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ACTIVE EXTRAPOLATION OF DIMSIMS IN NORDSIECK REPRESENTATION

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Abstract

Diagonally implicit multistage integration methods (DIMSIMs) are widely utilized in finding the solution to any problems in the subject of ordinary differential equations. These methods are selected from the general linear methods, which is considerable potential for efficient implementations. The extrapolation is derived from the stability of the explicit Runge-Kutta methods. In this paper, the combination of DIMSIMs with Richardson extrapolation of different orders shows that numerical solutions give higher accuracy when the extrapolation is applied with the base method.

Keywords: Diagonally implicit multistage integration methods, General linear methods, Active extrapolation

Abstrak

Kaedah penyepaduan berbilang peringkat tersirat (DIMSIMs) digunakan secara meluas untuk mencari penyelesaian bagi sebarang masalah dalam subjek persamaan pembezaan biasa. Kaedah ini dipilih daripada kaedah linear umum, yang berpotensi besar untuk pelaksanaan yang cekap. Ekstrapolasi diperoleh daripada kestabilan kaedah Runge-Kutta yang eksplisit. Dalam makalah ini, gabungan DIMSIM dengan ekstrapolasi Richardson bagi susunan yang berbeza menunjukkan bahawa penyelesaian berangka memberikan ketepatan yang lebih tinggi apabila ekstrapolasi digunakan dengan kaedah asas.

Kata kunci: Kaedah penyepaduan berbilang peringkat tersirat secara menyerong, Kaedah linear am, Ekstrapolasi aktif

1.0 INTRODUCTION

Consider the initial value problem given by

$$\begin{aligned} y'(x) &= f\big(y(x)\big), \qquad x \in [x_0, X] \\ y(x_0) &= y_0 \in \mathbb{R}^m, \end{aligned} \tag{1}$$

on the uniform grid point

$$x_n = x_0 + nh, \qquad n = 0,1,\dots,N, \qquad Nh = X - x_0$$

Diagonally implicit multistage integration methods can be defined as follows :

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

where $n = 1,2,\dots,N$. For these methods, the internal stages Y_i are approximation to $y(x_{n-1} + c_i h)$ within stage order q. This leads to

$$Y_i = y(x_{n-1} + c_i h) + O(h^{q+1}), \qquad i = 1,2,\dots,s,$$

and the external stages $y_i^{[n]}$ are approximating to the linear combination $h^k y^{(k)}$ within order p, that gives

$$y_i^{[n]} = \sum_{k=0}^{p} \alpha_{ik} h^k y^{(k)}(x_n) + O(h^{p+1}), \qquad i = 1,2,\dots,r,$$

where the vectors α_{ik} will be collect in the matrix W as follows:

$$W = [\alpha_0 \quad \alpha_1 \; \dots \; \alpha_p]. \tag{3}$$

In order to explain the stability of DIMSIMs, consider applying (2) to the following test problem.

$$y' = \xi y, \qquad t \geq 0,$$

where ξ denotes as complex parameter, then

$$y^{[n]} = M(z) y^{[n-1]}, \qquad n = 1,2,\dots,$$

where $z = h\xi$ and the stability matrix $M(z)$ is defined as follows:

$$M(z) = V + zB(I - zA)^{-1} U.$$

The stability of explicit type of DIMSIMs is similar to the stability of explicit Runge-Kutta methods which is in the form of a polynomial function,

$$R(z) = 1 + z + \frac{z^2}{2!} + \frac{z^3}{3!} + \dots + \frac{z^p}{p!},$$

for order-*p* method. On the other hand, the stability of implicit type of DIMSIMs is constructed based on the stability of Singly Diagonal Implicit Runge-Kutta methods (SDIRK).

In this paper, we consider the first type of DIMSIMs with condition $p = q = r = s$. These four itegers are defined as: p is order condition, q stage order, r is the number on external stages and s is the number on internal stages.

DIMSIMs have been considered by many researchers mainly Butcher in [3], and further investigation given by [7, 4, 2, 5, 6]. DIMSIMs were also studied by Wright in [16] and Huang in [11] as for their PhD research. In the resent years, DIMSIMs are becoming popular between the researchers such as studies by [10, 1, 8]. In addition to this, there is also an article for solving Volterra integro-differential equations which is based on a subclass of explicit general linear methods with and without Runge-Kutta stability property [13]. This stability properly is explained in Section 3.0.

