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Abstract

The need to have L-stablegeneral linear method (GLM) with higher order than Runge-Kutta methods has provided the need to propose second derivative GLM (SDGLM) and also multi-derivative GLM. This paper therefore describes somethird derivative general linear methods (TDGLM) which incorporates up to the third derivative terms. The methods which are diagonally implicit are A(α)-stable.

Keywords: Diagonally implicit Runge-Kutta methods; third derivative RK methods, GLM, $A(\alpha)$ -stable. *AMS subject classification:* 65L05, 65L06.

1.0 Introduction

Recently TDRK methods (Third derivative Runge-Kutta methods) which has a simple transformation to TDGLM were introduced in [1]for the numerical solution of the initial value problems(IVPs) in ordinary differential equations (ODEs)

$$\begin{cases} y' = f(x, y(x)), x \in [x_0, X], \\ y_0 = y(x_0), \quad y \in R^m, f \in R \times R^m, m \ge 1. \end{cases}$$
(1)

Interestingly, these methods can be derived to possess inherent RK stability [2] and nearly ARK stability [1] properties. In a related study, Ezzeddine and Hojjati [3] had considered third derivative linear multistep methods (TDLMM) for stiff problems. In particular, the TDGLM introduced in [1] is

$$\begin{cases} Y_{i} = h^{3} \sum_{j=1}^{s} a_{ij}^{(3)}(c_{i})F_{j}'' + h^{2} \sum_{j=1}^{s} a_{ij}^{(2)}(c_{i})F_{j}' + h \sum_{j=1}^{s} a_{ij}^{(1)}(c_{i})F_{j} + \sum_{j=1}^{r} u_{ij}(c_{i}) + y_{j}^{[n-1]}, \quad i = 1, ..., s, \\ y_{i}^{[n]} = h^{3} \sum_{j=1}^{s} b_{ij}^{(3)}(t)F_{j}'' + h^{2} \sum_{j=1}^{s} b_{ij}^{(2)}(t)F_{j}' + h \sum_{j=1}^{s} b_{ij}^{(1)}(t)F_{j} + \sum_{j=1}^{r} v_{ij}(t) + y_{j}^{[n-1]}, \quad i = 1, ..., r, \\ Y_{i} = y(x_{n-1} + c_{i}h), \quad F_{j} = F(x_{n-1} + c_{i}h, Y_{i}), \quad y_{1}^{[n-1]} = y_{n-1}, \quad y_{1}^{[n]} = y(x_{n-1} + th), \quad c_{s} = t = 1. \end{cases}$$

In matrix form

$$\begin{pmatrix} Y \\ y^{[n]} \end{pmatrix} = \begin{pmatrix} A_1 & A_2 & A_3 & U \\ B_1 & B_2 & B_3 & V \end{pmatrix} \begin{pmatrix} h F \\ h^2 F' \\ h^3 F'' \\ y^{[n-1]} \end{pmatrix}, c = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_s \end{pmatrix},$$
(3)

where, $h = x_n - x_{n-1}$ is the step length, $Y = (Y_1, Y_2, \dots, Y_S)^T$ denotes the stages, the $F = (F_1, F_2, \dots, F_S)^T$, $F' = (F_1', F_2', \dots, F_S')^T$, $F'' = (F_1'', F_2'', \dots, F_S'')^T$ are first, second, and third derivatives respectively. The $y^{[n-1]} = (y_1^{[n-1]}, y_2^{[n-1]}, \dots, y_r^{[n-1]})^T$ and $y^{[n]} = (y_1^{[n]}, y_2^{[n]}, \dots, y_r^{[n]})^T$ are the incoming and outgoing approximations

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evaluated at step n-1 and n respectively.

