

THREE-STEP BLOCK INTEGRATORS BASED ON TOP ORDER METHODS FOR SOLUTIONS OF STIFF CHEMICAL KINETICS PROBLEMS

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ABSTRACT

In this research, a three-step class of numerically stable block integrators based on top order methods was developed for solutions of stiff chemical kinetic problems. Firstly, the discrete schemes of the method were obtained from the same continuous formulation using the multistep collocation approach as block integrators. Secondly, Stability analysis of the newly derived method was carried out and it has shown to be consistent, zero-stable and A-stable. Numerical results were generated to investigate the influence of top order methods on stiff chemical kinetics problems. the results showed that the new method compare favorably with existing methods in the literature.

Keywords: Top order methods, Three-Step Block Integrators, Chemical kinetics, Stability analysis

INTRODUCTION

The foundation of many scientific and technical fields is chemical kinetics, which is the study of the rates and mechanisms of chemical reactions. The ability to precisely model and anticipate the temporal evolution of chemical systems is essential for understanding everything from intricate biochemical pathways in live beings to combustion processes in automobile engines. (Lambert, 1991; Fatunla, 1988). However, a significant challenge arises when dealing with what are known as "stiff" problems in chemical kinetics. Stiff differential equations typically involve multiple components that change at vastly different rates (multiple timescales). A common definition states that a differential equation is stiff if it contains some components with very small-time constants (fast-changing) alongside others with much larger time constants (slow-changing). The stiff equation is of the form:

$$y' = f(x, y), y'(x_0) = y_0 \quad x \in [a, b], y \in \mathbb{R} \quad (1)$$

Where $f: \mathbb{R} \times \mathbb{R}^m \rightarrow \mathbb{R}^m, y, y_0 \in \mathbb{R}^m, m \geq 1$ is a continuous and differentiable function, the jacobian of the equation (1) vary slowly and the eigen values have negative real parts. The function f in equation (1) is assumed to satisfy the conditions of existence and uniqueness of the solution in the interval $[a, b]$. (Joshua, 2022; Yelwa, I. A., et al., 2025).

MATERIALS AND METHODS

Generally, numerical methods for solving stiff ODEs have been widely used but some suffer from limitations that impact their effectiveness in certain areas. However, Second derivative methods have been known to be stable, convergent and suitable for numerical integration of stiff systems of ordinary differential equations. A lot of methods have been proposed for in the literature for the solution of stiff systems. Notably among them are Bakari, Skwame & Kumleng, (2018) proposed an application of second derivative backward differentiation formulae hybrid block method on stiff ordinary differential equations, Adoghe, Ukpebor & Akhanolu, (2024) developed a second derivative methods with hybrid predictors for solving stiff and non-stiff ordinary differential equations. Brugnano & Trigiante (1998) introduced Top order methods as Boundary Value Methods (BVMs) which belongs to the group of symmetric schemes. According to the authors, TOM methods cannot be obtained from the same continuous formulation hence, the need for additional methods as initial

method and final methods. Top order methods have specific characteristics such as; symmetric schemes, possible order of $2k$ and they have odd step numbers of $k = 2v - 1, v \geq 1$. Other scholars who have worked on top order methods (TOMs) include Awari, Taparki & Kumleng, (2021), they developed a second derivative block type top order method (SDBTOM) using the Rodriguez polynomial as a basis function.

In this paper, we derived all the discrete schemes from the same continuous formulation using multistep collocation approach as basis function to avoid the need of self-starters and pairing with any other method by evaluating the continuous formulation and their second derivatives at some grid points to obtain the discrete schemes that will be used in block form as Block Top Order Methods.

Definition 1: (Butcher, 2016)

A linear multistep method (LMM) is a numerical technique used to approximate the solutions of ordinary differential equations (ODEs). Mathematically, a LMM for solving initial value problem (1) can be written as:

$$\sum_{j=0}^k \alpha_j y_{n+j} = h \sum_{j=0}^k \beta_j f_{n+j} \quad (2)$$

Where α_j and β_j are the unknown coefficients of the method.

Definition 2: (Brugnano & Trigiante, 1998)

A linear multi-step method LMM (2), is said to be symmetric if the coefficients α_j and β_j of the polynomials $\rho(z)$ and $\sigma(z)$ respectively are symmetric (bilateral).

Definition 3: (Omar & Suleiman, 2005)

Block methods are the set of LMMs applied simultaneously to a problem in order to yield a better approximation.

Definition 4: (Lambert, 1991)

A numerical method is said to be A-stable if its region of absolute stability contains the whole of the left-hand plane ($\text{Re} h\lambda < 0$).