The organization of this paper is considered as follows. Section 2 includes the construction of DIMSIMs in Nordsieck representation. The methods through this representation are proved zero stable for most of selecting of variable mesh. The proves are also not complicated in the performances through the changing of step-size. Section 3 describes the extrapolation approach in order to construct an efficient method known as extrapolated DIMSIMs with assumed $p = q = r = s$. This approach gives advantages to the existing methods which are given in Section 4 on the numerical experiments. The last section concludes the article.

2.0 DIMSIMs IN NORDSIECK REPRESENTATION

To construct DIMSIMs in Nordsieck representation, consider another approximation $\eta^{[n]} \in \mathbb{R}^m$ defined as follows

$$\eta^{[n]} = h(b^T \otimes I_m) F(Y^{[n]}) + (v^T \otimes I_m) y^{[n-1]},$$

which can be approximate to $\sum_{k=0}^{p} h^k t_k y^{(k)}(x_n)$. In addition, suppose the matrix $\widetilde{W}$ given by

$$\widetilde{W} = \begin{bmatrix} W \\ t^T \end{bmatrix} = \begin{bmatrix} \alpha_0 & \alpha_1 & \dots & \alpha_p \\ t_0 & t_1 & \dots & t_p \end{bmatrix}.$$

The independence of the approximations $\eta^{[n]} \in \mathbb{R}^m$ and $y_i^{[n]}, i = 1,2,\dots,s$ ensures that $\widetilde{W}$ is non-singular.

As given in [5], putting $\tilde{y}^{[n]} = [y^{[n]^T}, \; \eta^{[n]^T}]$, DIMSIMs is given in Nordsieck representation as

$$\begin{aligned} Y^{[n]} &= h(A \otimes I_m) F(Y^{[n]}) + (\widetilde{U} \otimes I_m) \tilde{y}^{[n-1]}, \\ \tilde{y}^{[n]} &= h(\tilde{B} \otimes I_m) F(Y^{[n]}) + (\tilde{V} \otimes I_m) \tilde{y}^{[n-1]}, \end{aligned} \tag{5}$$

where

$$\widetilde{U} = [U \quad 0], \qquad \tilde{B} = \begin{bmatrix} B \\ b^T \end{bmatrix}, \qquad \tilde{V} = \begin{bmatrix} V & 0 \\ v^T & 0 \end{bmatrix}.$$

Since

$$\tilde{y}^{[n]} = (\widetilde{W} \otimes I_m) \begin{bmatrix} y(x_n) \\ h y'(x_n) \\ \vdots \\ h^p y^{(p)}(x_n) \end{bmatrix} + O(h^{p+1}), \tag{6}$$

and the vector $z^{[n]}$ can be defined by

$$\tilde{y}^{[n]} = (\widetilde{W} \otimes I_m) z^{[n]}.$$

Through the considerations of above, we can see

$$\widetilde{U}\widetilde{W} = [U \quad 0] \begin{bmatrix} W \\ t^T \end{bmatrix} = UM.$$

The resuting DIMSIMs methods in Nordsieck representation can be obtained by substituting (7) in (5).

$$Y^{[n]} = h(A\otimes I_m)F\big(Y^{[n]}\big) + (P\otimes I_m)z^{[n-1]},$$
$$z^{[n]} = h(G\otimes I_m)F\big(Y^{[n]}\big) + (Q\otimes I_m)z^{[n-1]}, \quad (8)$$

where $P = UM, G = \widetilde{W}^{-1}\tilde{B},\ Q = \widetilde{W}^{-1}\tilde{V}\widetilde{W}$ and $z^{([n])}$ given by

$$z^{[n]} = \big(\widetilde{W}^{-1}\otimes I_m\big)\tilde{y}^{[n]} = \begin{bmatrix} y(x_n) \\ hy'(x_n) \\ \vdots \\ h^p y^{(p)}(x_n) \end{bmatrix} + O(h^{p+1}). \quad (9)$$

The coefficient Q can be simplified as $\widetilde{W}[e^T, 1]^T = e_1$, where $e_1 = [1,0,\dots,0]^T$ that gives

$$Q = \widetilde{W}^{-1}\tilde{V}\widetilde{W},$$
$$= \widetilde{W}^{-1}\begin{bmatrix} e \\ 1 \end{bmatrix}[v^T \ \ 0]\begin{bmatrix} W \\ t^T \end{bmatrix} = e_1[1 \ \ v^T\alpha_1 \ \ \dots \ \ v^T\alpha_p]. \quad (10)$$

The marix G is defined by the following theorem.

