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Original Research Article

A family of Nested General Linear Methods for solving Ordinary Differential Equations

Abstract

General linear methods (GLMs) was introduced as a generalization of Runge–Kutta methods (RKMs) and linear multistep methods (LMMs). The discovery of general linear method gave insight into the discovery of new methods that are neither RKMs or LMMs. Here, new classes of GLMs that are nested in their stages and mono-implicit in the output are presented, these methods are referred to as nested general linear methods (NGLMs). Procedures for deriving members that are algebraically stable are discussed herein and algebraically stable NGLMs have been derived up to order $p = 5$. Implementation procedure of these nested general linear methods which include the solution of non-linear systems of equations by simplified Newton iterations and step size changing strategy are discussed. The order $p = 3$ NGLM has been implemented on two test problems by variable step size, and the results compared with the results of MATLAB ode15s and RADAU IIA.
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1 Introduction

This paper focuses on the numerical solution of ordinary differential equations (ODEs) in its non-autonomous general form

$$f(x, y(x)) = 0; \qquad y, f \in \mathbb{R}^m, \tag{1.1}$$

where f and y have same dimensions and f is assumed to be sufficiently differentiable. Here, the numerical solution of (1.1) is obtained by the general linear method (GLM) of the form

$$\begin{aligned} Y_i^{[n]} &= h\sum_{j=1}^{s} a_{ij} f(Y_j) + \sum_{j=1}^{r} u_{ij} y_j^{[n-1]}, \quad i = 1, 2, ..., s, \\ y_i^{[n]} &= h\sum_{j=1}^{s} b_{ij} f(Y_j) + \sum_{j=1}^{r} v_{ij} y_j^{[n-1]}, \quad i = 1, 2, ..., r, \end{aligned} \tag{1.2}$$

where h is the step size, $Y_i^{[n]}$ is an approximation of the stages $y(x_n + c_i h)$, for $i = 1, 2, ...s$, having stage order q, i.e.

$$Y_i^{[n]} = y(x_n + c_i h) + O(h^{q+1}),\ i = 1, 2, ..., s,$$

and $y_i^{[n]}$ is the output approximation of order p satisfying

$$y_i^{[n]} = \sum_{j=0}^{p} \alpha_{ij} h^j y^{(j)}(x_{n+1}) + O(h^{p+1}),\ i = 1, 2, ..., r,$$

with real constants α_{ij}. The GLM (1.2) in matrix form is

$$\left[\begin{array}{c} Y \\ \hline y^{[n]} \end{array}\right] = \left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] \left[\begin{array}{c} hF \\ \hline y^{[n-1]} \end{array}\right], \tag{1.3}$$

where the matrices A, U, B and V are the matrices defining the constant coefficients a_{ij}, u_{ij}, b_{ij} and v_{ij} respectively.

Physical problems arising in many applications, circuit analysis, singular perturbation, control theories and chemical process simulations are modelled as ODEs [5, 6, 16]. Several numerical methods have been developed and implemented for solving several type of ODEs. Some of these methods include the backward difference formulae of [4, 6, 15, 17, 37], implicit Runge - Kutta methods of [6, 16, 18], General linear methods of [12, 21, 35, 36, 39, 40, 42], hybrid methods of [22, 29, 30, 31, 32, 33, 34, 38, 41], block methods of [2, 3, 5, 7, 8, 28, 38], boundary value methods of [2, 3, 7, 8], among others.
ODEs having rapidly and slowly decaying transients in their solution are regarded as stiff ODEs [18, 35]. Thus, it is appropriate to solve stiff ODEs with numerical methods having reasonably wide region of stability. A-stability property of numerical methods introduced by Dahlquist in [13] are methods possessing unbounded region of absolute stability, thus making A-stable methods a good option for solving stiff ODEs. However, as it was discussed in [9], the concept of A-stability suffers from two draw backs; first, it is difficult to determine if a method satisfies this property for non-linear problems, and secondly, A-stability does not give concise details of the behaviour of the method when applied to problems that are either non-autonomous or non-linear or both, in other to circumvent these two draw backs, the stability of non-linear problems when linear multistep methods (LMMs) are applied was studied in [14] and the idea gave rise to ***G-stability***, while [10] used the same concept in the case of Runge - Kutta methods (RKMs), which also gave rise to ***B-stability***. In the same spirit, [9] included non-autonomous problems following the approach of [14] and [10] and the concept of ***algebraic stability*** was introduced. Here in, we present general linear methods (GLMs) that are nested in their stages, mono-implicit in the output and possessing algebraic stability property. Two questions were raised in [20] regarding GLMs with algebraic stability; first, how can algebraically stable GLMs be constructed? Secondly, given a GLM, is it algebraically stable? The second question was partly addressed by [20] where the procedures of how the G-matrix for an algebraically stable GLM can be found using a control technique leading to a generalized eigen-problem. As an example, [20] obtained the G-matrix of the algebraically stable second order backward difference formulae written as GLM (1.2) having the form

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] = \left[\begin{array}{c|cc} \frac{2}{3} & 0 & 1 \\ \hline -\frac{2}{9} & 0 & -\frac{1}{3} \\ \frac{8}{9} & 1 & \frac{4}{3} \end{array}\right]$$

the G-matrix is given by

$$G = 9\begin{bmatrix} \frac{5}{2} & 1 \\ 1 & \frac{1}{2} \end{bmatrix}$$

For the first question raised by [20], several authors have been able to propose conditions for constructing algebraically stable GLMs, some of which includes a class of multistep Runge - Kutta methods of order $p = 2s$ presented by [9], a special class of GLMs called diagonally implicit multistage integration methods (DIMSIMs). [19] constructed such methods with 2-stages up to a total order of $p = 4$. [23] investigated the algebraic stability of GLMs and acknowledge that it is difficult to satisfy exactly conditions for algebraic stability, especially for high order methods, thus introduced the weaker algebraically stable methods named ***ϵ-algebraic stability***. Such methods up to order $p = q = s = r = 4$ have been constructed there in. In the same spirit, we construct algebraically stable GLMs up to order $p = s = r = 5$.

