Quest for Research Excellence On Computing, Mathematics and Statistics

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Faculty of Computer and Mathematical Sciences

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Content

CHAPTER 17
Derivation of Four-Point Explicit Block Methods for Direct Solution of Initial Value Problems of Third Order Ordinary Differential Equations

Z. Omar, J. O. Kuboye, and Y.A. Abdullah

Abstract. Two block methods for solving third order ordinary differential equations directly are presented. These methods are derived using two different approaches; direct integration and collocation. Both methods are capable of approximating the numerical solutions at four points simultaneously. The advantages and drawbacks of each method are also discussed.

Keywords: Explicit Block method, Direct Integration, Collocation, Direct Solution, Initial Value Problems, Ordinary Differential Equations

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1 Introduction

We are interested in solving the following initial value problem of third order ordinary differential equation (ODE) directly

$$y''' = f(x, y, y', y''),\ y(a) = y_0,\ y'(a) = y'_0,\ \ y''(a) = y''_0,\ a \le x \le b. \tag{1}$$

Several methods for solving higher ODEs directly have been proposed by researchers such as Awoyemi and Kayode [1], Gear [2-4], Hall and Suleiman [5], Kayode and Obarhua [6], Odekunle et. al. [7] and Suleiman [8-9]. These methods are capable of solving higher order initial value problems of ODEs without going through the process of reduction. Reducing higher order ODE to its equivalent system of firstorder equations is not only enlarging the system of equations, it may also jeopardize the performance of the methods particularly in term of computational time.

In this paper, two explicit block methods for solving (1) are derived using two different approaches namely direct integration and collocation. The details derivations of both methods are described in the following sections

2 Derivation of Four-Point Explicit Block Method Using Direct Integration

Let $x_{n+j} = x_n + jh$, $j = 1,2,3,4.$ Integrating (1) once, twice and thrice and taking the limit from x_n to x_{n+j} gives

$$y''(x_{n+j}) - y''(x_n) = \int_{x_n}^{x_{n+j}} f(x, y, y')\,dx$$

$$y'(x_{n+j}) - y'(x_n) - jhy''(x_n) = \int_{x_n}^{x_{n+j}} \int_{x_n}^{x} f(x, y, y')\,dx\,dx = \int_{x_n}^{x_{n+j}} (x_{n+j} - x) f\ dx$$

$$y(x_{n+j}) - y(x_n) - jhy'(x_n) - \frac{(jh)^2}{2!} y''(x_t) = \int_{x_n}^{x_{n+j}} \int_{x_n}^{x} \int_{x_n}^{x} f(x, y, y')\,dx\,dx\,dx = \int_{x_n}^{x_{n+j}} \frac{(x_{n+j} - x)^2}{2!} f\ dx \tag{2}$$

Replacing $f(x,y,y')$ with a polynomial $P_{k,n}(x)=\sum_{m=0}^{k-1}(-1)^m\begin{pmatrix}-s\\m\end{pmatrix}\nabla^m f_n$ which interpolates $f(x,y,y')$ at the set of points (x_{n-i},f_{n-i}), $i=0,1,2,...,k-1$ gives the following results

$$y''_{n+j}-y''_n=\int_{x_n}^{x_{n+j}}\sum_{m=0}^{k-1}(-1)^m\begin{pmatrix}-s\\m\end{pmatrix}\nabla^m f_n\,dx.$$

$$y'(x_{n+j})-y'(x_n)-(jh)y''(x_n)=\int_{x_n}^{x_{n+j}}(x_{n+j}-x)\sum_{m=0}^{k-1}(-1)^m\begin{pmatrix}-s\\m\end{pmatrix}\nabla^m f_n\,dx.$$

$$y(x_{n+j})-y(x_n)-(jh)y'(x_n)-\frac{(jh)^2}{2!}y''(x_t)=\int_{x_n}^{x_{n+j}}\frac{(x_{n+j}-x)^2}{2!}\sum_{m=0}^{k-1}(-1)^m\begin{pmatrix}-s\\m\end{pmatrix}\nabla^m f_n\,dx. \quad (3)$$

where $s=\dfrac{x-x_n}{h}$.