Theorem 2.1

$$G = LC^{-1},$$

where C is the Vandermonde matrix and L is the matrix with columns L_k given by

$$L_k = (k-1)!\left(\sum_{j=0}^{k}\frac{e_{j+1}}{(k-j)!} - Q_{e_{k+1}}\right), \qquad k = 1,2,\dots,p, \quad (11)$$

where $e_i = 1,2,\dots,p+1$. In particular, the matrix G is independent of $t_1, t_2, \dots, t_p$. The proof of this theorem is given by [1]. Several other numerical methods derived for General Linear Methods using explicit Nordsieck representation is given in [15].

3.0 DIMSIMs WITH EXTRAPOLATION

The extrapolation technique is one of the popular numerical procedures that can be used efficiently in the efforts of some programs to improve the performance by which long-time-dependent engineering and scientific issues are dealing on computers. Richardson first introduced extrapolation in 1911. It is an approximation method in the numerical solution of differential equations. The different phenomenon that happens in engineering and science are successfully described by using some advanced large-scale mathematical models. The extrapolation in most of the applications is used as an initial technique to evaluate the magnitude of the computational errors and is used in the efforts to improve the accuracy of the model results [13].

The extrapolation can be performed by a couple of types focused on getting high accuracy of a time integration technique. In addition, the approximation improved in a good way by extrapolation technique for a given time which is not utilized in the next computations when the passive mode is applied. However, the extrapolation technique in its active mode will be used through the computation of the next approximation.The extrapolation technique can be applied with explicit DIMSIMs methods by depending on their stability property. This property is an important key to increase the efficiency of the computational procedure and also to get reliable and more accurate results.

Dahlquist in [9] introduced to study the stability properties by choosing numerical methods that are dealing with solving the ODEs and applying to the following test problem

$$\frac{dy}{dx} = \lambda y, \qquad x \in [0,\infty], \quad (12)$$

where λ is considered to be complex number, the exact solution of this test problem given by

$$y(x) = \eta e^{\lambda x}, \qquad x \in [0,\infty] \quad (13)$$

where η is assumed to be initial value which given also as complex number. In order to solve the system of ordinary differential equation $y' = f(x,y)$ by the numerical methods, consider the approximations of the exact solutions $y(x_n)$ are calculated for values x_n either of the grid point of

$$x_0 = a,\ x_n = x_{n-1} + h,\ x_N = b,\ h = \tfrac{b-a}{N}, \quad (14)$$

where $n = 1,2,\dots,N$, or of the grid point of

$$x_0 = a, \qquad x_n = x_{n-1} + h_n, \qquad x_N = b, \quad (14)$$

where $n = 1,2,\dots,N$. During these conditions, the formula of the extrapolation technique that will be dealing with the numerical methods.

There are critical conditions considered in this paper, first of all, the order condition p is assumed to be equal to the stage order q. The second condition is the approximation solution y_n of the exact value $y(x)$ of the test equation (12) can be calculated under the same assumption which is imposed to the approximation y_{n-1} has already computed.

The extrapolation technique can be formulated in cases where the test problem of Dahlquist is solved. Besides, the extrapolation technique in active mode can be applied with DIMSIMs methods in three practical ways. Firstly, implement one large step N with the stepsize *h* by applying y_{i-1} as a starting value to compute:

$$z_i = R(z)y_{i-1}, \tag{16}$$

Secondly, implement two small steps with the stepsize $0.5h$ by applying y_{i-1} as the starting value in the first of the two steps.

$$\widetilde{w}_i = R\left(\frac{z}{2}\right)y_{i-1}, \qquad w_i = R\left(\frac{z}{2}\right)\widetilde{w}_i = \left[R\left(\frac{z}{2}\right)\right]^2 y_{i-1}. \tag{17}$$