2 Nested General Linear Methods

Consider the GLM (1.2) for the numerical integration of (1.1) written in compact form (1.3), we assume the order p of the GLM equals the number of stages s, and s equals the number r of output approximations, (that is, $p = s = r$), the stage order $q = p - 1$ and the coefficient matrix A, U, B, V have the form

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] =$$

$$\left[\begin{array}{cccccccc|cccccc}
a_{11} & 0 & 0 & 0 & \cdots & 0 & 0 & a_{1s} & 1 & u_{12} & u_{13} & \cdots & u_{1s} \\
a_{21} & a_{22} & 0 & 0 & \cdots & 0 & 0 & a_{2s} & 1 & u_{22} & u_{23} & \cdots & u_{2s} \\
0 & a_{32} & a_{33} & 0 & \cdots & 0 & 0 & a_{3s} & 1 & u_{32} & u_{33} & \cdots & u_{3s} \\
0 & 0 & a_{43} & a_{44} & \ddots & 0 & 0 & a_{4s} & 1 & u_{42} & u_{43} & \cdots & u_{4s} \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & 0 & \cdots & a_{(s-1)(s-2)} & a_{(s-1)(s-1)} & a_{(s-1)s} & 1 & u_{(s-1)2} & u_{(s-1)3} & \cdots & u_{(s-1)s} \\
0 & 0 & 0 & 0 & \cdots & 0 & a_{s(s-1)} & a_{ss} & 1 & u_{s2} & u_{s3} & \cdots & u_{ss} \\
\hline
b_{11} & b_{12} & b_{13} & b_{14} & \cdots & b_{1(s-2)} & b_{1(s-1)} & b_{1s} & 1 & 0 & 0 & \cdots & 0 \\
0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & 0 & \cdots & 0 \\
b_{31} & b_{32} & b_{33} & b_{34} & \cdots & b_{3(s-2)} & b_{3(s-1)} & b_{3s} & 0 & 0 & 0 & \cdots & 0 \\
b_{41} & b_{42} & b_{43} & b_{44} & \cdots & b_{4(s-2)} & b_{4(s-1)} & b_{4s} & 0 & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
b_{s1} & b_{s2} & b_{s3} & b_{s4} & \cdots & b_{s(s-2)} & b_{s(s-1)} & b_{ss} & 0 & 0 & 0 & \cdots & 0
\end{array}\right], \tag{2.1}$$

where,

$$Y = \begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \\ \vdots \\ Y_s \end{bmatrix}; \quad F = \begin{bmatrix} f(Y_1) \\ f(Y_2) \\ f(Y_3) \\ \vdots \\ f(Y_s) \end{bmatrix}; \quad y^{[n]} = \begin{bmatrix} y_1^{[n]} \\ y_2^{[n]} \\ y_3^{[n]} \\ \vdots \\ y_{p+1}^{[n]} \end{bmatrix} = \begin{bmatrix} y_{n+1} \\ hy'_{n+1} \\ h^2 y''_{n+1} \\ \vdots \\ h^p y_{n+1}^{(p)} \end{bmatrix} \approx \begin{bmatrix} y(x_{n+1}) \\ hy'(x_{n+1}) \\ h^2 y''(x_{n+1}) \\ \vdots \\ h^p y^{(p)}(x_{n+1}) \end{bmatrix}.$$

GLMs having the representation of matrix A in the form (2.1) are referred to as nested general linear methods (NGLMs) [35, 36]. It is assumed that the last stage $Y_s^{[n]}$ equals the output $y_1^{[n]}$, thus the abscissa c_s is chosen to be $c_s = 1$.

2.1 Order Conditions of NGLM (2.1)

The NGLM (2.1) is preconsistent if there exist a preconsistency vector $\rho \in \mathbb{R}^r$ such that

$$\begin{aligned} U\rho &= e, \\ V\rho &= \rho, \end{aligned} \tag{2.2}$$

where $e = [1, 1, ...1, 1]^T \in \mathbb{R}^r$.

Lemma 2.1. *For the given NGLM (2.1), the preconsistency vector ρ is given as*

$$\rho = [1, 0, 0, ..., 0]^T \in \mathbb{R}^r. \tag{2.3}$$

For the NGLM (2.1), using the relation (2.2) the proof to Lemma 2.1 is trivial.

Theorem 2.2. *The NGLM (2.1) has stage order q and output order p if and only if*

$$\begin{aligned} e^{cz} &= zAe^{cz} + Uw + O(z^{q+1}), \\ e^z w &= zBe^{cz} + Vw + O(z^{p+1}), \end{aligned} \tag{2.4}$$

where, $e^{cz} = [e^{c_1 z}, e^{c_2 z}, ..., e^{c_s z}]$ and

$$w = \sum_{j=0}^{p} \omega_{jm} z^m; \quad j = 1, 2, \cdots, r.$$

Proof. The stage value $Y_i^{[n]}$ defined in (2.1) is an approximation to the solution $y(x_n + c_i h)$, satisfying

$$\begin{aligned} Y_i^{[n]} &= y(x_n + c_i h) + O(h^{q+1}) \\ &= \sum_{m=0}^{q} \frac{c_i^m}{m!} y^{(m)}(x_n) h^m + O(h^{q+1}), \end{aligned}$$

then,

$$\begin{aligned} hf(Y_i^{[n]}) &= hy'(x_n + c_i h) + O(h^{q+2}) \\ &= \sum_{m=1}^{q+1} \frac{c_i^{m-1}}{(m-1)!} y^{(m)}(x_n) h^m + O(h^{q+2}) \\ &= \sum_{m=1}^{q} \frac{c_i^{m-1}}{(m-1)!} y^{(m)}(x_n) h^m + O(h^{q+1}). \end{aligned}$$

Also, the Taylor series expansion of the first step in the output method can be written in the form

$$y_i^{[1]} = \sum_{m=0}^{p} \left(\sum_{l=0}^{m} \frac{1}{l!} \omega_{i,m-l} \right) y^{(m)}(x_n) h^m + O(h^{p+1}).$$

