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SIMULATION OF STIFF ORDINARY DIFFERENTIAL EQUATIONS VIA A SIMPSON THIRD-DERIVATIVE HYBRID-BLOCK INTEGRATOR

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ABSTRACT: *In this study, a Simpson's third derivative method is presented in hybrid-block form for the numerical simulation of stiff systems of ordinary differential equations. A multistep collocation approach has been adopted for the design of the new method. The new hybrid-block method is of order nine and has been examined to be consistent, zero-stable, convergent, and $A(\alpha)$-stable. These findings are supported by numerical tests on stiff problems. The results of this study are compared with exact solutions and other existing methods.*

KEYWORDS: Stiff Ordinary Differential Equations, Simpson's Third Derivative Method, Hybrid-Block Method, Stability properties.

INTRODUCTION

The linear system,

$$y' = Ay + \omega(x) \qquad (1)$$

where A is an $n \times n$ matrix and $\omega(x)$ is an n- dimensional vector, is called stiff if:

i) $Re\lambda_i < 0,\ i = 1,2,\ldots,n$ and,

ii) $\dfrac{\max\limits_{i=1,2,\ldots,n} |Re\lambda_i|}{\min\limits_{i=1,2,\ldots,n} |Re\lambda_i|} \gg 0$

Where λ_i $(i = 1,2,\ldots,n)$ are eigenvalues of A (Aware et al., 2020).

As a result of the rapid changes associated with certain elements of the system in (1), explicit numerical methods rely on a very small step size to be stable. Stiff ODEs always arise in pharmacokinetics models, engineering, chemical reactions, quantum mechanics, circuit theory, and control systems (Anongo et al., 2022; Adoghe et al., 2022).

Numerical techniques have been presented for numerical simulation of the initial value problems (IVPs) of stiff systems in (1), via hybrid-block methods. Most of the methods for solving (1) are of low orders and are not A-stable; therefore, they are not suitable for such differential equations (Yakubu, 2016).

LITERATURE/THEORETICAL UNDERPINNING

This study introduces a third-derivative method with an off-step point designed for the numerical simulation of initial value problems of stiff systems. Several authors have presented methods with derivative functions, such as Anongo (2022), Adoghe (2022), Akali (2023), andOlusheye (2018). According to Akali (2023), hybrid methods share the property of utilizing data at off-step points and the flexibility of changing step length. According to Adoghe (2022), higher-order derivative methods ensure adequate stability to cope with the system's stiffness. The fact that block methods are self-starting, that is, they do not require predictors or starting values, has been reiterated in Sunday (2022). Another advantage is that they are cheaper to implement than the predictor-corrector methods.

Simpson's method, frequently used for numerical integration, has also been extended to stiff ODEs, owing to its potential for greater accuracy and more reliable performance under specific constraints. When dealing with stiff ODEs, an implicit Simpson's rule can provide stable solutions, even with larger step sizes. This makes it a great option for systems where accuracy and efficiency are key (Butcher, 2003). A method of a new family of self-starting second derivative Simpson's type block methods (SDSMs) specifically designed for stiff ODEs has been presented (Nengem, 2020). Also, Akinfenwa, Abdulganiy and Okunuga (2023) delve into a family of block hybrid Simpson's methods to solve stiff ODEs.

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METHODOLOGY

Derivation of the New Method

The new hybrid-block method is derived using a k-step multistep collocation technique as adopted in Buba (2025). Taking $j = \frac{1}{2}, 1, 2,$ we define the following polynomial of degree as $p = t + 3m - 1, t = 1, m = 3$:

$$\bar{y}(x) = \alpha_0(x)y(x_n) + h\left[\sum_{j=1}^{2}\beta_j(x)f(\bar{x}_j, \bar{y}(\bar{x}_j)) + \beta_{\frac{1}{2}}(x)f\left(\bar{x}_{\frac{1}{2}}, \bar{y}\left(\bar{x}_{\frac{1}{2}}\right)\right)\right]$$

$$+h^2\left[\sum_{j=1}^{2}\gamma_j(x)g(\bar{x}_j, \bar{y}(\bar{x}_j)) + \gamma_{\frac{1}{2}}(x)g\left(\bar{x}_{\frac{1}{2}}, \bar{y}\left(\bar{x}_{\frac{1}{2}}\right)\right)\right]$$

$$+h^3\left[\sum_{j=1}^{2}\eta_j(x)q(\bar{x}_j, \bar{y}(\bar{x}_j)) + +\eta_{\frac{1}{2}}(x)q\left(\bar{x}_{\frac{1}{2}}, \bar{y}\left(\bar{x}_{\frac{1}{2}}\right)\right)\right] \quad (2)$$

where,

$\alpha_0(x), \beta_j(x), \gamma_j(x)$ and $\eta_j(x)$, for $j = \frac{1}{2}, 1, 2,$ are assumed polynomials to be determined.

