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3 Point Block Backward Differentiation with Multiple Off-step Points for the Solution of Stiff Problems

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Abstract

In this study, a three-point block backward differentiation formula (3PBBDF) method is derived for solving first-order stiff initial value problems (IVPs) of ordinary differential equations (ODEs). The newly proposed method is analyzed for its key properties and is found to be A-stable, zero-stable, and effective in handling stiff IVPs. To evaluate the performance of the 3PBBDF method, several stiff IVPs are solved, and the results are compared against existing numerical schemes. The comparison, based on tabulated results and plotted graphs, demonstrates that the proposed method offers superior accuracy in terms of error scaling over three competing methods and also outperforms two methods in terms of execution time. Consequently, the proposed 3PBBDF scheme proves to be an efficient tool for integrating stiff IVPs in ODEs.

Keywords: Backward differentiation formula, block multiple off-step point, linear multistep methods, stiff ordinary differential equations

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Introduction

The Backward Differentiation Formula (BDF) is a widely used numerical method for solving ordinary differential equations (ODEs). It belongs to the class of linear multistep methods, which estimate a function's derivative at a given point based on its values at previous points. The BDF method is particularly effective for solving stiff ODEs, which are common in fields such as chemical kinetics, fluid dynamics, and structural mechanics.

The general expression for a backward differentiation formula (BDF) can be formulated as

$$y = \sum_{j=0}^{k-1} \alpha_k y_{n+j} + h\beta_k f_{n+k} \qquad (1)$$

Where h and k represent the step size and step number, respectively, α, β define specific multistep used to approximate the derivative, while n is the current step index. The selection of coefficients is done in a manner that ensures the method attains order k, which is the highest achievable.

Implicit in nature, backward differentiation formula methods necessitate the resolution of nonlinear equations at every step. Typically, a modified form of Newton's method is applied for the solution of these nonlinear equations. The stability of numerical techniques in handling stiff equations is denoted by their domain of absolute stability. The stability characteristic of BDF methods diminishes as the step number rises. To address stiff systems, BDF methods must consider factors such as step size, stability, accuracy, and computational cost. A new fixed-coefficient diagonally implicit block backward differentiation formula was proposed to solve stiff initial value problems [1].

A diagonally implicit extended 2-point super-class of block backward differentiation formula with two off-step points was developed for solving first-order stiff initial value problems [2].

Recent innovations include the development of a 3-point variable step block hybrid method (3-point VSBHM) using Lagrange polynomials and an increment of step sizes [3]. Another innovation aimed at improving the numerical resolution of stiff ODEs was proposed which established a special class of multiderivative multistep methods with two free parameters [4]. Husin *et al.* presented accuracy improvement of block backward differentiation formulas for solving stiff ordinary differential equations using modified versions of Euler's method [5].

In this work, we wish to derivea three-point block backward differentiation formula (3PBBDF) and apply it to solve first-order stiff initial value problems (IVPs) of ordinary differential equations (ODEs). Furthermore, we shall carry out convergence analysis and compare the results obtained with other existing methods.

Materials and Methods

A stiff equation is a differential equation that exhibits unstable behavior when solved numerically using certain methods, unless the step size is extremely small. This is due to rapid variations in the solution caused by certain terms, which demand the use of very small-time steps to maintain stability when using explicit methods. As a result, stiff equations can lead to slow and inefficient computations, making it important to choose

appropriate numerical methods and step sizes to achieve accurate and efficient solutions.
A general form of a stiff ordinary differential equation (ODE) can be expressed as:

$$y'(t) = f(t, y(t)), \qquad y(0) = y_0$$

where $f(t, y(t))$contains terms that exhibit fast decay or rapid changes, making the system stiff. A classic stiff equation is characterized by the presence of a small parameter that forces some solution components to vary quickly, while others evolve more slowly.

Stiff equations are common in scientific and engineering applications, such as chemical kinetics, control systems, and fluid dynamics, where processes with vastly different timescales are modeled [6]. To tackle these challenges, researchers have developed methods specifically designed for stiff ordinary differential equations (ODEs). Additionally, a variable step-size multi-block backward differentiation formula approach has been developed to improve numerical solutions for stiff problems by dynamically adjusting the step size to accommodate rapid changes in the solution [7]. These advancements enhance the stability and efficiency of solving stiff ODEs, making them more applicable in complex scientific and engineering systems.