Derivation of the Method

we shall derive the continuous formulae of the generalized k -step top order method using the multistep collocation approach by Onumanyi, et al., (1994). Here, the number of interpolation points $t = k$ and collocation points $m = k + 1$, the generalized continuous formula of a k - step Top Order Method is given in the form:

$$y(x) = \sum_{j=0}^{k-1} \alpha_j(x) y_{n+j} + h \sum_{j=0}^k \beta_j(x) f_{n+j} \quad (3)$$

where $x \in [x_n, x_{n+k}]$ and $\alpha_j(x)$ and $\beta_j(x)$ are the continuous coefficients of the method and defined as:

$$\alpha_j(x) = \sum_{i=0}^{t+m-1} \alpha_{j,i+1} x^i, \quad j = 0, 1, \dots, t-1;$$

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

using matrix equation of the form

$$DC = I \quad (4)$$

$$D = \begin{pmatrix} 1 & x_n & x_n^2 & \dots & x_n^{t+m-1} \\ 1 & x_{n+1} & x_{n+1}^2 & \dots & x_{n+1}^{t+m-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n+t-1} & x_{n+t-1}^2 & \dots & x_{n+t-1}^{t+m-1} \\ 0 & 1 & 2x_0 & \dots & (t+m-1)x_0^{t+m-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 1 & 2x_{m-1} & \dots & (t+m-1)x_{m-1}^{t+m-2} \end{pmatrix} \quad (5)$$

And

$$C = \begin{pmatrix} \alpha_{0,1} & \alpha_{1,1} & \dots & \alpha_{t-1,1} & h\beta_{0,1} & \dots & h\beta_{m-1,1} \\ \alpha_{0,2} & \alpha_{1,2} & \dots & \alpha_{t-1,2} & h\beta_{0,2} & \dots & h\beta_{m-1,2} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \alpha_{0,t+m} & \alpha_{1,t+m} & \dots & \alpha_{t-1,t+m} & h\beta_{0,t+m} & \dots & h\beta_{m-1,t+m} \end{pmatrix} \quad (6)$$

It follows from (6) that the columns of $C = D^{-1}$, gives the continuous coefficients $\alpha_j(x)$ and $\beta_j(x)$. Block top order methods for $k = 3$ was derived.

To derive the method for $k=3$, we shall obtain the continuous formula from the generalized K-step continuous formula as:

$$y(x) = \alpha_0(x)y_n + \alpha_1(x)y_{n+1} + \alpha_2(x)y_{n+2} + h[\beta_0(x)f_n + \beta_1(x)f_{n+1} + \beta_2(x)f_{n+2} + \beta_3(x)f_{n+3}] \quad (7)$$

The D-matrix for $k=3$ was extracted from the K-step D-matrix using the multistep collocation approach as:

$$D = \begin{pmatrix} 1 & x_n & x_n^2 & x_n^3 & x_n^4 & x_n^5 & x_n^6 \\ 1 & x_{n+1} & x_{n+1}^2 & x_{n+1}^3 & x_{n+1}^4 & x_{n+1}^5 & x_{n+1}^6 \\ 1 & x_{n+2} & x_{n+2}^2 & x_{n+2}^3 & x_{n+2}^4 & x_{n+2}^5 & x_{n+2}^6 \\ 0 & 1 & 2x_n & 3x_n^2 & 4x_n^3 & 5x_n^4 & 6x_n^5 \\ 0 & 1 & 2x_{n+1} & 3x_{n+1}^2 & 4x_{n+1}^3 & 5x_{n+1}^4 & 6x_{n+1}^5 \\ 0 & 1 & 2x_{n+2} & 3x_{n+2}^2 & 4x_{n+2}^3 & 5x_{n+2}^4 & 6x_{n+2}^5 \\ 0 & 1 & 2x_{n+3} & 3x_{n+3}^2 & 4x_{n+3}^3 & 5x_{n+3}^4 & 6x_{n+3}^5 \end{pmatrix} \quad (8)$$