Thus, (2.1) can be expressed as

$$\begin{aligned} \sum_{m=0}^{q} \left(c_i^m - \sum_{j=1}^{s} m a_{ij} c_j^{m-1} - m! \sum_{j=1}^{r} u_{ij} \omega_{jm} \right) \frac{h^m}{m!} y^{(m)}(x_n) = O(h^{q+1}), \\ \sum_{m=0}^{p} \left(\sum_{l=0}^{m} \frac{1}{l!} \omega_{i,m-l} - \sum_{j=1}^{s} m b_{ij} c_j^{m-1} - m! \sum_{j=1}^{r} v_{ij} \omega_{jm} \right) \frac{h^m}{m!} y^{(m)}(x_n) = O(h^{p+1}). \end{aligned} \tag{2.5}$$

Equating the coefficients of $\frac{h^m}{m!} y^{(m)}(x_n)$ in (2.5) to zero, and multiplying these coefficients by $\frac{z^m}{m!}$ gives

$$\begin{aligned} e^{c_i z} - z \sum_{i=1}^{s} a_{ij} e^{c_i z} - \sum_{i=1}^{r} u_{ij} w_j = O(z^{q+1}) \quad i = 1, 2, ..., s, \\ e^z w_i - z \sum_{i=1}^{s} b_{ij} e^{c_i z} - \sum_{i=1}^{r} v_{ij} w_j = O(z^{p+1}) \quad i = 1, 2, ..., r, \end{aligned} \tag{2.6}$$

Hence, obtaining (2.4) respectively. □

2.2 Conditions for Algebraic Stability

Algebraic stability of GLM has been considered in [9, 11, 25, 26, 27]. The same concept has been used in investigating the algebraic stability of NGLM in this paper. Algebraic stability of NGLMs (2.1) is defined as follows

Definition 2.3. The NGLM is algebraically stable if there exist a real, symmetric, and positive definite matrix $G \in \mathbb{R}^{r \times r}$ and a real, diagonal and positive definite matrix $D \in \mathbb{R}^{s \times s}$, such that the matrix M defined by

$$M = \left[\begin{array}{c|c} DA + A^T D - B^T GB & DU - B^T GV \\ \hline U^T D - V^T GB & G - V^T GV \end{array} \right] \tag{2.7}$$

is non-negative definite.

Here, $M \geq 0$ denotes that M is non-negative definite, and $G > 0$, $D > 0$ denote that G and D are positive definite respectively. The matrices G and D are related by the equation [9]

$$D = diag \left(B^T G \rho \right). \tag{2.8}$$

3 Construction of Algebraically Stable NGLM

For the NGLM (2.1), define a positive definite matrix $G \in \mathbb{R}^{r\times r}$ and sub-vectors $u, v \in \mathbb{R}^{rN}$, where $u = u_1, u_2, \cdots, u_r \in \mathbb{R}^N$ and $v = v_1, v_2, \cdots, v_r \in \mathbb{R}^N$, define also an inner product $\langle \cdot,\cdot\rangle_G$ and the corresponding semi-norm $\| \cdot \|_G$ as in [11],

$$\langle u, v\rangle_G = \sum_{i=1}^{r}\sum_{j=1}^{r} g_{ij} \langle u_i, v_j\rangle_G ,$$

with an induced norm,

$$\| u \|_G^2 = \langle u, u\rangle_G .$$

The NGLM (2.1) is monotonic if

$$\| y^{[n]} \|_G \leq \| y^{[n-1]} \|_G, \quad n = 1, 2, ...$$

For the stage values Y, stage derivatives F, the input $y^{[n-1]}$ and output $y^{[n]}$ respectively, the NGLM (2.1) is algebraically stable if it satisfies definition 2.3, then

$$\begin{aligned}\| y^{[n]} \|_G^2 - \| y^{[n-1]} \|_G^2 &= 2 \langle Y, hF(Y)\rangle_D - \| hF(Y) \oplus y^{[n-1]} \|_M^2 \\ &= 2\sum_{i=1}^{s} d_i \langle Y_i, hF(Y_i)\rangle - \sum_{i=1}^{r+s}\sum_{j=1}^{r+s} m_{ij} \langle \alpha_i, \alpha_j\rangle ,\end{aligned}$$

where d_i are the diagonal elements of the matrix D defined in (2.8), m_{ij} are the elements of the matrix M defined in (2.7) and the vector $\alpha \in \mathbb{R}^{m(r+s)}$ is defined as

$$\alpha = \left[(y_1^{[n-1]})^T, (y_2^{[n-1]})^T, \cdots (y_r^{[n-1]})^T, hF(Y_1)^T hF(Y_2)^T, \cdots hF(Y_s)^T, \right]^T .$$

Constructing algebraically sable GLM is highly tasking [23]. The approach used by [19] and [23] have been used in constructing NGLMs that are algebraically stable. [19] demonstrated a simplified approach based on Albert theorem [1] by taking the partitioned matrix M defined in (2.7) as

$$M = \left[\begin{array}{c|c} M_{11} & M_{12} \\ \hline M_{12}^T & M_{22}\end{array}\right]. \tag{3.1}$$

By results in [1], $M \geq 0$ if and only if

$$M_{11} \geq 0, \quad M_{22} - M_{12}^T M_{11}^+ M_{12} \geq 0, \quad M_{11} M_{11}^+ M_{12} = M_{12}, \tag{3.2}$$

or

$$M_{22} \geq 0, \quad M_{11} - M_{12} M_{22}^+ M_{12}^T \geq 0, \quad M_{22} M_{22}^+ M_{12}^T = M_{12}^T, \tag{3.3}$$

where M^+ stands for the Moore - Penrose pseudo-inverse of the matrix M. Thus, the problem of checking the non-negative definiteness of the matrix M defined in (2.7) is made simpler by using either (3.2) or (3.3). Just as in [19, 23], we assume $G = I$ (where I is the identity matrix $I \in \mathbb{R}^{r\times r}$), so that if $M_{22} \geq 0$, $M_{22} M_{22}^+ M_{12}^T = M_{12}^T$ and $R = 0$, where

$$R = M_{11} - M_{12} M_{22}^+ M_{12}^T, \tag{3.2a}$$

then $M \geq 0$ is achieved.