Derivation through multistep collocation method

The approach proposed by Soomro *et al.* [8] shall be used in this derivation where a k-step multistep collocation method with t interpolation points and m collocation points was obtained as:

$$y(x) = \sum_{j=0}^{t-1} \alpha_j(x) y_{n+j} + h \sum_{j=0}^{m-1} \beta_j(x) f[x_j, y(x_j)],$$

$$x_n \le x \le x_{n+k} \qquad (2)$$

The continuous coefficients $\alpha_j(x)$ and $\beta_j(x)$ are defined as:

$$\alpha_j(x) = \sum_{i=0}^{t+m-1} \alpha_{j,i+1} x^i, \text{J} \in \{0,1,\dots,t-1\} \qquad (3)$$

$$\beta_j(x) = \sum_{i=0}^{t+m-1} h\beta_{j,i+1} x^i, \text{j} \in \{0,1,\dots,t-1\} \qquad (4)$$

To get $\alpha_j(x)$ and $\beta_j(x)$, [8] arrived at a matrix equation of the form:

$$DC = I \qquad (5)$$

Where I is the identity matrix of dimension $(t+m) \times (t+m)$ while D and C are matrices defined as:

$$D = \begin{pmatrix} 1 & x_n & x_n^2 & \dots & x_n^{t+m-1} \\ 1 & x_{n+1} & x_{n+1}^2 & \dots & x_{n+1}^{t+m-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n+t-1} & x_{n+t-1}^2 & \dots & x_{n+t-1}^{t+m-1} \\ 0 & 1 & 2x_0 & \dots & (t+m-1)x_0^{t+m-2} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 1 & 2x_{m-1} & \dots & (t+m-1)x_{m-1}^{t+m-2} \end{pmatrix} \qquad (6)$$

$$C = \begin{pmatrix} \alpha_{0,1} & \alpha_{1,1} & \dots & \alpha_{t-1,1} & h\beta_{0,1} & \dots & h\beta_{m-1,2} \\ \alpha_{0,2} & \alpha_{1,2} & \dots & \alpha_{t-1,2} & h\beta_{0,2} & \dots & h\beta_{m-1,2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \alpha_{0,t+m} & \alpha_{1,t+m} & \dots & \alpha_{t-1,t+m} & h\beta_{0,t+m} & \dots & h\beta_{m-1,t+m} \end{pmatrix} \qquad (7)$$

From (5) it follows that C=D^{-1}, where the columns of C give the continuous coefficients of the continuous scheme (2).

Derivation of the Continuous Formulation of Backward Differentiation Formula for Step Number $k = 3$ Incorporating two Off-Grid Collocation Point

In this case, the number of interpolation points, $t = 5$ and the number of collocation points, $m = 1$, then:

$$y(x) = \alpha_0(x)y_n + \alpha_1(x)y_{n+1} + \alpha_{\frac{1}{2}}(x)y_{n+\frac{1}{2}} + \alpha_{\frac{3}{2}}(x)y_{n+\frac{3}{2}} + \alpha_2(x)y_{n+2} + h\beta_3(x)f_{n+3} \qquad (8)$$

Thus, the matrix D become:

$$D = \begin{pmatrix} 1 & x_n & x_n^2 & x_n^3 & x_n^4 & x_n^5 \\ 1 & x_n + \frac{1}{2}h & (x_n + \frac{1}{2}h)^2 & (x_n + \frac{1}{2}h)^3 & (x_n + \frac{1}{2}h)^4 & (x_n + \frac{1}{2}h)^5 \\ 1 & x_n + h & (x_n + h)^2 & (x_n + h)^3 & (x_n + h)^4 & (x_n + h)^5 \\ 1 & x_n + \frac{3}{2}h & (x_n + \frac{3}{2}h)^2 & (x_n + \frac{3}{2}h)^3 & (x_n + \frac{3}{2}h)^4 & (x_n + \frac{3}{2}h)^5 \\ 1 & x_n + 2h & (x_n + 2h)^2 & (x_n + 2h)^3 & (x_n + 2h)^4 & (x_n + 2h)^5 \\ 0 & 1 & 2x_n + 6h & 3(x_n + 3h)^2 & 4(x_n + 3h)^3 & 5(x_n + 3h)^4 \end{pmatrix} \qquad (9)$$

