New Multiple FDMs Through Multistep Collocation for
$y'' = f(x.y)$

by

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Abstract
In this paper we show that a link between the Finite Difference Methods (FDMs) and the Multistep Collocation (MC) procedure leads to new Multiple FDMs among the global methods. They are applied to ordinary differential equations (ODEs) of the form $y'' = f(\mathrm{x}, y), a \leq \mathrm{x} \leq b$ with specified initial, boundary or mixed conditions at the two end points a and b or at multi-points in [a,b]. The resulting piecewise continuous approximate solution (interpolant) belongs to the space C^1[a, b] over sub-intervals, which do not overlap. Two specific methods of order four associated with the standard Numerov method are used to illustrate the new approach.

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1. Introduction

The finite difference methods (FDMs) and the k-step multistep collocation (MC) procedure are two important global methods which have been used with piecewise continuous approximate solutions of ordinary differential equations (ODEs) (see for instance, Gladwell and Sayers (1976), Lie and Norsett (1989), Atkinson (1989), Onumanyi et al (1994, 1999).

Let us consider the initial-value problem (IVP) and boundary-value problem (BVP) for the ODEs of the form:

$$y''(\mathrm{x}) = \mathrm{f(x,y)}, \ \mathrm{a} \leq \mathrm{x} \leq \mathrm{b} \tag{1.1}$$

With specified initial, boundary or mixed conditions only.

In this paper we show that a link between FDMs and the MC procedure leads to new Multiple FDMs for solving (1.1). The methods consist of more than one FDM, which are simultaneously applied to (1.1) over sub-intervals, which do not overlap. This is a desirable feature for the uniqueness of the interpolant between mesh points. This is not possible with the single FDM, i.e. the conventional FDM (see Lambert (1991), p. 53 and Jennings (1989), p. 59). In Onumanyi et al (1999), Multiple FDMs were constructed for the first order ODE's of the form y'' (x) = f(x,y). The Adams and the BDF methods were shown to be special cases. The extension of these multiple FDMs to (1.1) directly is not immediately obvious. Therefore this paper generalizes the results of Fatunla (1991), Onumanyi et al (1994, 1999) and Awoyemi (1992) to piecewise continuous approximate solutions in the $C^1[a,b]$ space for (1.1).

2. The Method for Continuous Approximations

We seek the method of the form

$$y(x) \cong U(x) = \sum_{v-0}^{1-1} \phi_v(x) y_{n=v} + h^2 \sum_{v=0}^{m-1} \psi_v(x) f_{n+v} \qquad (2.1)$$

Where x [x $\in X_{n,} X_{n+k}$] and we introduce the following notations. The positive integer k $\leq$ 2 denotes the step number of the method, (2.1) is sought on a given mesh:

$a=x_0 < x_1 < x_n < x_{n+1} < ... < x_{n+k} < ... < x_N = b;$

$h=x_{n+1} - x_n$, n=0, ... N; is a constant step-size; m > 0 is the number of distinct collocation points used and t is the number of interpolation points used, $2 \leq t \leq k$.

The values of k and m are arbitrary except for collocation at the mesh points only, where $0 < m \leq k + 1$. Let

$U(x_{n+v}) = y(x_{n+v})$, v = 0, ..., k - 1

Then a k-step multistep collocation method with m collocation points is constructed using (2.1) which yields a polynomial U(x) of degree p = t + m – 1 and such that it satisfies the conditions:

$$U(x_{n+v}) = y_{n+v} \in \{0,..., t\text{-}1); U''(\overline{X}) = f_{n+v,\ v = 0,\ ...,\ m - 1,} \qquad (2.2)$$

where f_{n+v} denotes $f(\overline{x}_{v,} U(\overline{x}_v))$, ϕ_v) and $\Psi_v(x)$ are assumed polynomial basis functions.