The continuous coefficients $\alpha_j(x)$ and $\beta_j(x)$ were obtained from the column of the inverse matrix C multiplied with a row matrix $[1 \ x \ x^2 \ x^3 \ x^4 \ x^5 \ x^6]$ as follows:

$$\alpha_0(x) = \alpha_{0,1} + \alpha_{0,2}x + \alpha_{0,3}x^2 + \alpha_{0,4}x^3 + \alpha_{0,5}x^4 + \alpha_{0,6}x^5 + \alpha_{0,7}x^6$$

$$\alpha_1(x) = \alpha_{1,1} + \alpha_{1,2}x + \alpha_{1,3}x^2 + \alpha_{1,4}x^3 + \alpha_{1,5}x^4 + \alpha_{1,6}x^5 + \alpha_{1,7}x^6$$

$$\alpha_2(x) = \alpha_{2,1} + \alpha_{2,2}x + \alpha_{2,3}x^2 + \alpha_{2,4}x^3 + \alpha_{2,5}x^4 + \alpha_{2,6}x^5 + \alpha_{2,7}x^6$$

$$h\beta_0(x) = h\beta_{0,1} + h\beta_{0,2}x + h\beta_{0,3}x^2 + h\beta_{0,4}x^3 + h\beta_{0,5}x^4 + h\beta_{0,6}x^5 + h\beta_{0,7}x^6$$

$$h\beta_1(x) = h\beta_{1,1} + h\beta_{1,2}x + h\beta_{1,3}x^2 + h\beta_{1,4}x^3 + h\beta_{1,5}x^4 + h\beta_{1,6}x^5 + h\beta_{1,7}x^6$$

$$h\beta_2(x) = h\beta_{2,1} + h\beta_{2,2}x + h\beta_{2,3}x^2 + h\beta_{2,4}x^3 + h\beta_{2,5}x^4 + h\beta_{2,6}x^5 + h\beta_{2,7}x^6$$

$$h\beta_3(x) = h\beta_{3,1} + h\beta_{3,2}x + h\beta_{3,3}x^2 + h\beta_{3,4}x^3 + h\beta_{3,5}x^4 + h\beta_{3,6}x^5 + h\beta_{3,7}x^6$$

$$h\beta_4(x) = h\beta_{4,1} + h\beta_{4,2}x + h\beta_{4,3}x^2 + h\beta_{4,4}x^3 + h\beta_{4,5}x^4 + h\beta_{4,6}x^5 + h\beta_{4,7}x^6$$

$$h\beta_5(x) = h\beta_{5,1} + h\beta_{5,2}x + h\beta_{5,3}x^2 + h\beta_{5,4}x^3 + h\beta_{5,5}x^4 + h\beta_{5,6}x^5 + h\beta_{5,7}x^6$$

$$h\beta_6(x) = h\beta_{6,1} + h\beta_{6,2}x + h\beta_{6,3}x^2 + h\beta_{6,4}x^3 + h\beta_{6,5}x^4 + h\beta_{6,6}x^5 + h\beta_{6,7}x^6$$

$$h\beta_7(x) = h\beta_{7,1} + h\beta_{7,2}x + h\beta_{7,3}x^2 + h\beta_{7,4}x^3 + h\beta_{7,5}x^4 + h\beta_{7,6}x^5 + h\beta_{7,7}x^6$$

$$h\beta_8(x) = h\beta_{8,1} + h\beta_{8,2}x + h\beta_{8,3}x^2 + h\beta_{8,4}x^3 + h\beta_{8,5}x^4 + h\beta_{8,6}x^5 + h\beta_{8,7}x^6$$

$$h\beta_9(x) = h\beta_{9,1} + h\beta_{9,2}x + h\beta_{9,3}x^2 + h\beta_{9,4}x^3 + h\beta_{9,5}x^4 + h\beta_{9,6}x^5 + h\beta_{9,7}x^6$$

$$h\beta_{10}(x) = h\beta_{10,1} + h\beta_{10,2}x + h\beta_{10,3}x^2 + h\beta_{10,4}x^3 + h\beta_{10,5}x^4 + h\beta_{10,6}x^5 + h\beta_{10,7}x^6$$

$$h\beta_{11}(x) = h\beta_{11,1} + h\beta_{11,2}x + h\beta_{11,3}x^2 + h\beta_{11,4}x^3 + h\beta_{11,5}x^4 + h\beta_{11,6}x^5 + h\beta_{11,7}x^6$$

$$h\beta_{12}(x) = h\beta_{12,1} + h\beta_{12,2}x + h\beta_{12,3}x^2 + h\beta_{12,4}x^3 + h\beta_{12,5}x^4 + h\beta_{12,6}x^5 + h\beta_{12,7}x^6$$

$$h\beta_{13}(x) = h\beta_{13,1} + h\beta_{13,2}x + h\beta_{13,3}x^2 + h\beta_{13,4}x^3 + h\beta_{13,5}x^4 + h\beta_{13,6}x^5 + h\beta_{13,7}x^6$$