Lemma 3.1. *For the given matrix V in the NGLM (2.1) and $G = I$, then for order $p = s = r$, then $M_{22} \geq 0$.*

Proof. By definition, $M_{22} = G - V^T G V$ in (2.7), then if the matrix $G = I$, and V is as defined in (2.1)

$$M_{22} = I - V^T V.$$

It can be verified that M_{22} has the form

$$M_{22} = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 1 \end{bmatrix},$$

whose eigenvalues are 1 ($p-1$ times) and 0. Thus, $M_{22} \geq 0$. □

Also, the condition $M_{22}M_{22}^{+}M_{12}^{T} = M_{12}^{T}$ is true for the NGLM (2.1), thus, we are only faced with enforcing the condition $R = M_{11} - M_{12}M_{22}^{+}M_{12}^{T} = 0$.

Lemma 3.2. *For $G = I$ and for ρ defined in (2.3), then for order $p = s = r$ in NGLM (2.1), the matrix D is defined as*

$$D = diag\,(b_{11}, b_{12}, ..., b_{1s})\,. \tag{3.4}$$

Proof. Substituting $G = I$ and $\rho = [1, 0, 0, ..., 0]^T \in \mathbb{R}^r$ into (2.8), gives

$$D = diag(B^T G\rho) = diag\left(\begin{bmatrix} b_{11} & 0 & b_{31} & \cdots & b_{s1} \\ b_{12} & 0 & b_{32} & \cdots & b_{s2} \\ b_{13} & 0 & b_{33} & \cdots & b_{s3} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ b_{1s} & 1 & b_{3s} & \cdots & b_{ss} \end{bmatrix}\begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}\right).$$

Hence, yielding the result (3.4). □

For $G = I$, the matrix M simplifies into

$$M = \left[\begin{array}{c|c} DA + A^T D - B^T B & DU - B^T V \\ \hline U^T D - V^T B & I - V^T V \end{array}\right]. \tag{3.5}$$

Thus, the following algorithm (compare [19, 23]) is used to derive algebraically stable NGLMs:

(i) Choose the matrix $G = I$.

(ii) Ensure that $D = diag\,(b_{11}, b_{12}, ..., b_{1s}) > 0$.

(iii) Enforce the condition $R = 0$.

We give examples of algebraically stable NGLMs of stage order $q = p - 1$ and output order $p = s = r$.

3.1 Examples of Methods

Here, we combine both the order conditions (2.4) and the algorithmic steps above to achieve the desired stability (algebraic stability) of the NGLMs to be constructed.
Methods with p=s=r=2
The structure A, U, B, V for the second order method is given by

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] = \left[\begin{array}{cc|cc} a_{11} & a_{12} & 1 & u_{12} \\ a_{21} & a_{22} & 1 & u_{22} \\ \hline b_{11} & b_{12} & 1 & 0 \\ 0 & 1 & 0 & 0 \end{array}\right] \tag{3.6}$$

Solving the stage order conditions with $q = 1$ and output order conditions with $p = 2$, then the following system of equation is obtained,

$$\begin{aligned} a_{11} + a_{12} + u_{12} = c_1,\ a_{21} + a_{22} + u_{22} = c_2, \\ b_{11} + b_{12} = 1,\ b_{11}c_1 + b_{12}c_2 = \frac{1}{2}. \end{aligned} \tag{3.7}$$

Solving (3.7) to obtain u_{12}, u_{22}, b_{11} and b_{12} yields

$$u_{12} = -a_{11} - a_{12} + c_1,\ u_{22} = -a_{21} - a_{22} + c_2,\ b_{11} = -\frac{2c_2 - 1}{2(c_1 - c_2)},\ b_{12} = -\frac{1 - 2c_1}{2(c_1 - c_2)}. \tag{3.8}$$

Then D is expressed as

$$D = \begin{bmatrix} -\frac{2c_2-1}{2(c_1-c_2)} & 0 \\ 0 & -\frac{1-2c_1}{2(c_1-c_2)} \end{bmatrix}.$$

By definition, $c_2 = 1$, then matrix $D > 0$ if and only if $c_1 < \frac{1}{2}$. Therefore, choosing $c_1 = \frac{1}{4}$, matrix D becomes

$$D = \begin{bmatrix} \frac{2}{3} & 0 \\ 0 & \frac{1}{3} \end{bmatrix} > 0,$$

then

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] = \left[\begin{array}{cc|cc} a_{11} & a_{12} & 1 & \frac{1}{4} - a_{11} - a_{12} \\ a_{21} & a_{22} & 1 & 1 - a_{21} - a_{22} \\ \hline \frac{2}{3} & \frac{1}{3} & 1 & 0 \\ 0 & 1 & 0 & 0 \end{array}\right],$$

and computing the matrix M defined in (3.5), the matrices M_{11}, M_{12} and M_{22} yields

$$M_{11} = \begin{bmatrix} \frac{4a_{11}}{3} - \frac{4}{9} & \frac{2a_{12}}{3} + \frac{a_{21}}{3} - \frac{2}{9} \\ \frac{2a_{12}}{3} + \frac{a_{21}}{3} - \frac{2}{9} & \frac{2a_{22}}{3} - \frac{10}{9} \end{bmatrix},\ M_{12} = \begin{bmatrix} 0 & \frac{2}{3}\left(-a_{11} - a_{12} + \frac{1}{4}\right) \\ 0 & \frac{1}{3}\left(-a_{21} - a_{22} + 1\right) \end{bmatrix},\ M_{22} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}. \tag{3.9}$$

