^{hk}\right) - \ln \mu}{h} = \frac{1}{h}\left(\frac{e^{hk} - \mu}{\mu}\right) \approx \frac{h^4 k^5}{1536}$$

for large x and small h. The relative error for the Runge-Kutta method is $F \approx \frac{h^4 k^5}{120}$, for the Runge-Kutta Nyström method is $F \approx \frac{h^4 k^5}{320}$ and for the method proposed by Chang and Gnepp ([3]) it is $F \approx \frac{h^4 k^5}{720}$.

8 – Chebyshev-Galerkin methods as hybrid symmetric two-step methods

Now we show that methods (11) may be formulated as symmetric two-step hybrid methods in which the position of the off-step points are determined by the x_i defined in (7). In [5] it was proved that a collocation method on the points $t_{k+c_i} = t_k + c_i h$, $i = 1, \ldots, n+1$ with $c_i = \frac{1}{2}(x_i + 1)$ is symmetric (that is the nodes are such that (18) holds). Then the approximations $y_i \approx y(t_i)$ and $z_i \approx y'(t_i)$ satisfy the equations

$$c_i h z_{k+1} = y_{k+1} - y_{k+c_{n+1-i}} + h^2 \sum_{j=1}^{n} b_{ij} f_{k+c_{n+1-j}} \tag{24}$$

for $i = 1, \ldots, n$, $k = 0, 1, \ldots$, where $f_{k+c_{n+1-j}} = f\left(t_k + c_{n+1-j} h, y_{k+c_{n+1-j}}\right)$. (Using the 18) and replacing $k+1$ by k in (24), we have:

$$c_i h z_k = y_k - y_{k-c_i} + h^2 \sum_{j=1}^{n} b_{ij} f_{k-c_j} \tag{25}$$

which, for $i = n+1$, may be written as

$$h z_k = y_k - y_{k-1} + h^2 \sum_{j=1}^{n} b_{n+1,j} f_{k-c_j} \tag{26}$$

and $b_{n+1,j} = \dfrac{1}{4}\beta_j(x_{n+1}) = b_j$.

Equations (15), (16), (17) may be put in the form:

$$\begin{cases} y_{k+1} = y_k + h z_k + h^2 \displaystyle\sum_{j=1}^{n} b_j f_{k+c_j} \\ y_{k+c_j} = y_k + h c_j z_k + h^2 \displaystyle\sum_{i=1}^{n} b_{ji} f_{k+c_i} \\ z_{k+1} = z_k + h \displaystyle\sum_{i=1}^{n} a_i f_{k+c_i} \end{cases} \tag{27}$$

so the method becomes:

$$(28)\qquad \begin{cases} y_{k+1} = 2y_k - y_{k-1} + h^2 \sum_{j=1}^{n} b_j \left(f_{k-c_j} + f_{k+c_j} \right) \\ y_{k+c_j} = 2y_k - y_{k-c_j} + h^2 \sum_{i=1}^{n} b_{ji} \left(f_{k-c_i} + f_{k+c_i} \right) \end{cases}$$

which is a symmetric, hybrid two-step method with $2n$ off-step points between t_{k-1} and t_{k+1} for each k.

If $x_i = \cos \dfrac{(n-i)\pi}{n}$, $i = 0, \ldots, n$, (28) coincides with Panovsky-Richardson implicit method [13]. In this case CRK method may be seen as an alternative formulation of Panovsky-Richardson method.

Equations (28) require starting values at x_0, x_1 and at any off-step points between x_0 and x_1. If these starting values provided by (28) are the approximations generated by CRK method on $[t_0, t_1]$, then, in exact arithmetic the two methods would yield identical results at all subsequent steps [13].

9 – Conclusions

This paper provides a family of numerical collocation methods for initial value problems of the form (1). For each positive integer n two polynomials, one of degree $n+1$, which approximates the exact solution of (1), and the other, of degree n, which approximates its first derivative, are given explicitly.

Numerical tests show that these methods perform as well as other existing methods in terms of stability, of magnitude of the absolute error, and of function evaluations.

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Lavoro pervenuto alla redazione il 15 febbraio 2003
ed accettato per la pubblicazione il 4 dicembre 2003.
Bozze licenziate il 6 dicembre 2004

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