$$h\beta_{14}(x) = h\beta_{14,1} + h\beta_{14,2}x + h\beta_{14,3}x^2 + h\beta_{14,4}x^3 + h\beta_{14,5}x^4 + h\beta_{14,6}x^5 + h\beta_{14,7}x^6$$

$$h\beta_{15}(x) = h\beta_{15,1} + h\beta_{15,2}x + h\beta_{15,3}x^2 + h\beta_{15,4}x^3 + h\beta_{15,5}x^4 + h\beta_{15,6}x^5 + h\beta_{15,7}x^6$$

$$h\beta_{16}(x) = h\beta_{16,1} + h\beta_{16,2}x + h\beta_{16,3}x^2 + h\beta_{16,4}x^3 + h\beta_{16,5}x^4 + h\beta_{16,6}x^5 + h\beta_{16,7}x^6$$

$$h\beta_{17}(x) = h\beta_{17,1} + h\beta_{17,2}x + h\beta_{17,3}x^2 + h\beta_{17,4}x^3 + h\beta_{17,5}x^4 + h\beta_{17,6}x^5 + h\beta_{17,7}x^6$$

$$h\beta_{18}(x) = h\beta_{18,1} + h\beta_{18,2}x + h\beta_{18,3}x^2 + h\beta_{18,4}x^3 + h\beta_{18,5}x^4 + h\beta_{18,6}x^5 + h\beta_{18,7}x^6$$

$$h\beta_{19}(x) = h\beta_{19,1} + h\beta_{19,2}x + h\beta_{19,3}x^2 + h\beta_{19,4}x^3 + h\beta_{19,5}x^4 + h\beta_{19,6}x^5 + h\beta_{19,7}x^6$$

$$h\beta_{20}(x) = h\beta_{20,1} + h\beta_{20,2}x + h\beta_{20,3}x^2 + h\beta_{20,4}x^3 + h\beta_{20,5}x^4 + h\beta_{20,6}x^5 + h\beta_{20,7}x^6$$

$$h\beta_{21}(x) = h\beta_{21,1} + h\beta_{21,2}x + h\beta_{21,3}x^2 + h\beta_{21,4}x^3 + h\beta_{21,5}x^4 + h\beta_{21,6}x^5 + h\beta_{21,7}x^6$$

$$h\beta_{22}(x) = h\beta_{22,1} + h\beta_{22,2}x + h\beta_{22,3}x^2 + h\beta_{22,4}x^3 + h\beta_{22,5}x^4 + h\beta_{22,6}x^5 + h\beta_{22,7}x^6$$

$$h\beta_{23}(x) = h\beta_{23,1} + h\beta_{23,2}x + h\beta_{23,3}x^2 + h\beta_{23,4}x^3 + h\beta_{23,5}x^4 + h\beta_{23,6}x^5 + h\beta_{23,7}x^6$$

$$h\beta_{24}(x) = h\beta_{24,1} + h\beta_{24,2}x + h\beta_{24,3}x^2 + h\beta_{24,4}x^3 + h\beta_{24,5}x^4 + h\beta_{24,6}x^5 + h\beta_{24,7}x^6$$

$$h\beta_{25}(x) = h\beta_{25,1} + h\beta_{25,2}x + h\beta_{25,3}x^2 + h\beta_{25,4}x^3 + h\beta_{25,5}x^4 + h\beta_{25,6}x^5 + h\beta_{25,7}x^6$$

$$h\beta_{26}(x) = h\beta_{26,1} + h\beta_{26,2}x + h\beta_{26,3}x^2 + h\beta_{26,4}x^3 + h\beta_{26,5}x^4 + h\beta_{26,6}x^5 + h\beta_{26,7}x^6$$

$$h\beta_{27}(x) = h\beta_{27,1} + h\beta_{27,2}x + h\beta_{27,3}x^2 + h\beta_{27,4}x^3 + h\beta_{27,5}x^4 + h\beta_{27,6}x^5 + h\beta_{27,7}x^6$$

$$h\beta_{28}(x) = h\beta_{28,1} + h\beta_{28,2}x + h\beta_{28,3}x^2 + h\beta_{28,4}x^3 + h\beta_{28,5}x^4 + h\beta_{28,6}x^5 + h\beta_{28,7}x^6$$

$$h\beta_{29}(x) = h\beta_{29,1} + h\beta_{29,2}x + h\beta_{29,3}x^2 + h\beta_{29,4}x^3 + h\beta_{29,5}x^4 + h\beta_{29,6}x^5 + h\beta_{29,7}x^6$$

$$h\beta_{30}(x) = h\beta_{30,1} + h\beta_{30,2}x + h\beta_{30,3}x^2 + h\beta_{30,4}x^3 + h\beta_{30,5}x^4 + h\beta_{30,6}x^5 + h\beta_{30,7}x^6$$