Then solve for R using (3.9) defined in (3.2a), gives

$$R = \begin{bmatrix} -\frac{4}{9}\rho_1^2 + \frac{4a_{11}}{3} - \frac{4}{9} & \frac{2a_{12}}{3} + \frac{a_{21}}{3} - \frac{2}{9}\rho_1\rho_2 - \frac{2}{9} \\ \frac{2a_{12}}{3} + \frac{a_{21}}{3} - \frac{2}{9}\rho_1\rho_2 - \frac{2}{9} & -\frac{1}{9}\rho_2^2 + \frac{2a_{22}}{3} - \frac{10}{9} \end{bmatrix},$$

where $\rho_1 = \frac{1}{4} - a_{11} - a_{12}$, $\rho_2 = 1 - a_{21} - a_{22}$. To ensure that $R = 0$, enforce that

$$-\frac{4}{9}\left(\frac{1}{4} - a_{11} - a_{12}\right)^2 + \frac{4a_{11}}{3} - \frac{4}{9} = 0, \qquad -\frac{1}{9}\left(1 - a_{21} - a_{22}\right)^2 + \frac{2a_{22}}{3} - \frac{10}{9} = 0,$$
$$\frac{2a_{12}}{3} + \frac{a_{21}}{3} - \frac{2}{9}\left(\frac{1}{4} - a_{11} - a_{12}\right)\left(1 - a_{21} - a_{22}\right) - \frac{2}{9} = 0.$$

In this, we have three system of equations with four unknowns, the Solve function of MATHEMATICA is used to obtain the possible solutions. The possible solutions obtained are

$$a_{11} = \frac{1}{3},\ a_{12} = -\frac{1}{12},\ a_{21} = \frac{5}{6},\ a_{22} = \frac{19}{6}, \tag{3.10}$$

and

$$a_{11} = \frac{10}{3},\ a_{12} = -\frac{1}{12},\ a_{21} = -\frac{31}{6},\ a_{22} = \frac{19}{6}. \tag{3.11}$$

Thus, choosing (3.10),

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] = \left[\begin{array}{cc|cc} \frac{1}{3} & -\frac{1}{12} & 1 & 0 \\ \frac{5}{6} & \frac{19}{6} & 1 & -3 \\ \hline \frac{2}{3} & \frac{1}{3} & 1 & 0 \\ 0 & 1 & 0 & 0 \end{array}\right]. \tag{3.12}$$

For this method (3.12),

$$M = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 \end{bmatrix} \geq 0,$$

which eigenvalues are $\{2, 0, 0, 0\}$. Also, choosing (3.11),

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] = \left[\begin{array}{cc|cc} \frac{10}{3} & -\frac{1}{12} & 1 & -3 \\ -\frac{31}{6} & \frac{19}{6} & 1 & 3 \\ \hline \frac{2}{3} & \frac{1}{3} & 1 & 0 \\ 0 & 1 & 0 & 0 \end{array}\right]. \tag{3.13}$$

For this method (3.13),

$$M = \begin{bmatrix} 4 & -2 & 0 & -2 \\ -2 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ -2 & 1 & 0 & 1 \end{bmatrix} \geq 0,$$

having eigenvalues $\{6, 0, 0, 0\}$. Hence, NGLM (3.12) and (3.13) are algebraically stable.

Methods with p=s=r=3

Using the order conditions (2.4) and applying the algorithm above obtaining an algebraically stable method, as in the procedures done in the previous example, we obtain a method of order $p = s = r = 3$ and $q = 2$, depending on $a_{11}, a_{13}, a_{21}, a_{22}, a_{23}, a_{32}, a_{33}, c_1, c_2, c_3$. Choosing $c_1 = \frac{1}{4}$, $c_2 = \frac{1}{2}$, $c_3 = 1$, matrix D is

$$D = \begin{bmatrix} \frac{4}{9} & 0 & 0 \\ 0 & \frac{1}{3} & 0 \\ 0 & 0 & \frac{2}{9} \end{bmatrix} > 0. \tag{3.14}$$

Following the same procedure of enforcing $R = 0$, the third order NGLM derived is given as

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] = \left[\begin{array}{ccc|ccc} \frac{1053}{128} & 0 & \frac{485}{24} & 1 & -\frac{1}{8} & \frac{1}{16} \\ -\frac{17119}{360} & \frac{32501}{600} & \frac{1}{4} & 1 & 0 & \frac{1}{10} \\ 0 & -\frac{3601}{40} & \frac{3953}{144} & 1 & \frac{3}{4} & \frac{1}{2} \\ \hline \frac{4}{9} & \frac{1}{3} & \frac{2}{9} & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ \frac{8}{3} & -6 & \frac{10}{3} & 0 & 0 & 0 \end{array}\right]. \tag{3.15}$$

For this method (3.15),

$$M = \begin{bmatrix} \frac{5}{1296} & \frac{1}{1080} & -\frac{1}{162} & 0 & -\frac{1}{18} & \frac{1}{36} \\ \frac{1}{1080} & \frac{1}{900} & \frac{1}{270} & 0 & 0 & \frac{1}{30} \\ -\frac{1}{162} & \frac{1}{270} & \frac{13}{324} & 0 & \frac{1}{6} & \frac{1}{9} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{18} & 0 & \frac{1}{6} & 0 & 1 & 0 \\ \frac{1}{36} & \frac{1}{30} & \frac{1}{9} & 0 & 0 & 1 \end{bmatrix} \geq 0,$$

and $\sigma(M) = \{1.04145, 1.00364, 0, 0, 0, 0\}$. Thus, the NGLM (3.15) is algebraically stable.