To obtain these polynomials, Ayoo (2025) extracts a matrix equation from (2) of the form

$$DC = I \quad (3)$$

where I is an identity matrix of dimension 10×10, D, and C are square matrices defined as:

$$D = \left[D_{left} \mid D_{right}\right] \quad (4)$$

where,

$$D_{left} = \begin{bmatrix} 1 & x_n & x_n^2 & x_n^3 & x_n^4 & x_n^5 \\ 0 & 1 & 2\left(x_n + \frac{1}{2}h\right) & 3\left(x_n + \frac{1}{2}h\right)^2 & 4\left(x_n + \frac{1}{2}h\right)^3 & 5\left(x_n + \frac{1}{2}h\right)^4 \\ 0 & 1 & 2(x_n + h) & 3(x_n + h)^2 & 4(x_n + h)^3 & 5(x_n + h)^4 \\ 0 & 1 & 2(x_n + 2h) & 3(x_n + 2h)^2 & 4(x_n + 2h)^3 & 5(x_n + 2h)^4 \\ 0 & 0 & 2 & 6(x_n + \frac{1}{2}h) & 12\left(x_n + \frac{1}{2}h\right)^2 & 20\left(x_n + \frac{1}{2}h\right)^3 \\ 0 & 0 & 2 & 6(x_n + h) & 12(x_n + h)^2 & 20(x_n + h)^3 \\ 0 & 0 & 2 & 6(x_n + 2h) & 12(x_n + 2h)^2 & 20(x_n + 2h)^3 \\ 0 & 0 & 0 & 6 & 24\left(x_n + \frac{1}{2}h\right) & 60\left(x_n + \frac{1}{2}h\right)^2 \\ 0 & 0 & 0 & 6 & 24(x_n + h) & 60(x_n + h)^2 \\ 0 & 0 & 0 & 6 & 24(x_n + 2h) & 60(x_n + 2h)^2 \end{bmatrix} \quad (5)$$

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$$D_{right} = \begin{bmatrix} x_n^6 & x_n^7 & x_n^8 & x_n^9 \\ 6\left(x_n + \frac{1}{2}h\right)^5 & 7\left(x_n + \frac{1}{2}h\right)^6 & 8\left(x_n + \frac{1}{2}h\right)^7 & 9\left(x_n + \frac{1}{2}h\right)^8 \\ 6(x_n + h)^5 & 7(x_n + h)^6 & 8(x_n + h)^7 & 9(x_n + h)^8 \\ 6(x_n + 2h)^5 & 7(x_n + 2h)^6 & 8(x_n + 2h)^7 & 9(x_n + 2h)^8 \\ 30\left(x_n + \frac{1}{2}h\right)^4 & 42\left(x_n + \frac{1}{2}h\right)^5 & 56\left(x_n + \frac{1}{2}h\right)^6 & 72\left(x_n + \frac{1}{2}h\right)^7 \\ 30(x_n + h)^4 & 42(x_n + h)^5 & 56(x_n + h)^6 & 72(x_n + h)^7 \\ 30(x_n + 2h)^4 & 42(x_n + 2h)^5 & 56(x_n + 2h)^6 & 72(x_n + 2h)^7 \\ 120\left(x_n + \frac{1}{2}h\right)^3 & 210\left(x_n + \frac{1}{2}h\right)^4 & 336\left(x_n + \frac{1}{2}h\right)^5 & 504\left(x_n + \frac{1}{2}h\right)^6 \\ 120(x_n + h)^3 & 210(x_n + h)^4 & 336(x_n + h)^5 & 504(x_n + h)^6 \\ 120(x_n + 2h)^3 & 210(x_n + 2h)^4 & 336(x_n + 2h)^5 & 504(x_n + 2h)^6 \end{bmatrix} \quad (6)$$

and

$$C = D^{-1} \quad (7)$$

The columns of C are multiplied by a row matrix:

$$[1 \quad x \quad x^2 \quad x^3 \quad x^4 \quad x^5 \quad x^6 \quad x^7 \quad x^8 \quad x^9]$$

to generate the values of the continuous coefficients $\alpha_0(x)$, $\beta_j(x)$, $\gamma_j(x)$ and $\eta_j(x)$.