$$h\beta_{31}(x) = h\beta_{31,1} + h\beta_{31,2}x + h\beta_{31,3}x^2 + h\beta_{31,4}x^3 + h\beta_{31,5}x^4 + h\beta_{31,6}x^5 + h\beta_{31,7}x^6$$

$$h\beta_{32}(x) = h\beta_{32,1} + h\beta_{32,2}x + h\beta_{32,3}x^2 + h\beta_{32,4}x^3 + h\beta_{32,5}x^4 + h\beta_{32,6}x^5 + h\beta_{32,7}x^6$$

$$\begin{aligned} & \frac{195\tau^4}{22h^4} - \frac{147\tau^5}{44h^5} + \frac{19\tau^6}{44h^6} \Big) y_{n+2} + \left(\tau - \frac{109\tau^2}{33h} + \frac{183\tau^3}{44h^2} - \frac{82\tau^4}{33h^3} + \right. \\ & \frac{31\tau^5}{44h^4} - \frac{5\tau^6}{66h^5} \Big) f_n + \left(-\frac{63\tau^2}{11h} + \frac{145\tau^3}{11h^2} - \frac{467\tau^4}{44h^3} + \frac{79\tau^5}{22h^4} - \right. \\ & \frac{19\tau^6}{44h^5} \Big) f_{n+1} + \left(-\frac{27\tau^2}{22h} + \frac{151\tau^3}{44h^2} - \frac{37\tau^4}{11h^3} + \frac{59\tau^5}{44h^4} - \frac{2\tau^6}{11h^5} \right) f_{n+2} + \\ & \left(\frac{\tau^2}{33h} - \frac{\tau^3}{11h^2} + \frac{13\tau^4}{132h^3} - \frac{\tau^5}{22h^4} + \frac{\tau^6}{132h^5} \right) f_{n+3} \end{aligned} \quad (10)$$

Where $\tau = x - x_n$

Equation (10) was evaluated at $\tau = 3h$, and its second derivative at points $\tau = 3h, 2h$ to yield the three-step Block Top order method as:

$$y_{n+3} = y_n + \frac{27}{11}y_{n+1} - \frac{27}{11}y_{n+2} + \frac{3}{11}hf_n + \frac{27}{11}hf_{n+1} + \frac{27}{11}hf_{n+2} + \frac{3}{11}hf_{n+3}$$

$$y_{n+2} = \frac{22}{873}g_{n+3}h^2 - \frac{193}{2619}hf_{n+3} + \frac{53}{97}hf_{n+2} + \frac{75}{97}hf_{n+1} + \frac{247}{2619}hf_n + \frac{64}{97}y_{n+1} + \frac{33}{97}y_n$$

$$y_{n+1} = \frac{11}{72}g_{n+2}h^2 - \frac{1}{180}hf_{n+3} - \frac{25}{36}hf_{n+2} - \frac{25}{36}hf_{n+1} - \frac{13}{216}hf_n + \frac{59}{48}y_{n+2} - \frac{11}{48}y_n \quad (11)$$

The three step block top order method derived is now a second derivative method because we evaluated at the second derivative of the continuous formula.

Analysis and Implementation

In this subsection, the analysis of basic properties of the newly derived method shall be carried out. These properties include local truncation error, order, consistence, zero stability, convergence and stability regions. The convergence of the new block methods is determined using the approach of Fatunla, (1995) and Bakari et al., (2018).

Order and Error Constant

Adopting the approach of [3], we associate the linear difference operator \mathcal{L} defined by

$$\mathcal{L}[y(x); h] = \sum_{j=0}^k [\alpha_j y(x + jh) - h\beta_j y'(x + jh) - h^2 \gamma_j y''(x + jh)] \quad (12)$$

Where $y(x)$ is an arbitrary function, continuously differentiable on an interval $[a, b]$. If we assume that $y(x)$ has as many higher derivatives as we require, then on Taylor expanding about the point x , we obtain

$$\mathcal{L}[y(x); h] = c_0 y(x) + c_1 h y'(x) + \dots + c_q h^q y^{(q)}(x) + \dots \quad (13)$$

where

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

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

$$c_2 = \frac{1}{2!}(\alpha_1 + 2^2\alpha_2 + \dots + k^2\alpha_k) - (\beta_1 + 2\beta_2 + \dots + k\beta_k)$$

$$c_3 = \frac{1}{3!}(\alpha_1 + 2^3\alpha_2 + \dots + k^3\alpha_k) - \frac{1}{2!}(\beta_1 + 2^2\beta_2 + \dots + k^2\beta_k) - (\gamma_1 + 2\gamma_2 + \dots + k\gamma_k)$$

$$c_q = \frac{1}{q!}(\alpha_1 + 2^q\alpha_2 + \dots + k^q\alpha_k) - \frac{1}{(q-1)!}(\beta_1 + 2^{(q-1)}\beta_2 + \dots + k^{(q-1)}\beta_k) - \frac{1}{(q-2)!}(\gamma_1 + 2^{(q-2)}\gamma_2 + \dots + k^{(q-2)}\gamma_k),$$