Methods with p=s=r=4

Using the order conditions (2.4) and algorithm for achieving algebraically stable method, we obtain a 24 parameter method of order $p = s = r = 4$ and $q = 3$ depending on $a_{11}, a_{14}, a_{21}, a_{22}, a_{24}, a_{32}, a_{33}, a_{34}, a_{43}, a_{44}, c_1, c_2, c_3, c_4$. With the choice of $c_1 = \frac{1}{4}$, $c_2 = -\frac{1}{2}$, $c_3 = \frac{3}{4}, c_4 = 1$, matrix D is defined as

$$D = \begin{bmatrix} \frac{14}{27} & 0 & 0 & 0 \\ 0 & \frac{1}{135} & 0 & 0 \\ 0 & 0 & \frac{2}{5} & 0 \\ 0 & 0 & 0 & \frac{2}{27} \end{bmatrix} > 0 \tag{3.16}$$

Enforcing the condition $R = 0$ yields the fourth order NGLM,

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] = \left[\begin{array}{cccc|cccc} \frac{20847238}{137781} & 0 & 0 & \frac{6769180}{15309} & 1 & \frac{5}{189} & 0 & 0 \\ -\frac{15830458}{6561} & \frac{301231781}{2187000} & 0 & -\frac{38504902}{10935} & 1 & \frac{2}{9} & -\frac{2}{9} & -\frac{1}{10} \\ 0 & \frac{70578197}{328050} & \frac{1310174319336689}{1458000} & \frac{17523569}{65610} & 1 & \frac{335151}{5} & \frac{11}{108} & \frac{14}{27} \\ 0 & 0 & \frac{1}{27} & \frac{20848249}{8748} & 1 & \frac{1}{3} & \frac{5}{9} & -\frac{4}{3} \\ \hline \frac{14}{27} & \frac{1}{135} & \frac{2}{5} & \frac{2}{27} & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ \frac{4}{3} & -\frac{2}{15} & -\frac{36}{5} & 6 & 0 & 0 & 0 & 0 \\ \frac{112}{9} & -\frac{64}{45} & -\frac{144}{5} & \frac{160}{9} & 0 & 0 & 0 & 0 \end{array}\right]. \tag{3.17}$$

For this method (3.17),

$$M = \begin{bmatrix} \frac{100}{531441} & \frac{4}{177147} & \frac{49652}{135} & \frac{20}{59049} & 0 & \frac{10}{729} & 0 & 0 \\ \frac{4}{177147} & \frac{881}{147622500} & \frac{36196127}{820125} & \frac{68}{1476225} & 0 & \frac{2}{1215} & -\frac{2}{1215} & -\frac{1}{1350} \\ \frac{49652}{135} & \frac{36196127}{820125} & \frac{1310172712912289}{1822500} & \frac{108585839}{164025} & 0 & \frac{670302}{25} & \frac{11}{270} & \frac{28}{135} \\ \frac{20}{59049} & \frac{68}{1476225} & \frac{108585839}{164025} & \frac{712}{59049} & 0 & \frac{2}{81} & \frac{10}{243} & -\frac{8}{81} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{10}{729} & \frac{2}{1215} & \frac{670302}{25} & \frac{2}{81} & 0 & 1 & 0 & 0 \\ 0 & -\frac{2}{1215} & \frac{11}{270} & \frac{10}{243} & 0 & 0 & 1 & 0 \\ 0 & -\frac{1}{1350} & \frac{28}{135} & -\frac{8}{81} & 0 & 0 & 0 & 1 \end{bmatrix} \geq 0,$$

and $\sigma(M) = \{7.18888 \times 10^8, 1.01145, 1, 0, 0, 0, 0, 0\}$. The NGLM (3.17) is thus algebraically stable.

Methods with p=s=r=5

In this case, we obtain a 40 parameter method of order $p = s = r = 5$ and $q = 4$ depending on $a_{11}, a_{15}, a_{21}, a_{22}, a_{25}, a_{32}, a_{33}, a_{35}, a_{43}, a_{44}, a_{45}, a_{54}, a_{55}, c_1, c_2, c_3, c_4, c_5$. With the choice of $c_1 = \frac{1}{5}$, $c_2 = -\frac{2}{5}$, $c_3 = \frac{3}{5}, c_4 = \frac{4}{5}, c_5 = 1$, the matrix D is thus given as

$$D = \begin{bmatrix} \frac{185}{432} & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{216} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{4} & 0 & 0 \\ 0 & 0 & 0 & \frac{55}{216} & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{16} \end{bmatrix} > 0. \tag{3.18}$$

Enforcing $R = 0$ yields the fifth order algebraically stable NGLM, having matrices A, U, B, V defined as,

$$A = \begin{bmatrix} 12968.1 & 0 & 0 & 0 & -47727.5 \\ -191346. & 7633.78 & 0 & 0 & 351130 \\ 0 & 11.869 & 3.83094 \times 10^{11} & 0 & 361412. \\ 0 & 0 & -9.10946 \times 10^{11} & 5.51555 \times 10^{11} & 0.000174758 \\ 0 & 0 & 0 & -1.76064 \times 10^6 & 307287. \end{bmatrix},$$

$$U = \begin{bmatrix} 1 & \frac{153}{592} & 0 & 0 & 0 \\ 1 & -\frac{1333217673}{700597936} & \frac{1}{432} & \frac{1}{2} & -\frac{1}{3528} \\ 1 & \frac{267848240}{153} & -\frac{1}{216} & \frac{19}{72} & \frac{9}{8} \\ 1 & -\frac{3502989680}{1683} & 0 & 0 & 0 \\ 1 & \frac{1}{64} & \frac{5}{216} & \frac{31}{64} & -\frac{5}{216} \end{bmatrix},$$

$$B = \begin{bmatrix} \frac{185}{432} & \frac{1}{216} & \frac{1}{4} & \frac{55}{216} & \frac{1}{16} \\ 0 & 0 & 0 & 0 & 1 \\ -\frac{35}{36} & \frac{4}{63} & 7 & -\frac{140}{9} & \frac{265}{28} \\ -\frac{575}{36} & \frac{10}{9} & \frac{195}{2} & -\frac{1250}{9} & \frac{225}{4} \\ -\frac{625}{6} & \frac{25}{3} & 450 & -\frac{1625}{3} & \frac{375}{2} \end{bmatrix},$$

$$V = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

For this method $\sigma(M) = \{4.72431 \times 10^{11}, 1.04965, 1.00089, 1, 0, 0, 0, 0, 0, 0\}$. Higher order algebraically stable NGLMs can be constructed following the approach discussed above.