The matrices in (3) are $A_1 = \{a_{ij}^{(1)}\} \in \mathbb{R}^{(s \times s)}$, $A_2 = \{a_{ij}^{(2)}\} \in \mathbb{R}^{(s \times s)}$, $A_3 = \{a_{ij}^{(3)}\} \in \mathbb{R}^{(s \times s)}$, $B_1 = \{b_{ij}^{(1)}\} \in \mathbb{R}^{(r \times s)}$, $B_2 = \{b_{ij}^{(2)}\} \in \mathbb{R}^{(r \times s)}$, $B_3 = \{b_{ij}^{(3)}\} \in \mathbb{R}^{(r \times s)}$, $U = \{u_{ij}\} \in \mathbb{R}^{(s \times r)}$, and $V = \{v_{ij}\} \in \mathbb{R}^{(r \times r)}$. The stages $Y_i = y(x_{n-1} + c_ih) + O(h^{q+1})$

are of order q. The abscissa vector is $c_i = [c_1, c_2, \dots, c_s]^T$ and $c_i \in [0, 1]$. The output method

$$y_n = y(x_{n-1} + h) + O(h^{p+1})$$

is of order *p*. The dimension of the GLM in (3) is $(s+r) \times (3s+r)$. An example of the TDGLM (3) is

$$A_{1} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad A_{2} = \begin{pmatrix} 0 & 0 \\ \frac{1}{2} & 0 \end{pmatrix}, \quad A_{3} = \begin{pmatrix} 0 & 0 \\ \frac{1}{6} & 0 \end{pmatrix}, \quad B_{1} = \begin{pmatrix} 1 & 0 \end{pmatrix}, \quad B_{2} = \begin{pmatrix} \frac{1}{2} & 0 \end{pmatrix}, \quad B_{3} = \begin{pmatrix} \frac{1}{6} & 0 \end{pmatrix}, c = \begin{bmatrix} 0 & 1 \end{bmatrix}^{T},$$
$$U = \begin{pmatrix} 1 & 1 \end{pmatrix}, \quad V = 1, \quad Y = \begin{pmatrix} Y_{1}, Y_{2} \end{pmatrix}^{T}, \quad F = \begin{pmatrix} F_{1}, F_{2} \end{pmatrix}^{T}, \quad F' = \begin{pmatrix} F_{1}', F_{2}' \end{pmatrix}^{T}, \quad F'' = \begin{pmatrix} F_{1}', F_{2}' \end{pmatrix}^{T}.$$

The stability polynomial of this TDGLMis $\Pi(w, z) = w - 1 - z - \frac{z}{2} - \frac{z}{6}$. The stability polynomial is exactly the same

as that of the classical third order RK method. By implication, this method will behave like the third order RK method. The interval of absolute stability of this method is (-2.513, 0). The stability plot is given in Fig. 1.



Fig. 1: The stability region of the GLM (3a).

The stability matrix of (3) is

 $\psi(z) = V + z(B_1 + zB_2 + z^2B_3)(I - zA_1 - z^2A_2 - z^3A_3)^{-1}U, \quad z = \lambda h,$ (4) while the stability polynomial is

$$\Pi(w, z) = \det(wI - \psi(z)).$$
⁽⁵⁾

Definition 1. c.f. [4]: If M(z), known as the stability function, has the special form

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$$\Pi(w,z) = \det(wI - \psi(z)) = w^{r-1}(w - R(z)),$$

then the method is said to possess RK stability.

For implicit case, $R(z) = \frac{N(z)}{\Omega(z)}$, where N(z) and $\Omega(z)$ are polynomials. If the diagonal elements of the method (3) are

equal, we calculate the value of the stability function as the trace of $\psi(z)$ and we find

$$R(z) = \frac{N(z)}{\left(1 - \lambda z - \mu z^2 - \tau z^3\right)^s},$$

where the numerator satisfies the condition

$$N(z) = \exp(z) \left(1 - \lambda z - \mu z^2 - \tau z^3 \right)^s + O(z^{p+1}).$$

The values of λ , μ , and τ which yields a stable methods are determined from the following *E*-polynomial formula

$$E(y) = \left| \left(1 - \lambda i y - \mu (i y)^2 - \tau (i y)^3 \right)^{p+1} \right|^2 - \left| N(i y) \right|^2, \quad z = i y.$$