$$\phi_v(x) = \sum_{1=0}^{1+m-1} \phi_{i+1,v} p_i(x), v \in \{0,...,t-1\} \qquad (2.3)$$

and

$$h^2\psi_v(x) = \sum_{i=0}^{1+m-1} h^2 \psi_{i-1,v} p_i(x), v = 0,1,...m-1 \qquad (2.4)$$

and the collocation points $\overline{x}_v \in Q, Q \equiv \{x_n,...,\ x_{n+k}\} \cup (x_{n+k-1,}\ x_{n+k})$

$\phi_{i+1,v}$ and $h^2\psi_{i+1,v}$ are un-determined elements of the following (t + m) x (t + m) dimensional matrix:

$$\underline{\underline{C}}=\begin{bmatrix} \phi_{1,0} & \phi_{1.1} & \ldots & \phi_{1,t-1} & h^2\psi_{1.0} & \ldots & h^2\psi_{1,m-1} \\ \phi_{2,0} & \phi_{2,1} & \ldots & \phi_{2,t-1} & h^2\psi_{2,0} & \ldots & h^2\psi_{2,m-1} \\ . & . & & . & . & & . \\ . & . & & . & . & & . \\ . & . & & . & . & & . \\ \phi_{i+1,0} & \phi_{i+1,1} & \ldots & \phi_{i+1,t-1} & h^2\psi_{i+1,0} & \ldots & h^2\psi_{i+1,m-1} \\ . & . & & . & . & & . \\ . & . & & . & . & & . \\ . & . & & . & . & & . \\ \phi_{t+m,0} & \phi_{t+m,1} & \ldots & \phi_{t+m,t-1} & h^2\psi_{t+m,0} & \ldots & h^2\psi_{t+m,m-1} \end{bmatrix} \quad (2.5)$$

Where i = 0,1,…,1=m-1 in (2.5).

We define the following vectors

$$\underline{a} = (a_o, a_1, \ldots, a_{1+m-1})^T \quad (2.6)$$

where T denotes 'transpose of'

$$\underline{V} = (y_n, y_{n+1}, \ldots, y_{n+t-1}, f_n, f_{n+1}, \ldots, f_{n+m-1})^T \quad (2.7)$$

$$\underline{P}\ (x) = (P_o(x), P_1(x), \ldots, P_{t+m-1}(x))^T \quad (2.8)$$

denotes an arbitrary basis function, and

$$\underline{\underline{M}}=\begin{bmatrix} P_o(x_n) & \ldots & P_{t+m-1}(x_n) \\ P_o(x_{n+1}) & \ldots & P_{t+m-1}(x_{m+1}) \\ . & & . \\ . & & . \\ . & & . \\ P_o(x_{n+t-1}) & \ldots & P_{t+m-1}(x_{n+t-1}) \\ P_o''(\overline{x}_o) & \ldots & P''_{t+m-1}(\overline{x}_o) \\ P_o''(\overline{x}_1) & \ldots & P''_{t+m-1}(x_1) \\ . & & . \\ . & & . \\ . & & . \\ P_o''(\overline{x}_{m-1}) & \ldots & P''_{t+m-1}(\overline{x}_{m-1}) \end{bmatrix} \quad (2.9)$$

where the matrix $\underline{\underline{M}}$ is assumed non-singular. Then we can show that

(a) $U(x) = \underline{V}^T (\underline{\underline{M}}^{-1})^T \underline{P}(x)$

(b) $\underline{\underline{C}} = \underline{\underline{M}}^{-1}$,

Proof of (a)