Lastly, the extrapolation technique is computed by

$$\tilde{y}_i = \frac{2^p\widetilde{w}_i - z_i}{2^p - 1} = \frac{2^p\left[R\left(\frac{z}{2}\right)\right]^2 - R(z)}{2^p - 1}\, y_{i-1}, \tag{18}$$

where the stability function of the combined DIMSIMs with extrapolation can be considered as follows.

$$\bar{R}(z) = \frac{2^p\left[R\left(\frac{z}{2}\right)\right]^2 - R(z)}{2^p - 1}. \tag{29}$$

This way of applying extrapolation is known as active extrapolation on where the extrapolation solution $\tilde{y}_i$ is continued to be applied at every steps. However, passive extrapolation is also possible with the same equation (19) on where the extrapolation is only applied at the end of the iterations.

The stability function of explicit s-stage RK method of order $p = s \le 4$ is given by the following equation

$$R(z) = 1 + z + \frac{z^2}{2!} + \cdots + \frac{z^s}{s!}. \tag{20}$$

Since DIMSIMs considered here have similar stability as the RK methods, the derivation of the stability of the following order-2 and order-3 DIMSIMs methods are given next.

Order 2: $(\boldsymbol{p = q = s = 2})$

The DIMSIMs method is given by

$$\left[\begin{array}{c|c} A & P \\ \hline G & Q \end{array}\right] = \left[\begin{array}{cc|ccc} 0 & 0 & 1 & 0 & 0 \\ 2 & 0 & 1 & -1 & 1/2 \\ \hline 5/4 & 1/4 & 1 & -1/2 & 1/4 \\ 0 & 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \end{array}\right].$$

The stability function is given by

$$R(z) = 1 + z + \frac{z^2}{2},$$

which is similar as to the order-2 RK method.

Next by using the extrapolation of the stability equation (19), $\bar{R}(z)$ with $p = 2$ is given by

$$\bar{R}(z) = \frac{4}{3}\left[1 + \frac{z}{2} + \frac{z^2}{8}\right]^2 - \frac{1}{3}\left(1 + z + \frac{z^2}{2}\right).$$

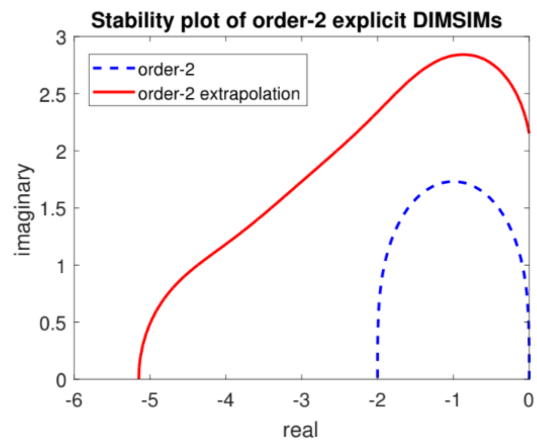


Figure 1 Stability regions of order-2 explicit DIMSIMs and extrapolated explicit DIMSIMs

Order 3: $(\boldsymbol{p = q = s = 3})$

The DIMSIMs method is given by

$$\left[\begin{array}{c|c} A & P \\ \hline G & Q \end{array}\right] = \left[\begin{array}{ccc|cccc} 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1/2 & 1/8 & 1/48 \\ 1/4 & 1 & 0 & 1 & -1/4 & 0 & 1/24 \\ \hline 5/4 & 1/3 & 1/6 & 1 & -3/4 & 1/6 & 1/24 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & -4 & 3 & 0 & 0 & 0 & 0 \end{array}\right].$$

The stability function is given by

$$R(z) = 1 + z + \frac{z^2}{2} + \frac{z^3}{6},$$

which is similar as to the order-3 RK method.

Next by using the extrapolation of the stability equation (19), $\bar{R}(z)$ with $p = 2$ is given by

$$\bar{R}(z) = \frac{8}{7}\left[1 + \frac{z}{2} + \frac{1}{2!}\left(\frac{z}{2}\right)^2 + \frac{1}{3!}\left(\frac{z}{2}\right)^3\right]^2 - \frac{1}{7}\left(1 + z + \frac{z^2}{2!} + \frac{z^3}{3!}\right).$$

The given order-2 and order-3 methods are considered in the numerical experiments.