For details see [5] and [6]. The example method is explicit; it is suitable for non-stiff IVPs. This paper briefly describes a new type of diagonally implicit counterpart with unequal elements on the diagonal. Methods of these kinds are in [7]. They are cheaper and simple to implement when compared with the so called fully implicit methods. One of the motivations for extending SDGLM to TDGLM is that the additional stage term introduced into the methods improves the order andpromotes accuracy and large stability region. If the GLM (3) have its diagonal elements unequal and is applied to the IVPs (1), theimplicitness arising from the stages can be resolvedusing the Newton Raphson method,

$$Y_{1}^{[r+1]} \to Y_{1}^{[r]} - D_{1}, \ Y_{2}^{[r+1]} \to Y_{1}^{[r]} - D_{2}, \ \cdots, \ Y_{s}^{[r+1]} \to Y_{s}^{[r]} - D_{s}, \tag{6}$$

where

$$\Delta \begin{pmatrix} D_1 \\ D_2 \\ \vdots \\ D_s \end{pmatrix} = \Phi; \quad \Delta = \begin{pmatrix} I - \frac{\partial \Phi_1}{\partial Y_1} & 0 & \cdots & 0 \\ 0 & I - \frac{\partial \Phi_2}{\partial Y_2} & \cdots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & I - \frac{\partial \Phi_s}{\partial Y_s} \end{pmatrix},$$

$$\Phi = \begin{pmatrix} \Phi_{1} \\ \Phi_{2} \\ \vdots \\ \Phi_{s} \end{pmatrix} = \begin{pmatrix} Y_{1} - h^{3} \sum_{j=1}^{s} a_{1j}^{(3)} F_{j}'' - h^{2} \sum_{j=1}^{s} a_{1j}^{(2)} F_{j}' - h \sum_{j=1}^{s} a_{1j}^{(1)} (c_{i}) F_{j} - \sum_{j=1}^{r} u_{1j} y_{j}^{[n-1]} \\ Y_{2} - h^{3} \sum_{j=1}^{s} a_{2j}^{(3)} F_{j}'' - h^{2} \sum_{j=1}^{s} a_{2j}^{(2)} F_{j}' - h \sum_{j=1}^{s} a_{2j}^{(1)} (c_{i}) F_{j} - \sum_{j=1}^{r} u_{2j} y_{j}^{[n-1]} \\ \vdots \\ Y_{s} - h^{3} \sum_{j=1}^{s} a_{sj}^{(3)} F_{j}'' - h^{2} \sum_{j=1}^{s} a_{sj}^{(2)} F_{j}' - h \sum_{j=1}^{s} a_{sj}^{(1)} (c_{i}) F_{j} - \sum_{j=1}^{r} u_{sj} y_{j}^{[n-1]} \end{pmatrix}$$

To start up the Newton method, an explicit starter such as RK method with multiple output is required and to obtain accurate solution from the output method, we keep doing (6) until

$$\left\|Y^{(i+1)} - Y^{(i)}\right\| \le Tol; \quad i = 0, 1, 2, \cdots, k.$$

The *Tol* is the tolerance requested by the user. The converged value of $Y^{(k)}$ is now the output from the step and $y^{[n]}$ is then computed in (2). This paper is organized in the following manner. Section 3 show the derivations of the two stagemethods of order p = 6 and three stage methods of order p = 9 and in Section 4 we demonstrates the application of the methods on stiff problems of (1).

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2.0 The construction of TDGLM

To derive (3) we use the following polynomial interpolant

$$y(x) = \sum_{j=0}^{N} \theta_j x^j .$$
⁽⁷⁾

The scale variable t in (2) is $\frac{x - x_{n-1}}{h}$, see [1]. The structure of the two stage diagonally implicit GLM in (3) is

$$\begin{cases} Y_{1} = h^{3} a_{11}^{(3)}(c_{1})F_{1}'' + h^{2} a_{11}^{(2)}(c_{1})F_{1}' + h a_{11}^{(1)}(c_{1})F_{1} + u_{11}(c_{1})y^{[n-1]}, \\ y^{[n]} = h^{3} \left(b_{11}^{(3)}(t)F_{1}'' + b_{12}^{(3)}(t)F_{2}'' \right) + h^{2} \left(b_{11}^{(2)}(t)F_{1}' + b_{12}^{(2)}(t)F_{2}' \right) \\ + h \left(b_{11}^{(1)}(t)F_{1} + b_{12}^{(1)}(t)F_{2} \right) + v_{11}(t)y^{[n-1]}, \\ Y_{1} = y(x_{n-1} + c_{1}h), \quad y^{[n]} = Y_{2} = y(x_{n-1} + th), \quad t = c_{2} = 1. \end{cases}$$
(8)