Using maple 18, the inverse matrix $C = D^{-1}$is obtained gives the continuous scheme

$$y_{n+1} = \frac{1}{108}hf_{n+3} - \frac{29}{12}f_{n+1}h + \frac{328}{81}y_{n+\frac{3}{2}} - \frac{8}{3}y_{n+\frac{1}{2}} - \frac{2}{3}y_{n+2} + \frac{23}{81}y_n:$$

$$y_{n+\frac{1}{2}} = -\frac{87}{175}f_{n+\frac{1}{2}}h - \frac{1}{350}hf_{n+3} - \frac{79}{105}y_{n+\frac{3}{2}} + \frac{23}{140}y_{n+2} + \frac{9}{5}y_{n+1} - \frac{89}{420}y_n:$$

$$y_{n+\frac{3}{2}} = \frac{261}{301}f_{n+\frac{3}{2}}h + \frac{3}{602}hf_{n+3} - \frac{171}{301}y_{n+\frac{1}{2}} - \frac{99}{172}y_{n+2} + \frac{621}{301}y_{n+1} + \frac{97}{1204}y_n \qquad (10)$$

$$y_{n+2} = -\frac{4}{611}hf_{n+3} + \frac{174}{611}f_{n+2}h + \frac{3104}{1833}y_{n+\frac{3}{2}} + \frac{224}{611}y_{n+\frac{1}{2}} - \frac{612}{611}y_{n+1} - \frac{107}{1833}y_n:$$

$$y_{n+3} = \frac{50}{87}y_n - \frac{96}{29}y_{n+\frac{1}{2}} + \frac{225}{29}y_{n+1} - \frac{800}{87}y_{n+\frac{3}{2}} + \frac{150}{29}y_{n+2} + \frac{10}{29}hf_{n+3}:$$

Convergence analysis

Here, the examinations of order, error constant, consistency, zero stability and region of the absolute stability of (10) are presented.

Order and error constant

A linear multistep method is said to be of order p if

$c_0 = c_1 = c_2 = \dots c_p = 0$, But $c_{p+1} \neq 0$ and c_{p+1} is called the error constant, where,

$$c_0 = \alpha_0 + \alpha_1 + \alpha_2 + \dots + \alpha_k$$

$$c_1 = (\alpha_1 + 2\alpha_2 + 3\alpha_3 + \dots + k\alpha_k) - (\beta_0 + \beta_1 + \beta_2 + \dots + \beta_k)$$

$$\vdots$$

$$c_q = \frac{1}{q!}(\alpha_1 + 2^q\alpha_2 + \dots k^q\alpha_k) - \frac{1}{(q-1)!}(\beta_0 + 2^{q-1}\beta_2 + \dots + k^{q-1}\beta_k)$$

$q = 2, 3, 4, 5 \dots$

The order and error constants of the discrete schemes in (10) are obtained as follows:

$$C_0 = \alpha_0 + \alpha_1 + \alpha_{\frac{1}{2}} + \alpha_{\frac{3}{2}} + \alpha_2 + \alpha_3 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$C_1 = \alpha_1 + \tfrac{1}{2}\alpha_{\frac{1}{2}} + \tfrac{3}{2}\alpha_{\frac{3}{2}} + 2\alpha_2 + 3\alpha_3 + \beta_0 - \beta_1 - \beta_{\frac{1}{2}} - \beta_{\frac{3}{2}} - \beta_2 - \beta_3 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$C_2 = \tfrac{1}{2}\alpha_1 + \tfrac{1}{8}\alpha_{\frac{1}{2}} + \tfrac{9}{8}\alpha_{\frac{3}{2}} + 2\alpha_2 + \tfrac{9}{2}\alpha_3 - \beta_1 - \tfrac{1}{2}\beta_{\frac{1}{2}} - \tfrac{3}{2}\beta_{\frac{3}{2}} - 2\beta_2 - 3\beta_3 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$C_3 = \tfrac{1}{6}\alpha_1 + \tfrac{1}{48}\alpha_{\frac{1}{2}} + \tfrac{9}{16}\alpha_{\frac{3}{2}} + \tfrac{4}{3}\alpha_2 + \tfrac{9}{2}\alpha_3 - \tfrac{1}{2}\beta_1 - \tfrac{1}{8}\beta_{\frac{1}{2}} - \tfrac{9}{8}\beta_{\frac{3}{2}} - 2\beta_2 - \tfrac{9}{2}\beta_3 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$C_4 = \tfrac{1}{24}\alpha_1 + \tfrac{1}{384}\alpha_{\frac{1}{2}} + \tfrac{27}{128}\alpha_{\frac{3}{2}} + \tfrac{2}{3}\alpha_2 + \tfrac{27}{8}\alpha_3 - \tfrac{1}{6}\beta_1 - \tfrac{1}{48}\beta_{\frac{1}{2}} - \tfrac{9}{16}\beta_{\frac{3}{2}} - \tfrac{4}{3}\beta_2 - \tfrac{9}{2}\beta_3 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$C_5 = \tfrac{1}{120}\alpha_1 + \tfrac{1}{3840}\alpha_{\frac{1}{2}} + \tfrac{81}{1280}\alpha_{\frac{3}{2}} + \tfrac{4}{15}\alpha_2 + \tfrac{81}{40}\alpha_3 - \tfrac{1}{24}\beta_1 - \tfrac{1}{384}\beta_{\frac{1}{2}} - \tfrac{27}{128}\beta_{\frac{3}{2}} - \tfrac{2}{3}\beta_2 - \tfrac{27}{8}\beta_3 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$C_6 = \tfrac{1}{720}\alpha_1 + \tfrac{1}{46080}\alpha_{\frac{1}{2}} + \tfrac{81}{5120}\alpha_{\frac{3}{2}} + \tfrac{4}{45}\alpha_2 + \tfrac{81}{80}\alpha_3 - \tfrac{1}{120}\beta_1 - \tfrac{1}{3840}\beta_{\frac{1}{2}} - \tfrac{81}{1280}\beta_{\frac{3}{2}} - \tfrac{4}{15}\beta_2 - \tfrac{81}{40}\beta_3 = \begin{bmatrix} -\frac{17}{8640} \\ \frac{33}{44800} \\ -\frac{321}{385280} \\ \frac{3}{3760} \\ -\frac{5}{454} \end{bmatrix}$$

Therefore, the developed method is of order 5, with error constant

$C_6 = -\frac{17}{8640}, \ \frac{33}{44800}, \ -\frac{321}{385280}, \ \frac{3}{3760}$, and $-\frac{5}{454}$

Zero stability

A linear multistep method is said to be zero stable if all the roots of first characteristics polynomial have modulus less than or equal to unity and those roots with modulus unity are simple.

Therefore, the zero stability of the discrete schemes in (10) will be obtained as follows:

$$A = \begin{bmatrix} 1+\frac{29}{12}z & \frac{8}{3} & -\frac{328}{81} & \frac{2}{3} & -\frac{1}{108}z \\ -\frac{9}{5} & 1+\frac{87}{175}z & \frac{79}{105} & -\frac{23}{140} & \frac{1}{350}z \\ -\frac{621}{301} & \frac{171}{301} & 1-\frac{261}{301}z & \frac{99}{172} & -\frac{3}{602}z \\ \frac{612}{611} & -\frac{224}{611} & \frac{3104}{1833} & 1-\frac{174}{611}z & \frac{4}{611}z \\ -\frac{225}{29} & \frac{96}{29} & \frac{800}{87} & -\frac{150}{29} & 1-\frac{10}{29}z \end{bmatrix}$$

$$B = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{23}{81} \\ 0 & 0 & 0 & 0 & -\frac{89}{420} \\ 0 & 0 & 0 & 0 & \frac{97}{1204} \\ 0 & 0 & 0 & 0 & -\frac{107}{1833} \\ 0 & 0 & 0 & 0 & \frac{50}{87} \end{bmatrix}$$