Therefore, putting $\zeta = x - x_n$, we have:

$$\alpha_0(\zeta + x_n) = 1 \quad (8)$$

$$\beta_{\frac{1}{2}}(\zeta + x_n) = \frac{64\zeta}{3645\,h^8}\Big(580\zeta^8 - 6390\zeta^7 h + 30060\zeta^6 h^2 - 78930\zeta^5 h^3 + 127008\zeta^4 h^4 - 129465\zeta^3 h^5 + 83400\zeta^2 h^6 - 32760\zeta\, h^7 + 7200\, h^8\Big) \quad (9)$$

$$\beta_1(\zeta + x_n) = -\frac{\zeta}{30\,h^8}(320\zeta^8 - 3510\zeta^7 h + 16440\zeta^6 h^2 - 42990\zeta^5 h^3 + 68922\zeta^4 h^4 - 70035\zeta^3 h^5 + 45000\zeta^2 h^6 - 17640\zeta\, h^7 + 3840\, h^8) \quad (10)$$

$$\beta_2(\zeta + x_n) = \frac{\zeta}{7290\,h^8}\Big(3520\zeta^8 - 35010\zeta^7 h + 147240\zeta^6 h^2 - 343530\zeta^5 h^3 + 491022\zeta^4 h^4 - 446985\zeta^3 h^5 + 259800\zeta^2 h^6 - 93240\zeta\, h^7 + 18810\, h^8\Big) \quad (11)$$

$$\gamma_{\frac{1}{2}}(\zeta + x_n) = \frac{8\zeta}{8505\,h^7}\Big(2240\zeta^8 - 24885\zeta^7 h + 118260\zeta^6 h^2 - 314370\zeta^5 h^3 + 513324\zeta^4 h^4 - 532035\zeta^3 h^5 + 348600\zeta^2 h^6 - 138600\zeta\, h^7 + 30240\, h^8\Big) \quad (12)$$

$$\gamma_1(\zeta + x_n) = \frac{\zeta}{210\,h^7}(560\zeta^8 - 6195\zeta^7 h + 29220\zeta^6 h^2 - 76755\zeta^5 h^3 + 123186\zeta^4 h^4 - 124845\zeta^3 h^5 + 79800\zeta^2 h^6 - 31080\zeta\, h^7 + 6720\, h^8) \quad (13)$$

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$$\gamma_2(\zeta + x_n) = -\frac{\zeta}{3402\, h^7}(560\zeta^8 - 5481\zeta^7 h + 22716\zeta^6 h^2 - 52353\zeta^5 h^3 + 74088\zeta^4 h^4 - 66906\zeta^3 h^5 + 38640\zeta^2 h^6 - 13797\zeta\, h^7 + 2772\, h^8) \quad (14)$$

$$\eta_{\frac{1}{2}}(\zeta + x_n) = \frac{2\zeta}{8505\, h^6}\left(560\zeta^8 - 6300\zeta^7 h + 30420\zeta^6 h^2 - 82530\zeta^5 h^3 + 138348\zeta^4 h^4 - 148365\zeta^3 h^5 + 101640\zeta^2 h^6 - 42840\zeta\, h^7 + 10080\, h^8\right) \quad (15)$$

$$\eta_1(\zeta + x_n) = -\frac{\zeta}{2520\, h^6}(1120\zeta^8 - 11970\zeta^7 h + 54360\zeta^6 h^2 - 137130\zeta^5 h^3 + 211176\zeta^4 h^4 - 205695\zeta^3 h^5 + 126840\zeta^2 h^6 - 47880\zeta\, h^7 + 10080\, h^8) \quad (16)$$

$$\eta_2(\zeta + x_n) = \frac{\zeta}{68040\, h^6}(1120\zeta^8 - 10710\zeta^7 h + 43560\zeta^6 h^2 - 98910\zeta^5 h^3 + 138348\zeta^4 h^4 - 123795\zeta^3 h^5 + 70980\zeta^2 h^6 - 25200\zeta\, h^7 + 5040\, h^8) \quad (17)$$

The continuous method is therefore obtained by substituting the values in (8)-(17) into (2). With further algebraic manipulation, the continuous method is simplified in the following form:

$$\begin{aligned}
\bar{y}(\zeta + x_n) = y(x_n) &+ h\left[\frac{64\zeta}{3645\, h^8}(580\zeta^8 - 6390\zeta^7 h + 30060\zeta^6 h^2 - 78930\zeta^5 h^3 + 127008\zeta^4 h^4 - 129465\zeta^3 h^5 + 83400\zeta^2 h^6 - 32760\zeta\, h^7 + 7200\, h^8)\right] f\left(x_{n+\frac{1}{2}}\right) \\
&+ h\left[-\frac{\zeta}{30\, h^8}(320\zeta^8 - 3510\zeta^7 h + 16440\zeta^6 h^2 - 42990\zeta^5 h^3 + 68922\zeta^4 h^4 - 70035\zeta^3 h^5 + 45000\zeta^2 h^6 - 17640\zeta\, h^7 + 3840\, h^8)\right] f(x_{n+1}) \\
&+ h\left[\frac{\zeta}{7290\, h^8}(3520\zeta^8 - 35010\zeta^7 h + 147240\zeta^6 h^2 - 343530\zeta^5 h^3 + 491022\zeta^4 h^4 - 446985\zeta^3 h^5 + 259800\zeta^2 h^6 - 93240\zeta\, h^7 + 18810\, h^8)\right] f(x_{n+2}) \\
&+ h^2\left[\frac{8\zeta}{8505\, h^7}(2240\zeta^8 - 24885\zeta^7 h + 118260\zeta^6 h^2 - 314370\zeta^5 h^3 + 513324\zeta^4 h^4 - 532035\zeta^3 h^5 + 348600\zeta^2 h^6 - 138600\zeta\, h^7 + 30240\, h^8)\right] g\left(x_{n+\frac{1}{2}}\right) \\
&+ h^2\left[\frac{\zeta}{210\, h^7}(560\zeta^8 - 6195\zeta^7 h + 29220\zeta^6 h^2 - 76755\zeta^5 h^3 + 123186\zeta^4 h^4 - 124845\zeta^3 h^5 + 79800\zeta^2 h^6 - 31080\zeta\, h^7 + 6720\, h^8)\right] g(x_{n+1}) \\
&+ h^2\left[-\frac{\zeta}{3402\, h^7}(560\zeta^8 - 5481\zeta^7 h + 22716\zeta^6 h^2 - 52353\zeta^5 h^3 + 74088\zeta^4 h^4 - 66906\zeta^3 h^5 + 38640\zeta^2 h^6 - 13797\zeta\, h^7 + 2772\, h^8)\right] g(x_{n+2}) \\
&+ h^3\left[\frac{2\zeta}{8505\, h^6}(560\zeta^8 - 6300\zeta^7 h + 30420\zeta^6 h^2 - 82530\zeta^5 h^3 + 138348\zeta^4 h^4 - 148365\zeta^3 h^5 + 101640\zeta^2 h^6 - 42840\zeta\, h^7 + 10080\, h^8)\right] q\left(x_{n+\frac{1}{2}}\right) \\
&+ h^3\left[-\frac{\zeta}{2520\, h^6}(1120\zeta^8 - 11970\zeta^7 h + 54360\zeta^6 h^2 - 137130\zeta^5 h^3 + 211176\zeta^4 h^4 - 205695\zeta^3 h^5 + 126840\zeta^2 h^6 - 47880\zeta\, h^7 + 10080\, h^8)\right] q(x_{n+1}) \\
&+ h^3\left[\frac{\zeta}{68040\, h^6}(1120\zeta^8 - 10710\zeta^7 h + 43560\zeta^6 h^2 - 98910\zeta^5 h^3 + 138348\zeta^4 h^4 - 123795\zeta^3 h^5 + 70980\zeta^2 h^6 - 25200\zeta\, h^7 + 5040\, h^8)\right] q(x_{n+2})
\end{aligned} \quad (18)$$

Evaluating the continuous method (18), at the points, $\zeta = \frac{h}{2}, h, 2h$, yields the following hybrid-block method of the form:

$$AY - By = hR^{(1)}F + h^2R^{(2)}G + h^3R^{(3)}Q \quad (19)$$

Multiplying (8) by the inverse of A, yields:

$$\bar{A}Y - \bar{B}y = h\overline{R^{(1)}}F + h^2\overline{R^{(2)}}G + h^3\overline{R^{(3)}}Q \quad (20)$$

where,

$$\bar{A} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, Y = \begin{bmatrix} y_{n+1} \\ y_{n+\frac{1}{2}} \\ y_{n+2} \end{bmatrix}, \bar{B} = \begin{bmatrix} -1 \\ -1 \\ -1 \end{bmatrix}, y = \begin{bmatrix} y_{n-2} \\ y_{n-1} \\ y_n \end{bmatrix},$$

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$$\overline{R^{(1)}} = \begin{bmatrix} -\frac{347}{30} & \frac{44992}{3645} & \frac{1627}{7290} \\ -\frac{45473}{3840} & \frac{44171}{3645} & \frac{208723}{933120} \\ -\frac{152}{15} & \frac{41984}{3645} & \frac{2242}{3645} \end{bmatrix}, \quad F = \begin{bmatrix} f_{n+1} \\ f_{n+\frac{1}{2}} \\ f_{n+2} \end{bmatrix}, \quad \overline{R^{(2)}} = \begin{bmatrix} \frac{611}{210} & \frac{22192}{8505} & -\frac{239}{3402} \\ \frac{158113}{53760} & \frac{704827}{272160} & -\frac{61315}{870912} \\ \frac{296}{105} & \frac{20864}{8505} & -\frac{218}{1701} \end{bmatrix}, \quad G = \begin{bmatrix} g_{n+1} \\ g_{n+\frac{1}{2}} \\ g_{n+2} \end{bmatrix}, \quad \overline{R^{(3)}} = \begin{bmatrix} -\frac{901}{2520} & \frac{2026}{8505} & \frac{433}{68040} \\ -\frac{115939}{322560} & \frac{64651}{272160} & \frac{55537}{8709120} \\ -\frac{94}{315} & \frac{1952}{8505} & \frac{82}{8505} \end{bmatrix}, Q = \begin{bmatrix} q_{n+1} \\ q_{n+\frac{1}{2}} \\ q_{n+2} \end{bmatrix}$$