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

According to [8], the method in equation (11) has order p if $c_0 = c_1 = c_2 = \dots = c_p = 0, c_{p+1} = 0$ but $c_{p+2} \neq 0$. Then c_{p+2} is called the error constant and $c_{p+2}h^{p+2}y^{(p+2)}(x_n)$ is the principal local truncation error at the point x_n . Therefore, the three-step block integrators based on top order method has uniform order $p = 5$ and error constant is $\bar{c}_7 =$

$$\begin{bmatrix} -1.95 \times 10^{-3} \\ -7.94 \times 10^{-4} \\ 3.09 \times 10^{-4} \end{bmatrix}$$

Consistency

The LMM is said to be consistent if it has order at least one, $p \geq 1$. The three-step block integrators based on top order

method are said to be consistent since the order is greater than one. According to Lambert, (1991) It is important to note that consistency controls the magnitude of the local truncation error committed at each stage of the computation.

Zero Stability

For a block method, the method is said to be zero-stable if the roots $\xi_s, s = 1, 2, \dots, k$ of its first characteristic polynomial $\rho(\xi) = \det(\xi A^{(0)} - E)$ satisfy $\xi_s \leq 1$, and any root with modulus one has multiplicity not exceeding the order of the differential equation [7]. The main consequence of zero-stability is to control the propagation of the error as the integration progresses. To determine the zero stability of the new method, using the approach of [11]. The derived method can be written in block form as

$$A^{(1)}Y_{w+1} = A^{(0)}Y_{w-1} + hBF_{w+1}$$

Whose first characteristics polynomial is given as

$$\rho(\xi) = \det[\xi A - B]$$

The first characteristic polynomial of the three-step block top order method (11) is given as:

$$A := \begin{bmatrix} -\frac{27}{11} & \frac{27}{11} & 1 \\ -\frac{64}{97} & 1 & 0 \\ 1 & -\frac{59}{48} & 0 \end{bmatrix}, B := \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & -\frac{33}{97} \\ 0 & 0 & \frac{11}{48} \end{bmatrix}$$

$$\rho(\xi) = \det(\xi A - B) = \begin{vmatrix} -\frac{27}{11}\xi & \frac{27}{11}\xi & \xi + 1 \\ -\frac{64}{97}\xi & \xi & \frac{33}{97} \\ \xi & -\frac{59}{48}\xi & -\frac{11}{48} \end{vmatrix} = -\frac{55}{291}\xi^2 - \frac{55}{291}\xi^3$$

The roots of the first characteristic equation $\rho(\xi)$ are obtained as $\xi_1 = 1, \xi_2 = \xi_3 = 0$

Convergence

Theorem 1 (Dahlquist, 1963)

The Dahlquist theorem of convergence states that for a LMM applied to a sufficiently smooth differential equation, convergence of the numerical solution to the exact solution occurs if and only if the method is consistent and zero-stable.

Region of Absolute Stability

The test equation $y' = \lambda y$ as used by Yatim et al., (2012) was inserted in the block methods to determine the regions of absolute stability. The equation $y' = \lambda y$ and $y'' = \lambda^2 y$ which is equivalent to $f_n = \lambda y_n, f_{n+1} = \lambda y_{n+1}, \dots, f_{n+k} = \lambda y_{n+k}$, and $g_n = \lambda^2 y_n, g_{n+1} = \lambda^2 y_{n+1}, \dots, g_{n+k} = \lambda^2 y_{n+k}$ was substituted in the new method.