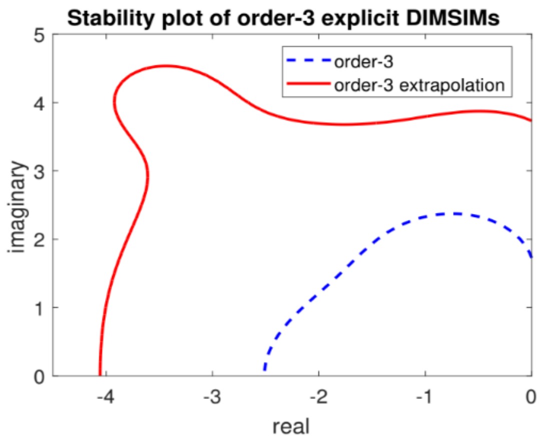


Figure 2 Stability regions of order-3 explicit DIMSIMs and extrapolated explicit DIMSIMs

Figure 1 and 2 give the stability regions of order-2 and order- 3 explicit DIMSIMs and extrapolated explicit DIMSIMs respectively. We can clearly see that the extrapolated order-2 and order-3 explicit DIMSIMs has a wider region then the base method without extrapolation.

3.0 RESULTS AND DISCUSSION

To test the efficiency of the explicit DIMSIMs methods with active extrapolation, the modified code *dim18.m* is used which is the variable order-variable stepsize given for $1 \leq p \leq 3$. This code was considered by Butcher [6]. Three test problems are considered to test the efficiency and accuracy of the methods. The test problems that are considered in this article are given in [12]. The class B problems that are selected are small systems that consists of linear and nonlinear equations. The numerical approximations are obtained for $x_n = 10$. The starting tolerance (tol) used is 10^{-3} and the solutions are obtained until $tol = 10^{-10}$. CPU time were measured using *tic* and *toc* build in functions in Matlab 2022.

To determine the accuracy of the approximations, the graphs of norm of global errors versus tolerances are given in Figures 4, 6 and 8, while to determine the efficiency of the approximations, the graphs of norm of global errors versus CPU Time are given in Figures 3, 5 and 7.

The two numerical methods thats are considered in the numerical experiments are DIMSIM order-2 (dim2x) and DIMSIM order-3 (dim3x) together with active extrapolations (dim2xactive) and (dim3xactive) respectively. These methods are compated with ode23 and ode45. The legends used in all the graphs is defined in Table 1.

Table 1 The legends used in all the graphs.

ode45	Six-stage, fifth-order, Runge-Kutta method
ode23	Three-stage, third-order, RK methods
dim2x	Order-2 DIMSIMs
dim2xactive	Order-2 DIMSIMs with active extrapolation
dim3x	Order-3 DIMSIMs
dim2xactive	Order-3 DIMSIMs with active extrapolation

B1 problem:

The first problem is the B1 problem which describes the growth of two conflicting populations.

$$y_1' = 2(y_1 - y_1 y_2),$$
$$y_2' = -y_2 + y_1 y_2,$$

$y_0 = [1,3]^T$.

B2 problem:

The second problem is the B2 problem which is a linear chemical reaction.

$$y_1' = -y_1 + y_2,$$
$$y_2' = y_1 - 2y_2 + y_3,$$
$$y_3' = y_2 - y_3,$$

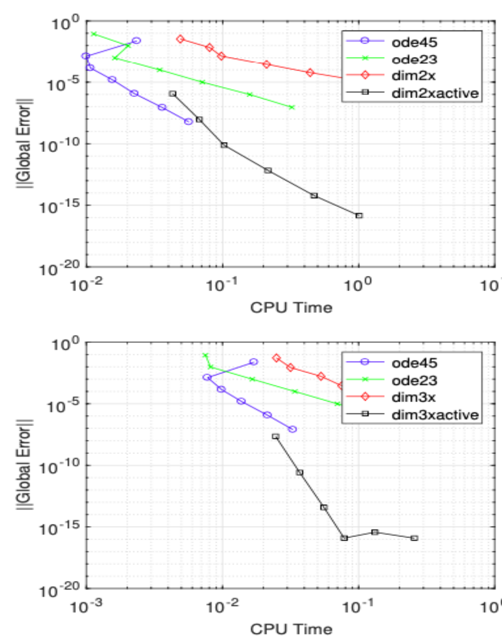
$y_0 = [2, 0, 1]^T$.