From (7) the coefficients of (8) are as follows:

$$a_{11}^{(1)}(c_1) = c_1, \ a_{11}^{(2)}(c_1) = -\frac{c_1^2}{2}, \ a_{11}^{(3)}(c_1) = \frac{c_1^3}{6}, \ u_{11}(c_1) = 1,$$

For the output method set t = 1, to obtain

$$a_{21}^{(1)}(c_{2}) = \frac{c_{2}^{4}(5c_{1}^{2} - 4c_{1}c_{2} + c_{2}^{2})}{2(-c_{1} + c_{2})^{5}},$$

$$a_{22}^{(1)}(c_{2}) = \frac{1}{2}c_{2}\left(1 + \frac{c_{1}\left(c_{1}^{4} - 5c_{1}^{3}c_{2} + 10c_{1}^{2}c_{2}^{2} - 5c_{1}c_{2}^{3} + c_{2}^{4}\right)}{(c_{1} - c_{2})^{5}}\right),$$

$$a_{21}^{(2)}(c_{2}) = \frac{c_{2}^{4}(10c_{1}^{2} - 6c_{1}c_{2} + c_{2}^{2})}{10(c_{1} - c_{2})^{4}},$$

$$a_{22}^{(2)}(c_{2}) = -\frac{c_{2}^{2}(5c_{1}^{4} - 20c_{1}^{3}c_{2} + 15c_{1}^{2}c_{2}^{2} - 6c_{1}c_{2}^{3} + c_{2}^{4})}{10(c_{1} - c_{2})^{4}},$$

$$a_{21}^{(3)}(c_{2}) = \frac{c_{2}^{4}(15c_{1}^{2} - 6c_{1}c_{2} + c_{2}^{2})}{120(-c_{1} + c_{2})^{3}}, a_{22}^{(3)}(c_{2}) = \frac{c_{2}^{3}(-20c_{1}^{3} + 15c_{1}^{2}c_{2} - 6c_{1}c_{2}^{2} + c_{2}^{3})}{120(-c_{1} + c_{2})^{3}}.$$
(9)

Setting $c_1 = \frac{1}{4}$, $c_2 = 1$ and t = 1 in (9) yields

$$Y_{1} = \frac{h^{3}}{384} F_{1}'' - \frac{h^{2}}{32} F_{1}' + \frac{h}{4} F_{1} + y^{[n-1]}, \quad p = 3,$$
(10)

$$y^{[n]} = h^3 \left(\frac{7}{810}F_1'' + \frac{1}{405}F_2''\right) + h^2 \left(\frac{16}{405}F_1' - \frac{37}{810}F_2'\right) + h \left(\frac{160}{243}F_1 + \frac{83}{243}F_2\right) + y^{[n-1]}, \quad p = 6. (11)$$

The matrix form in (3) of (10) and (11) is now.

The matrix form in (3) of (10) and (11) is now

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$$A_{1} = \begin{pmatrix} \frac{1}{4} & 0\\ \frac{160}{243} & \frac{83}{243} \end{pmatrix}, A_{2} = \begin{pmatrix} -\frac{1}{32} & 0\\ \frac{16}{405} & -\frac{37}{810} \end{pmatrix}, A_{3} = \begin{pmatrix} \frac{7}{810} & 0\\ \frac{7}{810} & \frac{1}{405} \end{pmatrix},$$
(12)
$$\begin{bmatrix} \frac{1}{4} & 1 \end{bmatrix}^{T}, B_{1} = \begin{pmatrix} \frac{160}{243} & \frac{83}{243} \end{pmatrix}, B_{2} = \begin{pmatrix} \frac{16}{405} & -\frac{37}{810} \end{pmatrix}, B_{3} = \begin{pmatrix} \frac{7}{810} & \frac{1}{405} \end{pmatrix},$$
(12)
$$Y = (Y, Y)^{T}, F = (F, F)^{T}, F' = (F', F')^{T}, F'' = (F'', F'')^{T}$$