Consider (2.1), (2.3) and (2.4) to obtain

$$U(x) = \sum_{i=0}^{t+m-1} \left\{ \sum_{v=0}^{t-1} \phi_{i+1,v} y_{n+v} + \sum_{v=0}^{m-1} h^2 \psi_{i+1,v} f_{n+v} \right\} P_i(x) \tag{2.10}$$

$$= \sum_{t=0}^{1+m-1} a_i P_i(x) \tag{2.11}$$

where, for i = 0, 1, …, t + m – 1,

$$a_i = \sum_{v=0}^{t-1} \phi_{i+1,v} y_{n+v} + \sum_{v=0}^{m-1} h^2 \psi_{i+1,v} f_{n+v} \tag{2.12}$$

and a_i in (2.12) are t + m undetermined constants. Now consider (2.11) in a vector form

$$U(x) = \underline{a}^T \underline{P}(x) \tag{2.13}$$

By imposing the conditions in (2.2) on (2.13) we obtain equation of the form:

$$\underline{\underline{M}}\ \underline{a} = \underline{V} \tag{2.14}$$

Thus

$$\underline{a} = \underline{\underline{M}}^{-1} \underline{V} \tag{2.15}$$

Since $\underline{\underline{M}}$ is assumed non-singular.

By (2.15), (2.13) becomes

$$U(x) = \underline{V}^T (M^{-1})^T \underline{P}(x) \tag{2.16}$$

Which proves (a) part.

Proof of (b)

We can write (2,12) in a vector form

$$a_i = (\phi_{i+1,0,...}\phi_{i+1,t-1}, h^2\psi_{i+1,m-1})\underline{V}, i = 0,1,...t+m-1 \quad (2.17)$$

By (2.5), (2.17) becomes

$$a_i = (\underline{\underline{C}}_{i+1}\underline{V}, \text{i = 0, 1, ..., t+m-1} \quad (2.18)$$

Where $\underline{C}_{i+1}$ denotes (i+1) the row vector of the matrix $\underline{C}$ in (2.5). Hence (2.18) can be put in the form

$$\underline{a}^T = (\underline{C}\ \underline{V})^T \ (or\ \underline{a} = \underline{C}\ \underline{V}) \quad (2.19)$$

Comprising (2.19) and (2.15) we obtain $\underline{\underline{C}} = \underline{\underline{M}}^{-1}$ which proves (b) part.

Comments (1)
We emphasize here that (a) and (b) proved above give a generalized derivation procedure for specific methods and under no circumstances should the method be used as a numerical integrator directly because obtaining $\underline{\underline{M}}^{-1}$ explicitly at each step of the integration process is expensive. In the next section we demonstrate (a) and (b) by two examples in which $\underline{\underline{M}}^{-1}$ is employed once for each example. The resulting specific case of U(x) can then be used as a continuous numerical integrator directly and singly in the conventional way on overlapping sub-intervals. A better approach is to derive Multiple FDMs from the evaluation of U(x and the first derivative function Z(x) at specified points.

3. Two Specified Method

3.1 A New Multiple FDMS Based on the Numerov Method

We consider the following parameter specifications:

$P_i(x) = X^i, i = 0,1,2,3,4;$
k = 2,t = 2, m = 3; $\{x_{n,}\ x_{n+1}\}$ as the interpolation points; $\{x_n,\ x_{n+2}\}$ as the collocation points;

$\underline{V} = (y_n, y_{n+1}, f_{n+1}, f_{n+2})^T$;

$$\underline{\underline{M}} = \begin{bmatrix} 1 & x_n & x_n^2 & x_n^3 & x_n^4 \\ 1 & x_{n+1} & x_{n+1}^2 & x_{n+1}^3 & x_{n+1}^4 \\ 0 & 0 & 2 & 6x_n & 12x_n^2 \\ 0 & 0 & 2 & 6x_{n+1} & 12_{n+1}^2 \\ 0 & 0 & 2 & 6x_{n+2} & 12x_{n+1} \end{bmatrix} \tag{3.1}$$

Hence

$$U(x) = \frac{-(x-x_{n+1})}{h} y_n + \frac{(h+(x-x_{n+1}))}{h} y_{n+1} + $$
$$+ \frac{((x-x_{n+1})^4 - 2h(x-x_{n+1})^3 + 3h^3(x-x_{n+1}))}{24h^2} f_n + $$
$$\frac{(-(x-x_{n+1})^4 - 6h^2(x-x_{n+1})^2 + 5h^3(x-x_{n+1}))}{12h^2} f_{n+1} + $$
$$\frac{+((x-x_{n+1})^4 - 12h(x-x_{n+1})^3 - h^3(x-x_{n+1}))}{24h^2} f_{n+2} \tag{3.2}$$