The stability polynomial, $\rho(r) = \det(rA - B)$

$$= \frac{11}{1164}r^3z^5 + \frac{55}{291}r^2z + \frac{385}{1746}r^2z + \frac{187}{1746}r^2z^2 + \frac{187}{6984}r^2z^3 + \frac{11}{3492}r^2z^4 + \frac{605}{1746}r^2z - \frac{517}{1746}r^3z^2 + \frac{11}{72}r^3z^3 - \frac{44}{873}r^3z^4 - \frac{55}{291}r^3$$

Is differentiated with respect to z to give

$$= \frac{55}{1164}r^3z^4 + \frac{385}{1746}r^2 + \frac{187}{873}r^2z + \frac{187}{2328}r^2z^2 + \frac{11}{873}r^2z^3 + \frac{605}{1746}r^3 - \frac{517}{873}r^3z + \frac{11}{24}r^3z^2 - \frac{176}{873}r^3z^3$$

The stability polynomial with its derivative are inserted into MATLAB code to plot the stability region as shown in the figure.

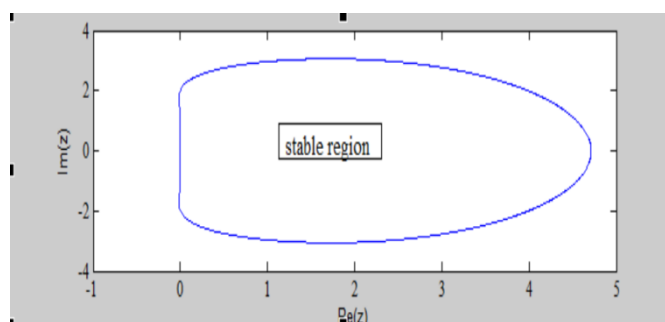


Figure 1: Region of Absolute Stability of 3SBITOM

Implementation

The three step block integrators based on top order methods derived in this research was implemented efficiently without requiring starting values and predictors. The implementation of the method was carried out with the aid of 2021 MATLAB programming language while the derivation of the method was carried out with the aid of maple 18.

RESULTS AND DISCUSSION

In this section, some numerical and graphical results for some stiff chemical kinetic problems shall be presented using the newly derived 3SBITOM. This is intended to show the performance of the methods on stiff chemical problems.

The following notations shall be used in the tables 1-3 and figure 2-3.

3SBITOM: newly derived three-step block integrators based on top order method.

EHPS: two-step second derivative method with equidistant hybrid point space by [9]

4SSDM: four-step hybrid block extended second derivative backward differentiation formula by [1].

Problem 1

Consider the Non-linear stiff chemical system in classical dynamics given by

$$y_1' = -1002y_1 + 1000y_2^2$$

$$y_2' = y_1 - y_2(1 + y_2)$$

$$y_1(0) = 1, y_2(0) = 1$$

This problem which is solved in the range $0 \leq x \leq 1$ has the exact solution,

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

The numerical and graphical results for problem 1 are presented in table 1 and figure 2 respectively.

Problem 2.

Consider the stiff linear chemical kinetic problem given by

$$y_1' = -100y_1 + 9.901y_2$$

$$y_2' = 0.1y_1 - y_2$$

$$y_1(0) = 1, y_2(0) = 10$$

$$\text{Exact soln: } y_1(x) = e^{-0.99x}, y_2(x) = 10e^{-0.99x}$$

The numerical and graphical results for problem 2 are presented in table 2-3 and figure 3 respectively.