 $U = \begin{pmatrix} 1 & 1 \end{pmatrix}, V = 1, Y = \begin{pmatrix} Y_1, Y_2 \end{pmatrix}^T, F = \begin{pmatrix} F_1, F_2 \end{pmatrix}^T, F' = \begin{pmatrix} F_1', F_2' \end{pmatrix}^T, F'' = \begin{pmatrix} F_1'', F_2'' \end{pmatrix}^T$. The stability function of the TDGLM (12) is

Third derivative GLM for stiff problems Okuonghae and Ikhile J of NAMP $\psi(z) = \frac{933120 + 381120 z + 66024 z^2 + 5634 z^3}{933120 - 552000 z + 151464z^2 - 25350 z^3 + 2738 z^4 - 183z^5 + 6 z^6}.$

The method (12) is $A(86^{\circ})$ -stable as seen from Fig. 2.



Fig. 2: The stability region of the GLM (12).

$$\begin{cases} Y_{1} = h^{3} a_{11}^{(3)}(c_{1})F_{1}'' + h^{2} a_{11}^{(2)}(c_{1})F_{1}' + h a_{11}^{(1)}(c_{1})F_{1} + u_{11}(c_{1})y^{[n-1]}, \\ Y_{2} = h^{3} \left(a_{21}^{(3)}(c_{2})F_{1}'' + a_{22}^{(3)}(c_{2})F_{2}''\right) + h^{2} \left(a_{21}^{(2)}(c_{2})F_{1}' + a_{22}^{(2)}(c_{2})F_{2}'\right) \\ + h \left(a_{21}^{(1)}(c_{2})F_{1} + b_{22}^{(1)}(c_{2})F_{2}\right) + u_{21}(c_{2})y^{[n-1]}, \\ y^{[n]} = h^{3} \left(b_{11}^{(3)}(t)F_{1}'' + b_{12}^{(3)}(t)F_{2}'' + b_{13}^{(3)}(t)F_{3}''\right) \\ + h^{2} \left(b_{11}^{(2)}(t)F_{1}' + b_{12}^{(2)}(t)F_{2}' + b_{13}^{(2)}(t)F_{3}'\right) \\ + h \left(b_{11}^{(1)}(t)F_{1} + b_{12}^{(1)}(t)F_{2} + b_{13}^{(1)}(t)F_{3}\right) + v_{11}(t)y^{[n-1]}, \end{cases}$$
(13)

Note that :

$$\left[Y_1 = y(x_{n-1} + c_1 h), \quad Y_2 = y(x_{n-1} + c_2 h), \quad y^{[n]} = Y_3 = y(x_{n-1} + th), \quad c_3 = t = 1.$$

$$a_{11}^{(1)}(c_{1}) = c_{1}, \ a_{11}^{(2)}(c_{1}) = -\frac{c_{1}^{2}}{2}, \ a_{11}^{(3)}(c_{1}) = \frac{c_{1}^{3}}{6}, \ u_{11}(c_{1}) = 1,$$

$$a_{21}^{(1)}(c_{2}) = \frac{c_{2}^{4}(5c_{1}^{2} - 4c_{1}c_{2} + c_{2}^{2})}{2(-c_{1} + c_{2})^{5}},$$

$$a_{22}^{(1)}(c_{2}) = \frac{1}{2}c_{2}\left(1 + \frac{c_{1}(c_{1}^{4} - 5c_{1}^{3}c_{2} + 10c_{1}^{2}c_{2}^{2} - 5c_{1}c_{2}^{3} + c_{2}^{4})}{(c_{1} - c_{2})^{5}}\right), (14)$$

$$a_{21}^{(2)}(c_{2}) = \frac{c_{2}^{4}(10c_{1}^{2} - 6c_{1}c_{2} + c_{2}^{2})}{10(c_{1} - c_{2})^{4}},$$

$$a_{22}^{(2)}(c_{2}) = -\frac{c_{2}^{2}(5c_{1}^{4} - 20c_{1}^{3}c_{2} + 15c_{1}^{2}c_{2}^{2} - 6c_{1}c_{2}^{3} + c_{2}^{4})}{10(c_{1} - c_{2})^{4}},$$