Changing the limit integration and substituting $dx=hds$ in (3) yields

$$y''(x_{n+j})-y''(x_n)=\int_0^j\sum_{m=0}^{k-1}(-1)^m\begin{pmatrix}-s\\m\end{pmatrix}\nabla^m f_n\,hds.$$

$$y'(x_{n+j})-y'(x_n)-(jh)y''(x_n)=\int_0^j h(j-s)\sum_{m=0}^{k-1}(-1)^m\begin{pmatrix}-s\\m\end{pmatrix}\nabla^m f_n\,hds.$$

$$y(x_{n+j})-y(x_n)-(jh)y'(x_n)-\frac{(jh)^2}{2!}y''(x_n)=\int_0^j\frac{(h(j-s))^2}{2!}\sum_{m=0}^{k-1}(-1)^m\begin{pmatrix}-s\\m\end{pmatrix}\nabla^m f_n\,hds. \quad (4)$$

which can be written as

$$y''(x_{n+j}) = y''(x_n) + h\sum_{m=0}^{k-1} \alpha_{j,m}^{(1)} \nabla^m f_n$$

$$y'(x_{n+j}) = y'(x_n) + (jh)y''(x_n) + h^2 \sum_{m=0}^{k-1} \alpha_{j,m}^{(2)} \nabla^m f_n$$

$$y(x_{n+j}) = y(x_n) + (jh)y'(x_n))\frac{(jh)^2}{2!} y''(x_n) + h^3 \sum_{m=0}^{k-1} \alpha_{j,m}^{(3)} \nabla^m f_n \tag{5}$$

where

$$\alpha_{j,m}^{(1)} = (-1)^m \int_0^j \binom{-s}{m} ds$$

$$\alpha_{j,m}^{(2)} = (-1)^m \int_0^j (j-s)\binom{-s}{m} ds$$

$$\alpha_{j,m}^{(3)} = (-1)^m \int_0^j \frac{(j-s)^2}{2!}\binom{-s}{m} ds \tag{6}$$

Let's $G_j^{(1)}(t)$, $G_j^{(2)}(t)$ and $G_j^{(3)}(t)$ be the generating functions defined as follows

$$G_j^{(1)}(t) = \sum_{m=0}^{\infty} \alpha_{j,m}^{(1)} t^m = \sum_{m=0}^{\infty} (-t)^m \int_0^j \binom{-s}{m} ds = \int_0^j (1-t)^{-s} ds = \int_0^j e^{-s\log(1-t)} ds$$

$$G_j^{(2)}(t) = \sum_{m=0}^{\infty} \alpha_{j,m}^{(2)} t^m = \sum_{m=0}^{\infty} (-t)^m \int_0^j (j-s)\binom{-s}{m} ds = \int_0^j (j-s)(1-t)^{-s} ds = \int_0^j (j-s)e^{-s\log(1-t)} ds$$

$$G_j^{(3)}(t) = \sum_{m=0}^{\infty} \alpha_{j,m}^{(3)} t^m = \sum_{m=0}^{\infty} (-t)^m \int_0^j \frac{(j-s)^2}{2!}\binom{-s}{m} ds = \int_0^j \frac{(j-s)^2}{2!}(1-t)^{-s} ds = \int_0^j \frac{(j-s)^2}{2!} e^{-s\log(1-t)} ds \tag{7}$$

The constant step size formulations of implicit k-step method corresponding to (5) are

$$\begin{aligned}
y''_{n+j} &= y''_n + h\sum_{m=0}^{k-1}\beta_{k-1,m}^{(j,1)} f_{n-m} \\
y'_{n+j} &= y'_n + (jh)y''_n + h^2\sum_{m=0}^{k-1}\beta_{k,m}^{(j,2)}\nabla^m f_{n-m} \\
y_{n+j} &= y_n + (jh)y'_n + \frac{(jh)^2}{2!}y''_n + h^3\sum_{m=0}^{k-1}\beta_{k,m}^{(j,3)}\nabla^m f_{n-m}
\end{aligned} \qquad (8)$$

respectively. The coefficients $\beta_{k,m}^{(j,p)}, m = 0,1,...k-1$ and $p = 1,2,3$ are well known and defined by Shampine and Gordon (1975) as follows

$$\beta_{k,m}^{(j,p)} = (-1)^m \sum_{r=m}^{k} \binom{r}{m} \alpha_{j,m}^{(p)}$$

The values of $\alpha_{j,m}^{(p)}$ are then substituted in (9) and subsequently in (8) respectively to get a four-point explicit block method. The most crucial part in deriving this method using direct integration approach is, therefore, to determine the values of $\alpha_{j,m}^{(p)}$ which we are going to discuss as follows.