If we also consider the first derivative function derived from the continuous method (3.2), we have

$$\frac{dU}{dx}(x) = Z(x), \frac{dU}{dx}(a) = Z_0 \tag{3.3}$$

The simultaneous application of (3.2) and (3.3) leads to the multiple FDMs of the form

$$y_{n+2} - 2y_{n+1} + y_n = \frac{h^2}{12}\left[f_{n+2} + 10f_{n+1} + f_n\right] \tag{3.4a}$$

$$-y_{n+1} + y_{n+2} + y_n = \frac{h^2}{24}(f_{n+4} - 6f_{n+3} - 16f_{n+2} - 26f_{n+1}f_n) \tag{3.4b}$$

Where n = 0,2, … for both (3.4a) is obtained from the first equation of (3.3) with a continuity equation imposed at $x = x_{n+2}$ of the form:

$$Z(x_{n+2})\Big|_{x, \le x \le x_{n+2}} Z(x_{n+2})\Big|_{x_{n+2} \le x \le x_{n+4}} \tag{3.5}$$

While (3.4a) is obtained from (3.2) evaluated at $x = x_{n+2}$ and the notation of page 3, Where $n = 0, 2, \ldots$ for (3.5).

Following Fatunla (1991), (3.4) has the normalized first characteristic polynomial of the form

$$
\begin{aligned}
P(R) &= \det\left[R\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} -1 & 2 \\ -2 & 3 \end{pmatrix} \right] \\
&= \det\begin{bmatrix} R+1 & -2 \\ 2 & R-3 \end{bmatrix} \\
&= (R-1)^2
\end{aligned}
$$

which satisfies the conditions for (3.4) to be zero-stable.

The analysis of (3.4) yields order P = 4 with an error constant $C_6 = \begin{pmatrix} -1/240 \\ 1/30 \end{pmatrix}$. Hence

(3.4) is consistent being of order $P > 1$. thus it is convergent (see Henrici (1962)) over $[x_{0,} x_2] \cup [x_2, x_4] \cup \ldots . \cup [x_{N-2,} x_N]$. we will now discuss three options to advance the integration process for the IVP after the first sub-interval $[x_{0,} x_2]$.

To start the IVP on the sub-interval $[x_0, x_2]$ we combine (3.4a) when $n = 0$ together with $\frac{dU}{dx}(a) = Z_0$ in (3.3).

That is, explicitly we obtain

$$
\left.
\begin{aligned}
y_2 - 2y_1 + y_0 &= \frac{h^2}{12}\left(f_2 + 10 f_1 + f_0\right) \\
hz_0 + y_0 - y_1 &= \frac{h^2}{24}\left(-f_2 + 6 f_1 + 7 f_0\right)
\end{aligned}
\right\} \qquad (3.6)
$$

where the form (3.6) has order three given by $(4,3)^T$ and an error constant

$\begin{pmatrix} -1/240 = C_6 \\ 1/45 = C_5 \end{pmatrix}$. It is thus convergent and simultaneously provides values for y_1 and y_2

Without looking for any other method to provide y_1. Hence, this is an improvement over the use of (3.4a) singly for the IVP. The first option is to proceed in the conventional approach with the single equation (3.4a) on the sub-intervals $[x_1, x_3],[x_2, x_4],...,$ which do overlap. The second option is to proceed by explicitly obtaining initial conditions at $x_{n+2,n} = 0,2,...,N-2$ using the computed values $U(x_{n+2}) = y_{n+2}$ and $Z(z_{n+2}) = Z_{n+2}$ over sub-intervals $[x_{0,}x_2],[x_{2,}x_4],...,[x_{N-2,}x_N]$, which do not overlap. The third option is to use (3.4) and a single matrix of finite difference equations is obtained which simultaneously provides the values $y_1, y_{2,}..., y_{N-1,}y_N$ over the same sub-intervals as in the second option, which do not overlap. The same matrix can be used directly for the BVP with adjustments for the boundary conditions.