B3 problem:

The third problem is the B3 problem which is a nonlinear chemical reaction.

$$y_1' = -y_1$$
$$y_2' = y_1 - y_2^2,$$
$$y_3' = y_2^2,$$

$y_0 = [1, 0, 0]^T$.



igure 3 Global error & CPU time for B1 problem

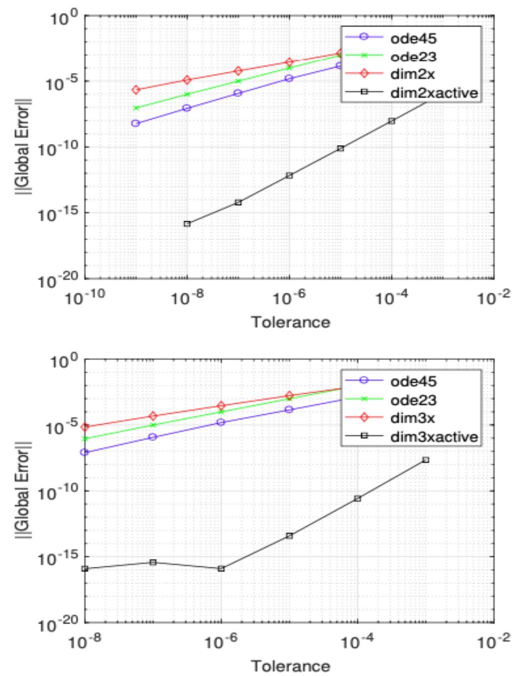


Figure 4 Global error & Tolerance for B1 problem

For B1 problem, dim2x and dim3x with extrapolations (dim2xactive and dim3xactive) have greater accuracy at different tolerance values (refer to Figure 3). Although these methods are also efficient (refer to Figure 4), both methods require slightly additional computational time. This is because as given in the extrapolation formula in equation (18), extrapolation is determined by using two different values of stepsize (h and h/2).

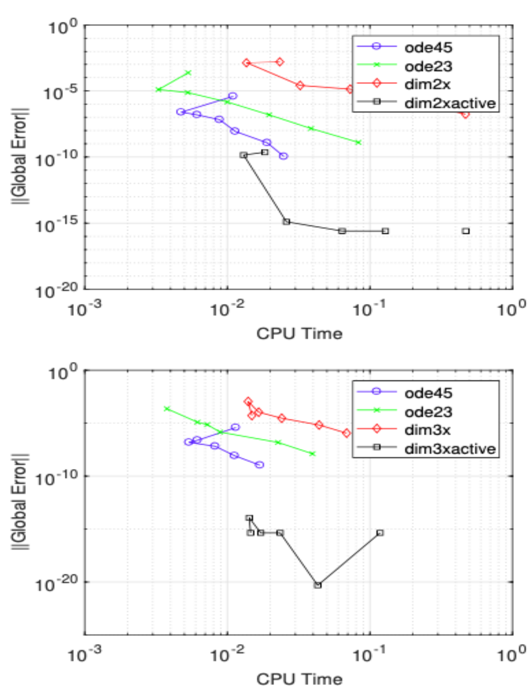


Figure 5 Global error & CPU Time for B2 problem.