4 Implementation and Numerical Experiment

There have been several procedures of implementing some classes of general linear methods in literature, some of which include: the implementation of DIMSIMs in [24], implementation of GLMs having inherent Runge-Kutta stability of [21, 24, 36, 42], just to mention a few. Here, we follow the ideas of these researchers mentioned. Since the NGLMs are implicit, the Newton's method used to resolve its implicitness. In the case of implementing the NGLMs, the procedure employed is to first predict the initial Nordsieck vectors $y^{[0]}$ and the last stage Y_s. The predicted value of the last stage Y_s is denoted as $\hat{Y}_s$. Solving the non-linear stiff ODE (1.1), the stages $Y_i,\ i = 1, 2, ..., s-1$ of the NGLM is computed using the iterative scheme

$$Y_i - ha_{ii}f(Y_i) = h\sum_{j=1}^{i-1} a_{ij}f(Y_i) + ha_{ss}f(\hat{Y}_s) + \sum_{j=1}^{r} u_{ij}y_j^{[n-1]}, \qquad i = 1, 2, ..., s-1. \tag{4.1}$$

The iterative scheme (4.1) is then used to improve the last stage $\hat{Y}_s$ by the scheme

$$Y_s - ha_{ss}f(Y_s) = h\sum_{j=1}^{s-1} a_{sj}f(Y_i) + \sum_{j=1}^{r} u_{sj}y_j^{[n-1]}. \tag{4.2}$$

In other to resolve the implicitness in (4.1), denote the right hand side of (4.1) as ϕ_i, (4.1) becomes

$$Y_i - ha_{ii}f(Y_i) = \phi_i, \qquad i = 1, 2, ..., s-1, \tag{4.3}$$

then (4.3) can be expressed as

$$\Gamma_i = Y_i - ha_{ii}f(Y_i) - \phi_i = 0, \qquad i = 1, 2, ..., s-1. \tag{4.3a}$$

Then the Newton's method for resolving the implicitness of (4.1) is defined as

$$Y_i^{[\zeta+1]} = Y_i^{[\zeta]} - J^{-1}\Gamma_i^{[\zeta]}, \qquad i = 1, 2, ..., s-1, \qquad \zeta = 0, 1, 2, ..., N, \tag{4.3b}$$

where ζ is the ζ-th Newton's iteration and J is the Jacobian of (4.3a) and defined as

$$J = I - ha_{ii}\frac{\partial f}{\partial y}(Y_i) \qquad i = 1, 2, ..., s-1.$$

Again, to resolve the implicitness of (4.2), denote the right hand side of (4.2) as ϕ_s, then (4.2) becomes

$$Y_s - ha_{ss}f(Y_s) = \phi_s, \tag{4.4}$$

we then express (4.4) as

$$\Gamma_s = Y_s - ha_{ss}f(Y_s) - \phi_s = 0. \tag{4.4a}$$

The Newton's iterative scheme for (4.2) is then defined as

$$Y_s^{[\zeta+1]} = Y_s^{[\zeta]} - \Delta^{-1}\Gamma_s^{[\zeta]}, \qquad \zeta = 0, 1, 2, ..., N, \tag{4.4b}$$

where Δ is the Jacobian of (4.4a). Equations (4.3a) and (4.4b) are repeated to obtain corrected solution to the stages $Y_i^{[N]},\ i = 1, 2, ..., s$.

The Newton's iterative process is repeated until

$$\| Y_i^{[\zeta+1]} - Y_i^{[\zeta]} \| < TOL; \quad \zeta = 0, 1, 2, ..., N.$$

The converged value $Y_i^{[N]}$ is now used for computing the output method $y^{[n]}$. Here, TOL is the supplied error tolerance in the stage approximations.

In variable step size implementation, the error control strategy used is computing the local truncation error using [36]

$$E_n = C_{p+1}h^{p+1}y^{(p+1)}(x_n) + O(h^{p+2}), \quad p \geq 1, \tag{4.5}$$

where C_{p+1} is the error constant of the method being used. Ignoring the terms of $O(h^{p+2})$ in (4.5), the error estimation is then expressed as

$$E_n \approx C_{p+1}h^{p+1}y^{(p+1)}(x_n), \quad p \geq 1. \tag{4.5a}$$

Define

$$h^{p+1}y^{(p+1)}(x_n) \approx h\left(d_1f(Y_1) + d_2f(Y_2) + \cdots + d_sf(Y_s)\right), \tag{4.6}$$

where $d_1, d_2, ..., d_s$ are coefficients obtained by expanding $f(Y_i)$ by Taylor's series about x_n, the local error estimate (4.5a) can now be defined as

$$E_n \approx C_{p+1}\left[d_1 hf(Y_1) + d_2 hf(Y_2) + \cdots + d_s hf(Y_s)\right]. \tag{4.7}$$

In this paper, the step size changing strategy used is defined as

$$h_{n+1} = \theta_n h_n, \tag{4.8}$$

where h_n is the stepsize at step n and h_{n+1} is the stepsize at the step $n+1$ (i.e. expected stepsize). The coefficient θ_n is obtained using

$$\theta_n = min\left(2, max\left(\hat{\theta_n}, \frac{1}{2}\right)\right); \qquad \hat{\theta_n} = \gamma\left(\frac{TOL}{\parallel E_n \parallel}\right)^{\frac{1}{p+1}}, \tag{4.9}$$

where γ is the safety factor chosen as $\gamma = 0.9$, and TOL is the supplied error tolerance.

The global error is computed using the equation

$$GE(h) = \parallel y(x) - y_h(x) \parallel_\infty,$$

where $y(x)$ and $y_h(x)$ is the exact and computed solution respectively.