We are going to be addressing this last option in the remaining part of this paper for a uniform and direct treatment of the IVP and the BVP.

In addition to providing the starting value y_1 and FDM solutions over sub-intervals, which do not overlap for the BVP in particular, $U(x)$ when obtained explicitly can provide a dense output and accurate global error estimates (see Onumanyi et al (1999)). This is done after the numerical values for $y_1, y_2,..., y_N$ are calculated and substituted into (2.1) which cause $U(x)$ to belong to $C^1[a,b]$.

3.2 **Improved Fatunla Block Method**

Let us consider the following parameter specifications

$P_i(x) = x^i, i = 0,1,2,3,4,5;\ k = 3, t = 2, m = 4, \{x_n, x_{n+1}\}$ as the interpolation points;

$$\underline{\underline{M}}=\begin{bmatrix} 1 & x_n & x_n^2 & x_n^3 & x_n^4 & x_n^5 \\ 1 & x_{n+1} & x_{n+1}^2 & x_{n+1}^3 & x_{n+1}^4 & x_{n+1}^5 \\ 0 & 0 & 2 & 6x_n & 12x_n^2 & 20x_n^3 \\ 0 & 0 & 2 & 6x_{n+1} & 12x_{n+1}^2 & 20x_{n+1}^3 \\ 0 & 0 & 2 & 6x_{n+1} & 12_{n+2}^2 & 20x_{n+2}^3 \\ 0 & 0 & 2 & 6x_{n+3} & 12x_{n+3}^2 & 20x_{n+3}^3 \end{bmatrix} \tag{3.7}$$

The resulting U(x) is evaluated at $x = x_{n+3}$ and $x = x_{n+2}$ to yield respectively the following three-step method of order four

$$y_{n+3} - 3y_{n+1} + 2y_n = \frac{h^2}{12}\left(f_{n+3} + 12f_{n+2} + 21f_{n+1} + 2f_n\right) \tag{3.8}$$

With $C_6 = 1/80$ like the method (3.4a). The combination of (3.8) and (3.4a) is zero-stable and hence convergent over single step integration with overlapping sub-intervals.

We can improve the Multiple FDM (3.8) and (3.4a) by considering an additional equation arising from the use of (3.5) at $x = x_{n+3}$ given in the form

$$-U_{n+4} + U_{n+3} + U_{n+1} - U_n$$
$$= \frac{h^2}{360}\left[-8f_{n+6} + 39f_{n+5} - 114f_{n+4} - 224f_{n+2} - 291f_{n+1} - 38f_n\right] \qquad (3.)$$

The improved Fatunla Block Method (Multiple FDMs) is then given by a simultaneous application of (3.8), (3.4a) and (3.9) yielding order four Multiple FDMs with an error constant

$$C_6 = \begin{pmatrix} 1/80 \\ -1/240 \\ 3/80 \end{pmatrix}, n = 0,3,6,...,N-3,N,$$

On the sub-intervals $[x_0, x_3],[x_3, x_6],...,[x_{N-3}, x_N]$.

For n = 0, to start the IVP, we use

$$hZ_0 = -U_0 + U1 + \frac{h^2}{360}\left[-97f_0 - 114f_1 + 39f_2 - 8f_3\right], C_6 = -7/480 \qquad (3.10)$$

The rest of the details follow section (3.1) similarly. The two specific multiple FDMs which have been presented are compared on the following numerical example to illustrate the new approach.