Stability Analysis of the Hybrid Block Methods

Based on Aware et al., (2020); Ramos et al., (2021), we define the following linear difference operator, L, associated with (20), as:

$$L[y(x);h] = \sum_{j=0}^{k}\left[\overline{\alpha_0}y(x) + \overline{\alpha_j}y(x+jh) - h\overline{\beta_j}y'(x+jh) - h^2\overline{\gamma_j}y''(x+jh) - h^3\overline{\eta_j}y'''(x+jh)\right] \tag{21}$$

Assuming that $y(x)$ has as many higher derivatives as required, then from the Taylor series expansion of (21) about the point x, we obtain the expression:

$$\mathcal{L}[y(x);h] = \overline{c_0}y(x) + \overline{c_1}hy'(x) + \overline{c_2}hy''(x) + \overline{c_3}hy'''(x) + \cdots + \overline{c_p}h^p y^{(p)}(x) + \cdots \tag{22}$$

where the constant coefficients are given as follows:

$$\overline{c_0} = \sum_{j=0}^{k}\overline{\alpha_j}$$

$$\overline{c_1} = \sum_{j=1}^{k} j\overline{\alpha_j} - \sum_{j=0}^{k}\overline{\beta_j}$$

$$\overline{c_2} = \frac{1}{2!}\sum_{j=1}^{k} j^2\overline{\alpha_j} - \sum_{j=1}^{k} j\overline{\beta_j} - \sum_{j=0}^{k}\overline{\gamma_j}$$

$$\overline{c_3} = \frac{1}{3!}\sum_{j=1}^{k} j^3\overline{\alpha_j} - \frac{1}{2}\sum_{j=1}^{k} j^2\overline{\beta_j} - \sum_{j=1}^{k} j\overline{\gamma_j} - \sum_{j=0}^{k}\overline{\eta_j}$$

$$\vdots$$

$$\overline{c_p} = \frac{1}{p!}\left[\sum_{j=1}^{k} j^p\overline{\alpha_j} - p\sum_{j=1}^{k} j^{p-1}\overline{\beta_j} - p(p-1)\sum_{j=1}^{k} j^{p-2}\overline{\gamma_j} - p(p-1)(p-2)\sum_{j=0}^{k} j^{p-3}\overline{\eta_j}\right]$$

$p = 4,5,\ldots$

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Definition (Order and Error Constant)

The method in (20) has order p if

$$\overline{c_0} = 0, \overline{c_1} = 0, \ldots, \overline{c_p} = 0, \qquad \overline{c_{p+3}} \neq 0$$

where $\overline{c_{p+3}}$ is defined as the error constant (Kumleng, Longwap, and Adee, 2013).

Hence,

$$\overline{\alpha_0} = \begin{bmatrix} -1 \\ -1 \\ -1 \end{bmatrix}, \overline{\alpha_1} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \overline{\alpha_{\frac{1}{4}}} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \overline{\alpha_2} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \overline{\beta_1} = \begin{bmatrix} -\frac{347}{30} \\ -\frac{45473}{3840} \\ -\frac{152}{15} \end{bmatrix}, \overline{\beta_{\frac{1}{4}}} = \begin{bmatrix} \frac{44992}{3645} \\ \frac{44171}{3645} \\ \frac{41984}{3645} \end{bmatrix}, \overline{\beta_2} = \begin{bmatrix} \frac{1627}{7290} \\ \frac{208723}{933120} \\ \frac{2242}{3645} \end{bmatrix},$$

$$\overline{\gamma_1} = \begin{bmatrix} \frac{611}{210} \\ \frac{158113}{53760} \\ \frac{296}{105} \end{bmatrix}, \overline{\gamma_{\frac{1}{4}}} = \begin{bmatrix} \frac{22192}{8505} \\ \frac{704827}{272160} \\ \frac{20864}{8505} \end{bmatrix}, \overline{\gamma_2} = \begin{bmatrix} -\frac{239}{3402} \\ -\frac{61315}{870912} \\ -\frac{218}{1701} \end{bmatrix}, \overline{\eta_1} = \begin{bmatrix} -\frac{901}{2520} \\ -\frac{115939}{322560} \\ -\frac{94}{315} \end{bmatrix}, \overline{\eta_{\frac{1}{4}}} = \begin{bmatrix} \frac{2026}{8505} \\ \frac{64651}{272160} \\ \frac{1952}{8505} \end{bmatrix}, \overline{\eta_2} = \begin{bmatrix} \frac{433}{68040} \\ \frac{55537}{8709120} \\ \frac{82}{8505} \end{bmatrix}$$