From (7), we have

$$\begin{aligned}
G_j^{(1)}(t) &= \sum_{m=0}^{\infty}\alpha_{j,m}^{(1)}t^m = \int_0^j e^{-s\log(1-t)}ds \\
G_j^{(2)}(t) &= \sum_{m=0}^{\infty}\alpha_{j,m}^{(2)}t^m = \int_0^j (j-s)e^{-s\log(1-t)}ds = \frac{j - G_j^{(1)}(t)}{\log(1-t)} \\
G_j^{(3)}(t) &= \sum_{m=0}^{\infty}\alpha_{j,m}^{(3)}t^m = \int_0^j \frac{(j-s)^2}{2!}e^{-s\log(1-t)}ds = \frac{j^2 - 2!G_j^{(2)}(t)}{2!\log(1-t)}
\end{aligned} \qquad (10)$$

which implies

$$\sum_{m=0}^{\infty}\alpha_{j,m}^{(1)}t^m = \int_0^j e^{-s\log(1-t)}ds$$

$$\sum_{m=0}^{\infty}\alpha_{j,m}^{(2)}t^m = \frac{j-\sum_{m=0}^{\infty}\alpha_{j,m}^{(1)}t^m}{\log(1-t)}$$

$$\sum_{m=0}^{\infty}\alpha_{j,m}^{(3)}t^m = \frac{j^2-2!\sum_{m=0}^{\infty}\alpha_{j,m}^{(2)}t^m}{2!\log(1-t)} \tag{11}$$

From Equation (11) it is observed that the integration coefficients depend very much on $\sum_{m=0}^{\infty}\alpha_{j,m}^{(1)}t^m$. Therefore, we will focus on determining the values of $\sum_{m=0}^{\infty}\alpha_{j,m}^{(1)}t^m$ for j=1,2,3,4. When j=1, we have

$$\sum_{m=0}^{\infty}\alpha_{1,m}^{(1)}t^m = \int_0^1 e^{-s\log(1-t)}ds = \frac{t}{-(1-t)\log(1-t)}$$

which leads to

$$\left(\sum_{m=0}^{\infty}\alpha_{1,m}^{(1)}t^m\right)\left(\frac{-\log(1-t)}{t}\right) = \frac{1}{1-t} \tag{12}$$

Replacing $\left(\frac{-\log(1-t)}{t}\right) = 1+\frac{1}{2}t+\frac{1}{3}t^2+\ldots$ and $\frac{1}{1-t} = 1+t+t^2+\ldots$ in (12), equating coefficients t^m and on simplifying we obtain

$$\alpha_{1,0}^{(1)} = 1$$

$$\alpha_{1,m+1}^{(1)} = 1 - \sum_{r=0}^{m} \frac{\alpha_{1,r}^{(1)} t^m}{m+2-r}$$

$$\alpha_{1,0}^{(p)} = \alpha_{1,1}^{(p-1)}$$

$$\alpha_{1,m+1}^{(p)} = \alpha_{1,m+2}^{(p-1)} - \sum_{r=0}^{m} \frac{\alpha_{1,r}^{(p)}}{m+2-r} \quad \textit{for } p = 2,3, \quad m = 0,1,\ldots,k-1 \tag{13}$$

Repeat the same procedure for *j*=2,3,4, we have

$$\alpha_{j,0}^{(1)} = j$$

$$\alpha_{j,m+1}^{(1)} = \frac{(m+j+1)(m+j)(m+j-1)\ldots(m+3)}{(j-1)!} - \sum_{r=o}^{m} \frac{\alpha_{j,r}^{(1)}}{m+2-r}$$

$$\alpha_{j,0}^{(p)} = \alpha_{j,1}^{(p-1)}$$

$$\alpha_{j,m+1}^{(p)} = \alpha_{j,m+2}^{(p-1)} - \sum_{r=0}^{m} \frac{\alpha_{j,r}^{(p)}}{m+2-r} \quad \textit{for } j = 2,3,4, \; p = 2,3, m = 0,1,\ldots,k-1. \tag{14}$$

Substituting the values of integration coefficients obtained in (13) and (14) into (9), followed by (9) into (8) produces a four-point explicit block method.

3 Derivation of Four-Point Explicit Block Method Using Collocation Approach

Let power series of the form

$$y(x) = \sum_{i=0}^{k+3} a_i x^i \tag{15}$$

be an approximate solution to (1) where the number of points k = 4. Differentiating (15) thrice we have

$$y''' = \sum_{i=3}^{k+3} i(i-1)(i-2) a_i x^{i-3} \tag{16}$$

Equation (15) is interpolated at $x = x_{n+j},\ j = 0,2,3$ and equation (16) is collocated at $x = x_{n+j},\ j = 0(1)3$. As a result, we have

$$\sum_{i=0}^{k+3} a_i x_{n+j}^i = y_{n+j}$$
$$\sum_{i=2}^{k+3} i(i-1)(i-2) a_i x_{n+j}^i = f_{n+j} \tag{17}$$