$Ar - B$

$$\begin{bmatrix} r(1+\frac{29}{12}z) & \frac{8}{3}r & -\frac{328}{81}r & \frac{2}{3}r & -\frac{1}{108}zr-\frac{23}{81} \\ -\frac{9}{5}r & r(1+\frac{87}{175}z) & \frac{79}{105}r & -\frac{23}{140}r & \frac{1}{350}zr+\frac{89}{420} \\ -\frac{621}{301}r & \frac{171}{301}r & r(1-\frac{261}{301}z) & \frac{99}{172}r & -\frac{3}{602}zr-\frac{97}{1204} \\ \frac{612}{611}r & -\frac{224}{611}r & -\frac{3104}{1833}r & r(1-\frac{174}{611}z) & \frac{4}{611}zr+\frac{107}{1833} \\ -\frac{225}{29}r & \frac{96}{29}r & \frac{800}{87}r & -\frac{150}{29}r & r\left(1-\frac{10}{29}z\right)-\frac{50}{87} \end{bmatrix}$$

Taking the determinant of the above matrix, differentiate the determinant with respect to z and solving for r, we obtained

$$\left[[r=0],[r=0],[r=0],[r=0],\left[r=-\frac{20z^3+77z^3+142z+112}{15z^4-54z^3+130z^2-190z+128}\right]\right]$$

Evaluating r at z=0, we obtained

$[[r=0],\ [r=0],\ [r=0],\ [r=0],\ [r=\frac{7}{8}]]$

Therefore, the method is zero stable.

Region of Absolute Stability

The region of absolute stability for all the discrete schemes is all the points on the complex plane excluding the points inside the enclosed region (Fig. 1).

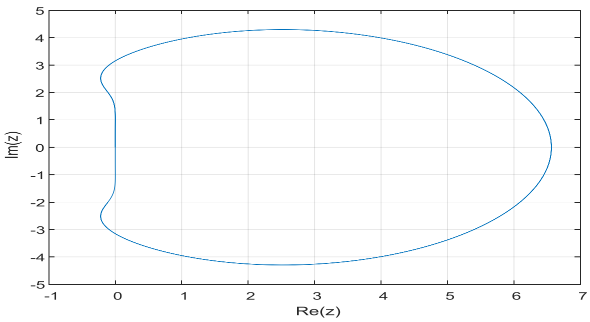

Figure 1: Region of absolute stability of the proposed 3PBBDF method given in (10)

Results and Discussion

To test the reliability of the proposed 3POBBDF method, some numerical results are obtained by applying the method on some well-known chemical reaction problems. Comparison is done with other multistep methods.

Example 1 (stiff chemical reaction problem)

A chemistry problem with a stiff system is considered below,

$$y'_1 = -0.013y_2 - 1000y_1y_2 - 2500y_1y_3$$
$$y'_2 = -0.013y_2 - 1000y_1y_2$$
$$y'_3 = -2500y_1y_3$$

With initial value $y_1 = 0, y_2 = 1$ and $y_3 = 1,\ 0 \le x \le 2$.

This problem is solved using $h = 10^{-5}$ for 3POBBDF. Table 1 shows the integration results of this problem at $x = 2$ in comparison with other methods [8–10].

Table 1: Numerical solution of Problem 1

y_i	Exact solution	Error in 3POBBDF	Error in [8]	Error in [9]	Error in [10]
y_1	0.000003616933169289	1.6990E-17	1.1E-17	0.61E-16	0.82E-10
y_2	0.9815029948230	3.8059E-12	2.2E-11	0.53E-10	0.61E-05
y_3	1.0184933882440	-2.958E-12	4.39E-11	0.74E-10	0.57E-05

Example 2 (Chemical Akzo Noble Problem)
The chemical Akzo noble problem is a chemical process given by a stiff system with six non-linear differential equations. Mathematically the problem is described as,

$$\frac{dy}{dx} = F(y), \quad y(0) = y_0, \qquad y \in R^6, \qquad 0 \le x \le 180.$$