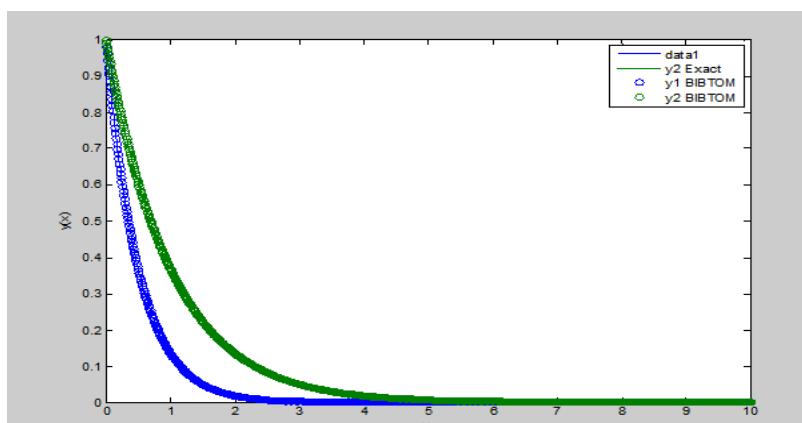


Figure 2: Solution Curve of 3SBITOM for Problem1

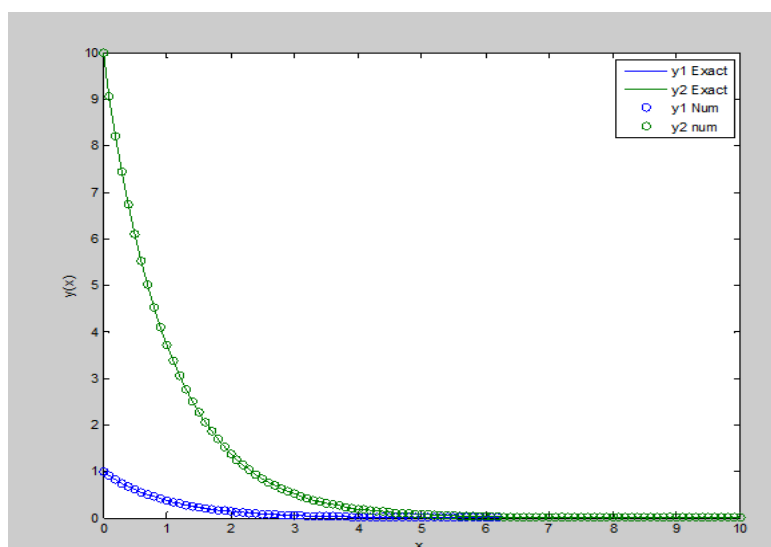


Figure 3. Solution Curve of 3SBITOM for Problem 2

Table 1: Showing the Absolute Errors for Problem 1

| H | y_k | 4SSDM | EHPS | 3SBITOM |
|-------|-------|------------|------------|------------|
| 0.01 | y_1 | 8.8401e-02 | 2.409e-03 | 2.1720e-07 |
| | y_2 | 9.7066e-02 | 3.7287e-04 | 1.4625e-09 |
| 0.05 | y_1 | 3.139e-02 | 6.9821e-04 | 3.9503e-05 |
| | y_2 | 7.9153e-02 | 9.1071e-05 | 1.0154e-08 |
| 0.001 | y_1 | 7.6391e-02 | 1.3262e-05 | 2.0928e-06 |
| | y_2 | 5.4312e-02 | 3.5891e-06 | 2.3542e-09 |
| 0.005 | y_1 | 5.8924e-02 | 2.2883e-06 | 2.3542e-09 |
| | y_2 | 9.0635e-02 | 8.9613e-07 | 2.3542e-10 |

Table 2: Solutions of Problem 2

| x | Num y1 | Num y2 | Exact y1 | Exact y2 |
|-----|----------|----------|----------|----------|
| 0 | 1 | 10 | 1 | 10 |
| 0.1 | 0.905743 | 9.057427 | 0.905743 | 9.057427 |
| 0.2 | 0.82037 | 8.203699 | 0.82037 | 8.203699 |
| 0.3 | 0.743044 | 7.43044 | 0.743044 | 7.43044 |
| 0.4 | 0.673007 | 6.730067 | 0.673007 | 6.730067 |
| 0.5 | 0.609571 | 6.095709 | 0.609571 | 6.095709 |
| 0.6 | 0.552114 | 5.521144 | 0.552114 | 5.521144 |
| 0.7 | 0.500074 | 5.000736 | 0.500074 | 5.000736 |
| 0.8 | 0.452938 | 4.52938 | 0.452938 | 4.52938 |
| 0.9 | 0.410245 | 4.102453 | 0.410245 | 4.102453 |

Table 3: Showing the Absolute Errors for Problem 2

| x | Error y1 | Error y2 |
|-----|----------|----------|
| 0 | 0 | 0 |
| 0.1 | 2.59E-10 | 2.59E-09 |
| 0.2 | 4.69E-10 | 4.69E-09 |
| 0.3 | 6.37E-10 | 6.37E-09 |
| 0.4 | 7.69E-10 | 7.69E-09 |
| 0.5 | 8.71E-10 | 8.71E-09 |
| 0.6 | 9.46E-10 | 9.46E-09 |
| 0.7 | 1.00E-09 | 1.00E-08 |
| 0.8 | 1.04E-09 | 1.04E-08 |
| 0.9 | 1.05E-09 | 1.05E-08 |

A class of three-step block integrator based on top order methods was derived for the solutions of stiff chemical kinetic problems using the multistep collocation as basis function. We obtained the main scheme and the corresponding schemes from the same continuous formula thereby, eradicating the need for starting values associated with top order methods. The method have uniform order of 5 thus, consistent. The newly derived method is convergent and A-stable. The method was implemented on two chemical kinetic problems, and from table 1 and 3, the method is computationally reliable.

CONCLUSION

Here, we have another configuration of TOM for the solution of stiff chemical kinetic problems is now available. It has a uniform order of $2k - 1$, is zero stable and convergent. The method's efficacy and accuracy were demonstrated by comparing the method's results to those acquired using other existing methods.

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