$$A_{3} = \begin{pmatrix} \frac{1}{20250} & 0 & 0\\ \frac{110}{59049} & \frac{106}{59049} & 0\\ \frac{59875}{74680704} & \frac{389}{34020} & \frac{-5311}{4609920} \end{pmatrix}, B_{1} = \begin{pmatrix} \frac{3345709375}{10978063488} & \frac{616}{729} & \frac{-2255191}{15059072} \end{pmatrix},$$

$$B_{2} = \begin{pmatrix} \frac{10061875}{522764928} & \frac{179}{9720} & \frac{305989}{10756480} \end{pmatrix}, B_{3} = \begin{pmatrix} \frac{59875}{74680704} & \frac{389}{34020} & \frac{-5311}{4609920} \end{pmatrix}, c = \begin{pmatrix} \frac{1}{15} & \frac{2}{3} & 1 \end{pmatrix}^{T},$$

$$U = \begin{pmatrix} 1 & 1 & 1 \end{pmatrix}, V = 1, Y = \begin{pmatrix} Y_{1}, Y_{2}, Y_{3} \end{pmatrix}^{T}, F = \begin{pmatrix} F_{1}, F_{2}, F_{3} \end{pmatrix}^{T}, F' = \begin{pmatrix} F_{1}', F_{2}', F_{3}' \end{pmatrix}^{T}$$
 and $F'' = \begin{pmatrix} F_{1}'', F_{2}'', F_{3}'' \end{pmatrix}^{T}.$
The stability function of (18) is $\Pi(w, z) = \frac{N(z)}{\Omega(z)}$;
$$N(z) = 810304588628640000 + 634751998657692750z + 209198268924273450z^{2} + 39332184113473290z^{3} + 4658412195637140z^{4} + 352149979888728z^{5} + 15708183177708z^{6},$$

$$\Omega(z) = 810304588628640000 - 175552589970947250z - 2040143541909300z^{2} + 12459149746606215z^{3} - 2103946039121550z^{4} + 188710140596658z^{5} \end{pmatrix}$$

1

 $-10148408580315z^6 + 343705900366z^7 - 7424096106z^8 + 82756002z^9.$

The method is $A(50^{\circ})$ -stable, in Fig. 3.



Fig. 3: The stability region of the GLM (18).

3.0 **Implementation of the methods**

To demonstrate the application of the methods apply the TDGLM in (12) to the following IVPs: Problem 1:Linear Problem [1]

$$\begin{cases} y_1' = -8y_1 + 7y_2, & y(0) = 1, & y_1(x) = 2e^{-x} - e^{-50x}, \\ y_2' = 42y_1 - 43y_2, & y(0) = 8, & y_2(x) = 2e^{-x} + 6e^{-50x}, \\ x \in [0, 10]. \end{cases}$$

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Problem 2:Non-linear problem [8]

$$\begin{cases} y_1' = -10004y_1 + 10000y_2^4, & y_1(0) = 1, & y_1(x) = e^{-4x}, \\ y_2' = y_1 - y_2(1 + y_2^3), & y_2(0) = 1, & y_2(x) = e^{-x}, \\ x \in [0, 10]. \end{cases}$$

Find in Tables 1, 2 the numerical results.

Table 1:	Results	for	Problem	1	for	comparison
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x	TDGLM error	Ode15serror
2.0	1.58e - 09	6.78e - 05
4.0	4.28e - 10	1.28e - 04
6.0	8.69e - 11	1.41e - 05
8.0	1.56e - 11	3.52e -07
10.0	2.65e-12	1.51e -07

Table 2:	Results	for Prob	olem 2 for	comparison
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x	TDGLM error	Ode15s error
2.0	2.27e - 11	1.39e - 07
4.0	2.14e - 10	2.50e - 05
6.0	4.34e - 11	6.13e - 06
8.0	7.84 e - 12	6.75e -07
10.0	1.32 e - 12	7.85e -08

It is to be noted that the numerical results in Tables 1, 2 show that the TDGLM (12) outperformed the state of the art Ode15s Matlab code considered in [8] on problems 1, 2. This accuracy is as a result of high order of the TDGLM processes arising from the addition of the third derivative terms in their GLM. In fact, multi-derivative GLM are of recent introduction in [1] to which the methods therein are of a special case. The methods are with RK stability properties suitable for stiff problems.

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