$$\overline{c_0} = \sum_{j=0}^{2} \overline{\alpha_j} = \begin{bmatrix} -1 \\ -1 \\ -1 \end{bmatrix} + \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\overline{c_1} = \sum_{j=1}^{2} j\overline{\alpha_j} - \sum_{j=0}^{2} \overline{\beta_j} = \frac{1}{4}\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} + 2\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} - \left(\begin{bmatrix} -\frac{347}{30} \\ -\frac{45473}{3840} \\ -\frac{152}{15} \end{bmatrix} + \begin{bmatrix} \frac{44992}{3645} \\ \frac{44171}{3645} \\ \frac{41984}{3645} \end{bmatrix} + \begin{bmatrix} \frac{1627}{7290} \\ \frac{208723}{933120} \\ \frac{2242}{3645} \end{bmatrix} \right) = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\overline{c_2} = \frac{1}{2!}\sum_{j=1}^{2} j^2\overline{\alpha_j} - \sum_{j=1}^{2} j\overline{\beta_j} - \sum_{j=0}^{2} \overline{\gamma_j} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\overline{c_3} = \frac{1}{3!}\sum_{j=1}^{2} j^3\overline{\alpha_j} - \frac{1}{2}\sum_{j=1}^{2} j^2\overline{\beta_j} - \sum_{j=1}^{2} j\overline{\gamma_j} - \sum_{j=0}^{2} \overline{\eta_j} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\vdots$$

$$c_9 = \frac{1}{9!}\left[\sum_{j=1}^{2} j^9\overline{\alpha_j} - 9\sum_{j=1}^{2} j^8\overline{\beta_j} - 9(8)\sum_{j=1}^{2} j^7\overline{\gamma_j} - 9(8)(7)\sum_{j=1}^{2} j^6\overline{\eta_j} \right] = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

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Therefore,

$$\overline{c_0} = 0, \overline{c_1} = 0, \dots, \overline{c_9} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

but

$$\overline{c_{10}} = \begin{bmatrix} -1.0354 \times 10^{-8} \\ -1.7354 \times 10^{-8} \\ -5.0850 \times 10^{-8} \end{bmatrix}$$

Definition (Consistency)

The order $p \geq 3$ implies that the new hybrid-block form of the new method is consistent (Chollom, Ndam, and Kumleng, 2007).

Definition (Zero-Stability)

A block method is zero stable if all the roots ς_i of the first characteristic polynomial, $\rho(\varsigma)$, satisfy $|\varsigma_i| \leq 1$, any root that $|\varsigma_i| = 1$ is simple (Chollom, Ndam, and Kumleng, 2007).

Hence,

$$\rho(\varsigma) = det(\varsigma \underline{A} - \varsigma \underline{B}) = [\varsigma\ 0\ \ -1\ 0\ \varsigma\ \ -1\ 0\ 0\ \varsigma - 1\ ] = \varsigma^2(\varsigma - 1) = 0$$

The new hybrid block method is zero-stable since $|\varsigma_1| = |\varsigma_2| = 0,$ and $|\varsigma_3| = 1$.

Theorem (Fundamental Theorem of Dahlquist on LMM)

The necessary and sufficient conditions for a linear multi-step method (LMM) to be convergent are that it be consistent and zero-stable (Abdelrahim et al., 2019).

Thus, the new hybrid-block method is convergent since it satisfies the necessary and sufficient provisos of consistency and zero stability.

Definition (Absolute stability)

According to Cholom, Ndam, and Kumleng (2007), a method is said to be absolutely stable for a given $\underline{h}$, if for that $\underline{h}$, all the roots ς_s of the stability polynomial

$$\pi(\varsigma; \bar{h}) = \rho(\varsigma) - \bar{h}\sigma^2(\varsigma) - \bar{h}^2\sigma^3(\varsigma) - \bar{h}^3\sigma^4(\varsigma) = 0 \qquad (23)$$

satisfy $|\varsigma_s| < 1, s = 1,2, \dots, k$

The method of the form (20) is reformulated as a general linear method and is plotted using the Matlab program, as revealed in Figure 1, to be all $A(\alpha)$ stable:

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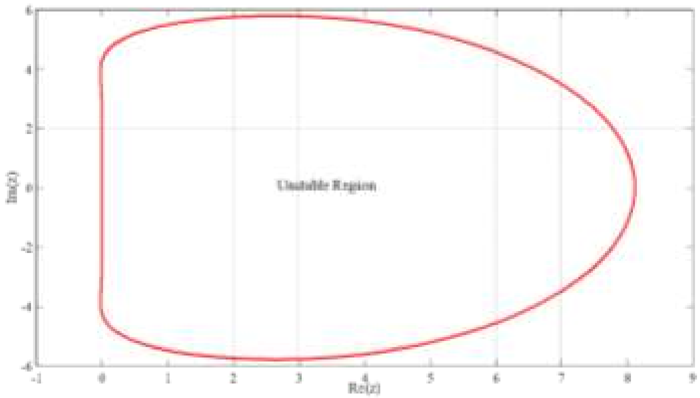
Figure 1: Region of Absolute stability of the new hybrid block methods



NUMERICAL EXAMPLES

Two linear Stiff PK models of the form (1) are considered. The calculated absolute errors are presented in tables, and the solution curves are shown in figures.

Example 4.1 (Pharmacokinetics Model)

Consider the pharmacokinetics model composed of two components, that is, the drug concentration in the gastrointestinal (GI) tract, $y_1(t,)$ and drug concentration in the bloodstream, $y_2(t)$ as a function of time, t given by,

$$\left.\begin{aligned} y_1 &= -k_1 y_1 + d,\ y_1(0) = 1 \\ y_2 &= k_1 y_1 - k_e y_2,\ y_2(0) = 0 \end{aligned}\right\} \tag{24}$$

where $k_e > 0$ and k_1 are the clearance rate constant and rate constants from one compartment to another, respectively. The parameter d is the regimen of drug intake. Taking $k_1 = 2(ln2)$ and $k_e = (ln2)/5$, the exact solution of equation (24) for $t \in [0,6]$ is given by:

$$\left.\begin{aligned} y_1(x) &= e^{-k_1 t} \\ y_2(t) &= -k_1(k_1 - k_e)e^{-k_1 t} - e^{-k_e t}\ ,\ k_1 \neq k_e \end{aligned}\right\} \tag{25}$$

Source: Sunday et al., (2022)

Example 4.2 (Stiff Chemical Reaction Problem)

$$\left.\begin{aligned} y_1' &= -1002y_1 + 1000y_2^2 \\ y_2' &= y_1 - y_2(1 + y_2) \end{aligned}\right\} \tag{26}$$

The initial conditions of the system is considered as $y_1(0) = 1,\ y_2(0) = 1$, and the exact solutions are :

$$\left.\begin{aligned} y_1(t) &= e^{-2x} \\ y_2(t) &= e^{-x} \end{aligned}\right\} \tag{27}$$

Source: Alkali et al., (2023)

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RESULTS/FINDINGS

The following abbreviations and their meanings are used in the study.

t: Point of evaluation

h: Step size

T/s: Computation/Execution time in seconds

MaxE: Maximum error

Ode 15s: MATLAB's built-in stiff solver

IFPHBI: Implicit four-point hybrid-block integrator in (Sunday et al., 2022)

NEHPS: Non-equidistant hybrid point spacing (Sunday, 2022)

EHPS: Equidistant hybrid point spacing (Sunday, 2022)

STDHBI: The new Simpson's third-derivative hybrid-block integrator

Table 1: Error comparison between the new hybrid-block method and the exact solution in example 4.1

h	*Methods*	*MaxE*	*T/s*
10^{-2}	STDHBI	1.78151×10^{-13}	1.112
	FPHBI	2.14126×10^{-6}	3.17921×10^{-7}
	Ode 15s	7.75030×10^{-3}	3.40630×10^{-2}

Figure 2: Solution curves for Example 4.1

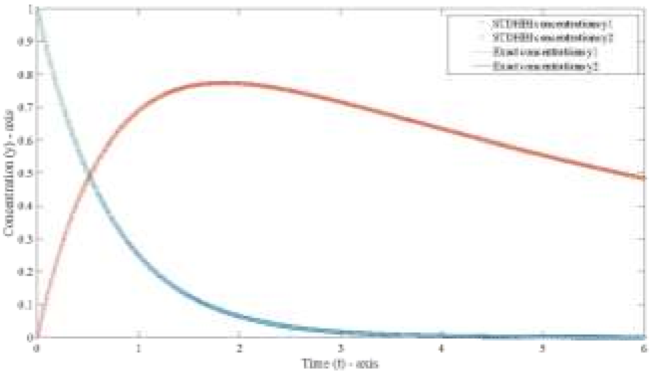

Table 2: Absolute errors for example 4.2

x	y_i	STDHBI	NEHPS	EHPS
0.01	Y_1	9.0214e-05	2.3092e-02	2.4609e-03
	Y_2	8.2653e-08	2.8129e-02	3.7287e-04
0.05	Y_1	8.3343e-05	8.4099e-03	6.9821e-04
	Y_2	4.8069e-08	1.0321e-02	9.1071e-05
0.001	Y_1	2.6488e-06	1.1352e-03	1.3262e-05