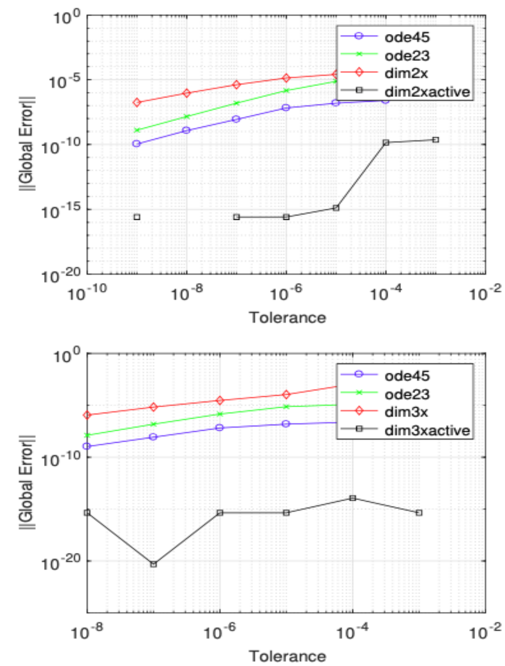
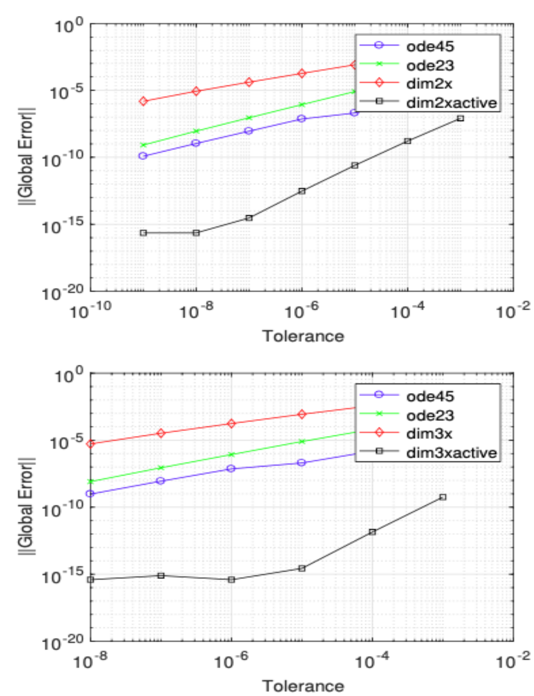


Figure 6 Global error & Tolerance for B2 problem

For B2 problem, similar results are shown as given for Problem B1 where both dim2x and dim3x with extrapolations (dim2xactive and dim3xactive) give greater accuracy and efficiency at different tolerance values (refer to Figure 5 and Figure 6 respectively). However, due to greater accuracy and efficiency as we have seen that the global errors are almost to $10^{-20,}$ the approximations started to be destroyed due to the round of errors. This can be overcome by using compensated summation or adjusting the, time interval and tolerance value.



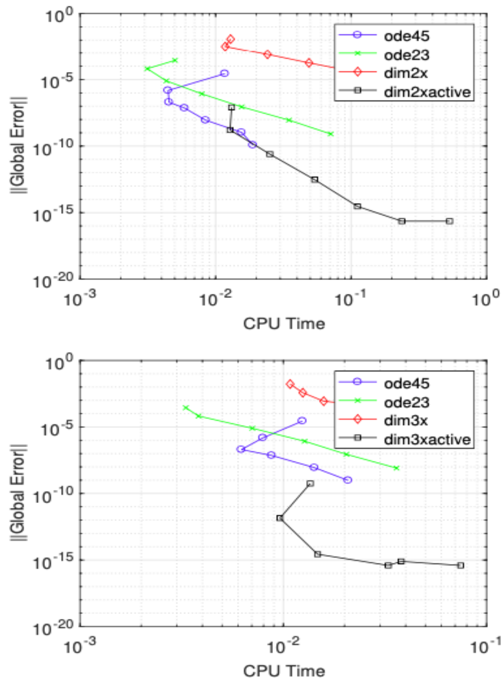


Figure 8 Global error & CPU time for B3 problem

Lastly, for B3 problems, similar results are obtained as given for problems B1 and B2 (Refer to Figure 7 and Figure 8).

The numerical results show that for all problems, active extrapolation is more efficient than ode45 and ode23. DIMSIMs with active extrapolation are seen to be superior than DIMSIMs without extrapolation.

4.0 CONCLUSION

The construction of diagonally implicit multistage integration methods has been considered to be a hard task. In this work, we apply the active extrapolation with DIMSIMs of order-2 and order-3 in solving non-stiff differential equations. These issues consider of the way of applying the active extrapolation with the choice of initial stepsize and order-changing strategies. Although the numerical results give promising results on the implementation of DIMSIMs with active extrapolation, theoretical analysis on the convergence of the extrapolation is also important to be studied in detail. Theoretically for Runge-Kutta methods, we know that the order of extrapolation will increased by one at a time for non-symmetric methods and two at a time for symmetric methods. Since type one DIMSIMs have similar stability as to explicit Runge-Kutta method, it is important to investigate whether the latter is also true for all the families of type one DIMSIMs with extrapolation. We wish to investigate the order behaviour in the future.

Conflicts of Interest

The author(s) declare(s) that there is no conflict of interest regarding the publication of this paper.

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