In order to find the values of *a's* in (17), Gaussian elimination method is employed. These values are then substituted into equation (15) and using transformation $t = \dfrac{x - x_{n+3}}{h}$, a continuous explicit scheme of the following form is obtained

$$y(t) = \alpha_0(t) y_n + \sum_{j=2}^{k-1} \alpha_j(t) y_{n+j} + h^3 \sum_{j=0}^{k-1} \beta_j(t) f_{n+j} \tag{18}$$

where

$$\alpha_0(t) = \frac{t}{6} + \frac{t^2}{6}$$
$$\alpha_2(t) = -\frac{3t}{2} - \frac{t^2}{2}$$
$$\alpha_3(t) = \frac{4t}{3} + \frac{t^2}{3}$$
$$\beta_0(t) = \frac{t}{120} + \frac{11t^2}{720} - \frac{t^4}{72} - \frac{t^5}{120} - \frac{t^6}{720}$$
$$\beta_1(t) = \frac{t}{20} + \frac{t^2}{60} + \frac{t^4}{16} + \frac{t^5}{30} + \frac{t^6}{240}$$
$$\beta_2(t) = \frac{3t}{8} + \frac{37t^2}{80} - \frac{t^4}{8} - \frac{t^5}{24} - \frac{t^6}{240}$$
$$\beta_3(t) = \frac{t}{15} + \frac{31t^2}{180} + \frac{t^3}{6} + \frac{11\,t^4}{144} + \frac{t^5}{60} + \frac{t^6}{720} \tag{19}$$

The first derivative of (19) yields

$$\alpha_0'(t) = \frac{1}{6} + \frac{t}{3}$$
$$\alpha_2'(t) = -\frac{3}{2} - t$$
$$\alpha_3'(t) = \frac{4}{3} + \frac{2}{3}t$$
$$\beta_0'(t) = \frac{1}{120} + \frac{11t}{360} - \frac{t^3}{18} - \frac{t^4}{24} - \frac{t^5}{120}$$
$$\beta_1'(t) = \frac{1}{20} + \frac{t}{30} + \frac{t^3}{4} + \frac{t^4}{6} + \frac{t^5}{40}$$
$$\beta_2'(t) = \frac{3}{8} + \frac{37}{40}t - \frac{t^3}{2} - \frac{5t^4}{24} - \frac{t^5}{40}$$
$$\beta_3'(t) = \frac{1}{15} + \frac{31}{90}t + \frac{t^2}{2} + \frac{11t^3}{36} + \frac{t^4}{12} + \frac{t^5}{120} \tag{20}$$

and the second derivative of (19) produces

$$\alpha_0''(t) = \frac{1}{3}$$
$$\alpha_2''(t) = -1$$
$$\alpha_3''(t) = \frac{2}{3}$$
$$\beta_0''(t) = \frac{11}{360} - \frac{t^2}{6} - \frac{t^3}{6} - \frac{t^4}{24}$$
$$\beta_1''(t) = \frac{1}{30} + \frac{3t^2}{4} + \frac{2t^3}{3} + \frac{t^4}{8}$$
$$\beta_2''(t) = \frac{37}{40} - \frac{3}{2}t^2 - \frac{5}{6}t^3 - \frac{t^4}{8}$$
$$\beta_3''(t) = \frac{31}{90} + t + \frac{11}{12}t^2 + \frac{t^3}{3} + \frac{t^4}{24} \tag{21}$$

Evaluating (19) at non-interpolating points i.e. at t = -2, 1 and evaluating (20) and (21) at all the grid points. i.e. t =-3, -2, -1, 0, and 1 produces the discrete schemes and its derivatives which are combined in a matrix form as follows

$$\begin{pmatrix} 1 & -1 & \frac{1}{3} & 0 \\ 0 & 2 & -\frac{8}{3} & 1 \\ 0 & -\frac{3}{2} & \frac{2}{3} & 0 \\ 0 & 1 & -\frac{2}{3} & 0 \end{pmatrix} \begin{pmatrix} y_{n+1} \\ y_{n+2} \\ y_{n+3} \\ y_{n+4} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & \frac{1}{3} \\ 0 & 0 & 0 & \frac{1}{3} \\ 0 & 0 & 0 & -\frac{5}{6} \\ 0 & 0 & 0 & \frac{1}{3} \end{pmatrix} \begin{pmatrix} y_{n-3} \\ y_{n-2} \\ y_{n-1} \\ y_n \end{pmatrix} + h \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} y'_{n-3} \\ y'_{n-2} \\ y'_{n-1} \\ y'_n \end{pmatrix}$$