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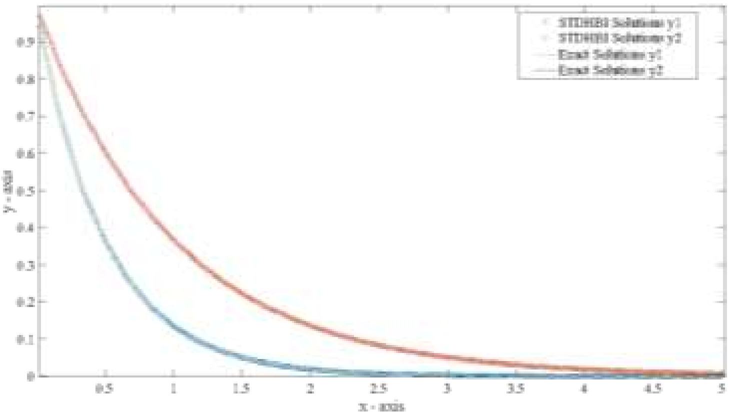
	Y_2	2.6537e-09	1.4494e-03	3.5891e-06
0.005	Y_1	4.1244e-06	5.2481e-04	2.2883e-06
	Y_2	4.1578e-09	6.8590e-04	8.9613e-07

Figure 3: Solution curves for Example 4.2



DISCUSSION

The numerical results clearly show that the proposed Simpson's Third-Derivative Hybrid-Block Integrator (STDHBI) performs very well when applied to stiff systems of ordinary differential equations. The numerical solutions from STDHBI in Example 4.1, which represent a pharmacokinetics problem, show high similarity to the exact solutions. The solution curves overlap almost completely, which demonstrates that the method achieves its highest level of precision. The maximum error reported is minimal, and the computation time is competitive when compared with existing methods such as the implicit four-point hybrid-block integrator (IFPHBI) and MATLAB's built-in solver ode15s.

The absolute errors produced by STDHBI in Example 4.2, which represents a stiff chemical reaction system, showed consistent results with much lower values than those of non-equidistant hybrid point spacing (NEHPS) and equidistant hybrid point spacing (EHPS) methods. The method can produce accurate results throughout all step sizes because its performance remains unchanged after the problem stiffness increases. The results show that the method maintains stability during small step size execution, which acts as an essential requirement for solving stiff problems.

STDHBI shows its strong performance because it uses order nine accuracy combined with third-derivative term inclusion and its $A(\alpha)$stability characteristic. The method can handle fast solution changes through its features, which enable it to operate without necessitating tiny step size intervals. The block structure enables method efficiency improvements because it operates as a self-starting system, which eliminates the need for predictor value acquisition. The numerical experiments provide evidence that the stability and convergence properties established earlier in the manuscript are indeed valid.

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IMPLICATIONS TO RESEARCH AND PRACTICE

The results of this research are significant for the study of numerical analysis and for computing stiff ordinary differential equation models in real-life practice. The proposed Simpson's Third-Derivative Hybrid-Block Integrator (STDHBI) illustrates that higher-order hybrid-block techniques are capable of offering high accuracy, stability, and convergence when solving stiff equations. In relation to the existing literature, this method is relevant due to the creation of the self-starting ninth-order technique, that can lower errors during numerical calculations. In practice, the method can be used in areas such as pharmacokinetics, chemical reaction modeling, engineering, and control theory because these processes involve stiff equations. The stability feature of the method allows its application with larger step sizes, thus lowering costs and improving efficiency in calculation.

CONCLUSION

The development of a Simpson's third-derivative hybrid-block integrator for numerical simulation of stiff ordinary differential equations stands as the principal achievement of this research. The method was derived by a multistep collocation approach, which proved its capability to achieve consistent zero-stability and $A(\alpha)$-stability along with successful convergence. The theoretical characteristics of the method enable its application to solve initial value problems that exhibit stiffness.

Numerical experiments conducted on stiff pharmacokinetics and chemical reaction models reveal that the proposed method demonstrates both high accuracy and operational efficiency. The results produce lower error magnitudes than existing methods. The block design of the method enables simple execution while maintaining low computational requirements.

The numerical results and analysis show that STDHBI functions as an effective and dependable solution method for solving stiff ordinary differential equations, which occur in both engineering and applied science fields.

FUTURE RESEARCH

With the stability features of this approach, the extension of the technique to other nonlinear and larger-scale stiff equations can be undertaken in future research studies.

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