A Numerical Example

$y'' = -y, 0 \le x \le 1.2, \quad = Cosx + Sinx$ is the exact solution,

$I.V.$ $\mathrm{y}(0) = 1, \quad \mathrm{y}'(0) = 1$

$B.V.$ y(0) =1, y(1.2) = Cos(1.2) + Sin(1.2)

Table 1 Comparison of the Theoretical/Approximate Solutions

X	Theoretical solution y(x)	Initial Value Problem		Boundary Value Problem	
		Numerov Block approx. solution y(x)	Improved Fatunla's Block Approx. Soln. y(x)	Numerov Block Approx. Soln. y(x)	Improved Fatunla's Block Approx. Soln. y(x)
0	1.0	1.0	1.0	1.0	1.0
0.1	1.094837582	1.094837379	1.094837566	1.094837464	1.094837678
0.2	1.178735909	1.1787355.01	1.178735872	1.178735671	1.178736095
0.3	1.250856696	1.250856127	1.250856633	1.25085638	1.250856966
0.4	1.310479336	1.310478608	1.310479212	1.310478943	1.310479649
0.5	1.357008101	1.357007268	1.35700791	1.357007679	1.35700845
0.6	1.389978088	1.389977155	1.389977825	1.389977637	1.389978461
0.7	1.409059875	1.409058895	1.409059502	1.409059446	1.4090660225
0.8	1.4140628	1.414061781	1.414062314	1.414062396	1.41406312
0.9	1.404936878	1.404935879	1.404936275	1.404936551	1.404937157
1.0	1.341773291	1.341772316	1.341772537	1.381773009	1.381773484
1.1	1.344803481	1.34480259	1.34480258	1.344803357	1.344803583
1.2	1.29439684	1.294396039	1.294395787	1.29439684*	1.2943964*

Table 2 Comparison of the Absolute Errors of the Two Block Methods With h = 0.1

X	Initial Value Problem		Boundary Value Problem	
	Numerov Block Method	Improved Fatunla Block Method	Numerov Block Method	Improved Fatunla Block Method
0	0	0	0	0
0.1	2.03×10^{-7}	1.60×10^{-8}	1.18×10^{-7}	9.60×10^{-8}
0.2	4.08×10^{-7}	3.70×10^{-8}	2.38×10^{-7}	1.86×10^{-7}
0.3	5.69×10^{-7}	6.30×10^{-8}	3.16×10^{-7}	2.70×10^{-7}
0.4	7.28×10^{-7}	1.24×10^{-7}	3.93×10^{-7}	3.13×10^{-7}
0.5	8.33×10^{-7}	1.90×10^{-7}	4.22×10^{-7}	3.49×10^{-7}
0.6	9.33×10^{-7}	2.63×10^{-7}	4.51×10^{-7}	3.73×10^{-7}
0.7	9.80×10^{-7}	3.73×10^{-7}	4.29×10^{-7}	3.50×10^{-7}
0.8	1.019×10^{-6}	4.86×10^{-7}	4.04×10^{-7}	3.20×10^{-7}
0.9	9.99×10^{-7}	6.03×10^{-7}	3.27×10^{-7}	2.79×10^{-7}
1.0	9.75×10^{-7}	7.54×10^{-7}	2.52×10^{-7}	1.93×10^{-7}
1.1	8.91×10^{-7}	9.01×10^{-7}	1.24×10^{-7}	1.02×10^{-7}
1.2	8.01×10^{-7}	1.053×10^{-6}	0	0

4. **Conclusion**

According to Lambert (1991) linear multistep methods are closely linked with the process of polynomial interpolation and that this link is a revealing one. On the other hand, according to Atkinson (1989) collocation is probably now the most important numerical procedure for obtaining continuous methods for ODEs.

We cannot agree less with both Lambert and Atkinson. This link has been very rewarding through the multistep collocation procedure as has been shown in our earlier works, Onumanyi et al (1994, 1999, 2001), Sirisena et al (2001) and in this paper. The scope of extensions is unlimited as a new direction for the future. For instance, the basis function $\underline{P}(x)$ is arbitrary and with flexibility it can be changed to new ones for special problems, like Stiff ODEs (see Onumanyi et al (2001b) and delay ODEs (see Ruibin Qu (1997)). Moreover P-Stable methods can be similarly treated using the proposed approach of this paper.

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