$$+ h^2 \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} y''_{n-3} \\ y''_{n-2} \\ y''_{n-1} \\ y''_n \end{pmatrix} + h^3 \begin{pmatrix} 0 & \frac{1}{6} & 0 & 0 \\ \frac{1}{6} & \frac{2}{3} & \frac{1}{2} & 0 \\ \frac{75}{120} & \frac{36}{120} & \frac{1}{120} & 0 \\ \frac{393}{360} & \frac{72}{360} & \frac{11}{360} & 0 \end{pmatrix} \begin{pmatrix} f_{n+1} \\ f_{n+2} \\ f_{n+3} \\ f_{n+4} \end{pmatrix} + h^3 \begin{pmatrix} 0 & 0 & 0 & \frac{1}{6} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{8}{120} \\ 0 & 0 & 0 & \frac{124}{360} \end{pmatrix} \begin{pmatrix} f_{n-3} \\ f_{n-2} \\ f_{n-1} \\ f_n \end{pmatrix}$$

Therefore, multiplying both y and f function by the inverse of the coefficients of $y_{n+i}, i = 0(1)4.$ This gives the explicit block method below

$$\begin{aligned}
y_{n+1} &= y_n + hy'_n + \frac{1}{2}h^2 y''_n + h^3 (\frac{19}{180} f_n + \frac{7}{80} f_{n+1} - \frac{1}{30} f_{n+2} + \frac{1}{144} f_{n+3}). \\
y_{n+2} &= y_n + 2hy'_n + 2h^2 y''_n + h^3 (\frac{5}{9} f_n + \frac{14}{15} f_{n+1} - \frac{1}{5} f_{n+2} + \frac{2}{45} f_{n+3}). \\
y_{n+3} &= y_n + 3hy'_n + \frac{9}{2}h^2 y''_n + h^3 (\frac{27}{20} f_n + \frac{243}{80} f_{n+1} + \frac{9}{80} f_{n+3}). \\
y_{n+4} &= y_n + 4hy'_n + 8h^2 y''_n + h^3 (\frac{112}{45} f_n + \frac{32}{5} f_{n+1} + \frac{16}{15} f_{n+2} + \frac{32}{45} f_{n+3})
\end{aligned} \tag{22}$$

The corresponding first derivatives of (22) are

$$\begin{aligned}
y'_{n+1} &= y'_n + hy'_n + h^2 (\frac{97}{360} f_n + \frac{37}{60} f_{n+1} - \frac{11}{120} f_{n+2} + \frac{1}{45} f_{n+3}). \\
y'_{n+2} &= y'_n + 2hy'_n + h^2 (\frac{28}{45} f_n + \frac{22}{15} f_{n+1} - \frac{2}{15} f_{n+2} + \frac{2}{45} f_{n+3}). \\
y'_{n+3} &= y'_n + 3hy'_n + h^2 (\frac{39}{40} f_n + \frac{27}{10} f_{n+1} + \frac{27}{40} f_{n+2} + \frac{3}{20} f_{n+3}).
\end{aligned}$$

$$y'_{n+4} = y'_n + 4hy'_n + h^2(\frac{56}{45} f_n + \frac{64}{15} f_{n+1} + \frac{16}{15} f_{n+2} + \frac{64}{45} f_{n+3}).$$

while the corresponding second derivatives of (22) are

$$y''_{n+1} = y''_n + h(\frac{3}{8} f_n + \frac{19}{24} f_{n+1} - \frac{5}{24} f_{n+2} + \frac{1}{24} f_{n+3}).$$
$$y''_{n+2} = y''_n + h(\frac{1}{3} f_n + \frac{4}{3} f_{n+1} + \frac{1}{3} f_{n+2}).$$
$$y''_{n+3} = y''_n + h(\frac{3}{8} f_n + \frac{9}{8} f_{n+1} + \frac{9}{8} f_{n+2} + \frac{3}{8} f_{n+3}).$$
$$y''_{n+4} = y''_n + h(0 f_n + \frac{8}{3} f_{n+1} - \frac{4}{3} f_{n+2} + \frac{8}{3} f_{n+3}).$$

4 Discussion and Conclusion

Two numerical methods for the solution of general second order initial value problems using direct integration and collocation approaches have been proposed in this paper. Both methods have their strengths and weaknesses. In terms of simplicity, the derivation of block method using collocation method seems simpler than its counterpart. But this approach fails to generalize the formulation of unknowns *a's* to any point since the order of differential equation that determines the number of interpolation points. In addition, the order of the approximated power series is also determined by the number of interpolation and collocation points. Although the derivation using direct integration method is more complicated, this approach is able to generalize the formulation of the integration coefficients for any back values used at any point.

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