The function $F(y)$ is defined by

$$\frac{dy}{dx} = \begin{bmatrix} -2r_1 + r_2 - r_3 - r_4 \\ \frac{1}{2}r_1 - r_4 - \frac{1}{2}r_5 + F_{in} \\ r_1 - r_2 + r_3 \\ -r_2 + r_3 - 2r_4 \\ -r_2 - r_3 + r_5 \\ -r_5 \end{bmatrix}$$

Where r_i and F_{in} are auxiliary variables given by

$$r_1 = k_1 y_1^4 y_2^{\frac{1}{2}}, \qquad k_1 = 18.7, \qquad r_2 = k_2 y_3 y_4,$$
$$k_2 = 0.58, \qquad r_3 = \frac{k_2}{k} y_3 y_5,$$
$$k = 34.4, \qquad r_4 = k_3 y_1 y_4^2,$$
$$k_3 = 0.09, \qquad r_5 = k_4 y_6^2 y_2^{\frac{1}{2}},$$
$$k_4 = 0.42$$
$$F_{in} = {}^{k}/_{A}\left(\frac{p(O_2)}{H} - y_2\right) {}^{k}/_{A} = 3.3p(O_2) = 0.9H = 737.$$

The initial vector $y_0 = (0.437, \ 0.00123, \ 0, \ 0, \ 0,$ *0.367)T.*
The numerical results by proposed method at the end point (x_{end} =180) are shown in Table 2

Table 2: Numerical solution of Problem 2

y_i	Error in 3POBBDF	Error in [8]	Error in [9]
y_1	1.936737E-12	6.92288E-6	1.16162E-1
y_2	1.936735E-12	1.16287E-8	1.11941E-3
y_3	1.936734E-12	3.55564E-6	1.62125E-1
y_4	-1.722661E-9	1.97555E-7	3.39591E-3
y_5	-1.722660E-9	1.71447E-5	1.64618E-1
y_6	-1.722660E-9	2.12229E-6	1.98954E-1

Example 3 (stiff chemical reaction problem)
Consider the stiff system IVPs.

$$y'_1 = -1002y_1 + 1000y_2^2$$
$$y'_2 = y_1 - y_2(1 + y_2)$$

With the initial value as $y_1(0) = 1$and $y_2(0) = 1$ having exact solutions as,

$$y_1 = \exp(-2x)$$
$$y_2 = \exp(-x)$$

This problem is solved at $x = 50$, by new method and compared the results with fourth order two step hybrid method with one off-step point. Here the stepsize $h = 0.05$ is used for compared and proposed methods. Table 3 shows the numerical results.

Table 3: Numerical solution of Problem 3

y_i	Error in 3POBBDF	Error in [8]	Error in [9]
y_1	4.1397092E-45	7.38E-24	7.14E-21
y_2	6.4422159E-23	4.83E-25	3.34E-19

Conclusion

In this work, an implicit 3 Point block backward differentiation formula (3PBBDF) was derived for the numerical solution of stiff systems of first order IVP arising from chemical reactions such as Chemical AKZO and Stiff Chemical Problems. The approach is based on the block backward differentiation formula (BBDF), in which at each step of the integration, four approximation are generated simultaneously. Based on the stability analysis of the method, it is consistent and zero-stable, thus is convergent. Since it has an A-stability properties, the method is declared suitable for solving stiff Ordinary differential equations (ODEs).
The numerical results obtained through the 3PBBDF and compared to the methods by Soomro *et al.* [8], Khalsaraei *et al.* [9], Ismail and Ibrahim [10], the accuracy of the numerical solutions in terms of absolute error at specific points is improved. Hence the proposed method can be successfully applied on stiff systems generated from chemical reactions because of their high order, accuracy and wider stability region. Therefore, the 3PBBDF can be considered a suitable solver for ordinary differential equations. Future research could improve efficiency by implementing variable step sizes for solving ODEs.

Conflict of interest: Authors have declared that there is no conflict of interest whatsoever.

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