We experiment by implementing the NGLMs on two stiff ODEs as test problems. Our results are also compared with the results obtained from the MATLAB ode15s (based on the backward differentiation formulae) and the algebraically stable RADAU IIA [18]. The following test problems have been considered.
Problem 1:

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} y'(x) + \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} y(x) = \begin{pmatrix} x^2 \\ 2x - e^x \end{pmatrix}, \qquad y(0) = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{4.10}$$

having exact solution

$$y(x) = \begin{pmatrix} e^x \\ x^2 - e^x \end{pmatrix}, \quad t \in [-0.5, 0.5].$$

Problem 2:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} y'(x) + \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} y(x) = \begin{pmatrix} \cos x \\ 0 \\ 0 \end{pmatrix}, \qquad y(0) = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \tag{4.11}$$

having exact solution

$$y(x) = \begin{pmatrix} 0 \\ 0 \\ \sin x \end{pmatrix}.$$

The third order nested general linear method with algebraic stability (NGLMAS), MATLAB ode15s, RADAU IIA were implemented on problems 1 and 2 with $x \in [0, 1]$. The results of the global error $\parallel e_h \parallel$ versus the number of function evaluations (nfe) for tolerances $TOL = 10^{-j}$, $j = 2(2)12$ are shown in figures 1 and 2 for problems 1 and 2 respectively. From the results, the NGLMAS (order $p = 3$) gives better accuracy in terms of global error than MATLAB ode15s and RADAU IIA for problems 1 and 2.

5 Conclusion

Developing numerical schemes for solving ODEs have gained popular interest among researchers due to the fact that real life problems are modelled as stiff ODEs. This paper is motivated to develop nested GLMs having non-linear stability (algebraic stability) for ODEs. Methods that are algebraically stable for orders $p = 2, 3, 4, 5$ have been derived. On implementation, the third order algebraically stable NGLM has been implemented on two test problems by variable step size, and the results compared with the results of MATLAB ode15s and RADAU IIA. The results from the algebraically stable NGLM has better accuracy than the MATLAB ode15s and RADAU IIA.
Future investigation would focus on the desire that the implementation of NGLMs are automated ODE solver using variable order - variable step size implementation. It is also desirable that these methods are extended to delay differential equations.

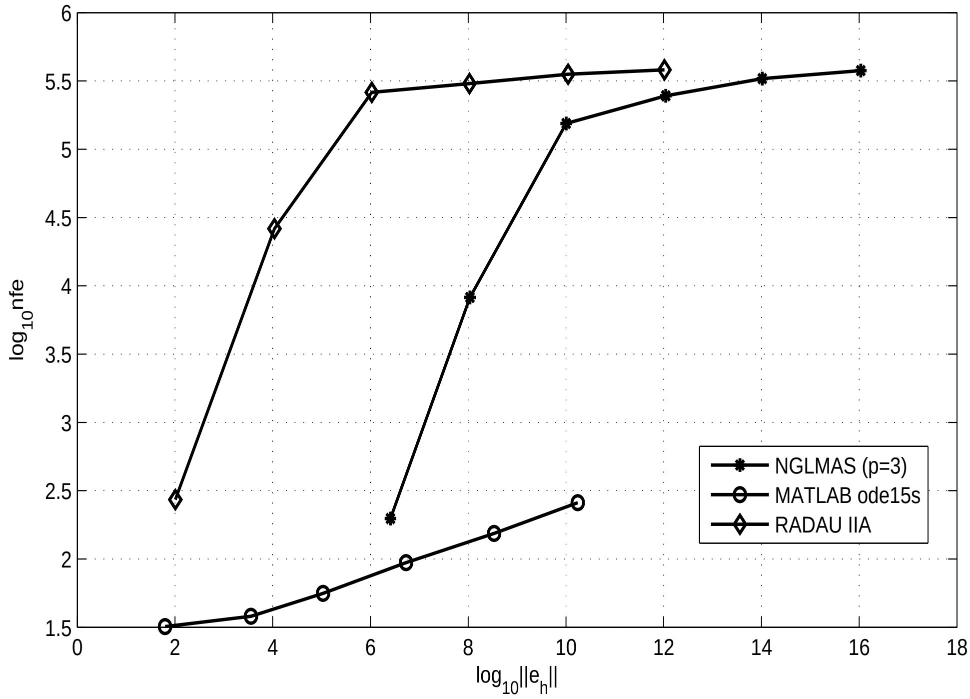

Figure 1: nfe versus $\| e_h \|$ at $x = 1$ for problem 1

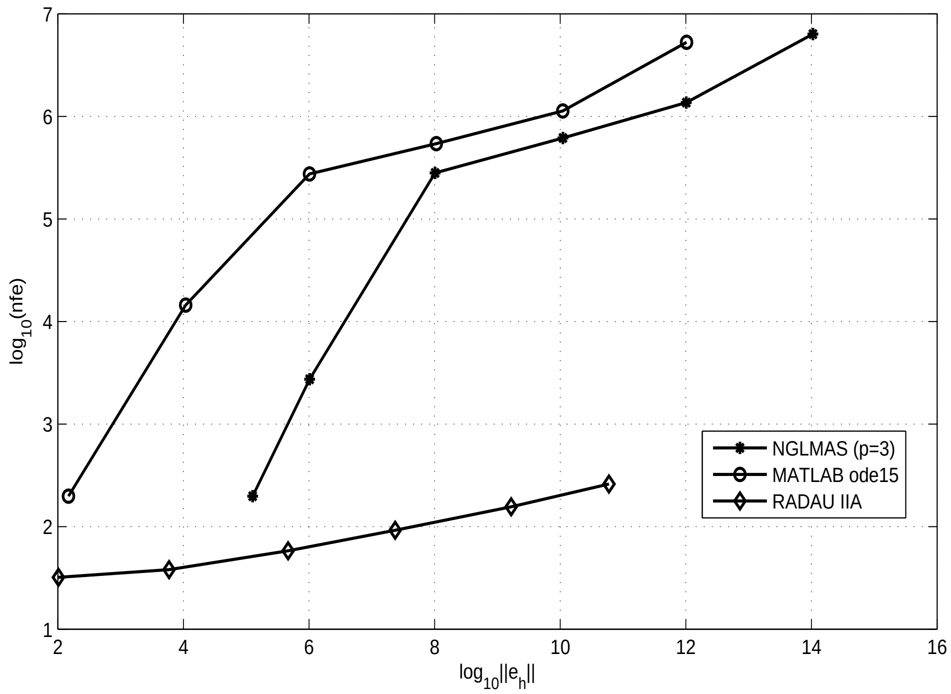

Figure 2: nfe versus $\| e_h \|$ at $x = 1$ for problem 2

6 Declarations

Availability of data and material: Not applicable.

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