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ACCURACY OF IMPLICIT DIMSIMS WITH EXTRAPOLATION

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ABSTRACT. The main aim of this article is to present recent results concerning diagonal implicit multistage integration methods (DIMSIMs) with extrapolation in solving stiff problems. Implicit methods with extrapolation have been proven to be very useful in solving problems with stiff components. There are many articles written on extrapolation of Runge-Kutta methods however fewer articles on extrapolation were written for general linear methods. Passive extrapolation is more stable than active extrapolation as proven in many literature when solving stiff problems by the Runge-Kutta methods. This article takes the first step by investigating the performance of passive extrapolation for DIMSIMs type-2 methods. In the variable stepsize and order codes, order-2 and order-3 DIMSIMs with extrapolation are investigated for Van der Pol and HIRES problems. Comparisons are made with ode23 solver and the numerical experiments showed that implicit DIMSIMs with extrapolation has greater accuracy than the method itself without extrapolation and ode23.

Key words and phrases: General linear method, Implicit methods, Passive extrapolation, Diagonally implicit multistage integration methods.

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1. INTRODUCTION

General linear methods (GLMs) was firstly considered by Butcher [11] as a system of methods for studying some important properties like the convergence, stability and consistency of the traditional methods. There are two traditional methods considered for solving stiff ordinary differential equations, such as backward differentiation formulas (BDF) and implicit Runge-Kutta (RK) methods. These methods have upsides and downsides. To take the upside and overcome the downside, a new subclasses of general linear methods are constructed for solving stiff equations. This subclasses are called as Diagonally Implicit Multistage Integration methods abbreviate as DIMSIMs [2].

This article is aimed to describe the construction of implicit DIMSIMs methods and the implementations of these methods with extrapolation for solving numerical solutions of initial value problems which is given by

$$y'(x) = f(y(x)), \quad x \in [x_0, X], \tag{1.1}$$

$$y(x_0) = y_0 \in \mathbb{R}^m, \tag{1.2}$$

where f defines as $f : \mathbb{R} \to \mathbb{R}^m$ are smooth functions.

Even though in the papers [14],[9], the derivations of explicit methods for nonstiff equations and implicit methods for stiff equations are given, it can only be constructed for a small subset of the big family of methods that appears to exist. In this article, we study the construction of different orders of implicit methods and the implementation of extrapolation technique to gain higher accuracy.

The result of construction the implicit DIMSIMs with extrapolation methods based on the Nordsieck representation for input and output. The order condition p is assumed equal to stage order q with consider the stability properties as similar as singly diagonally implicit Runge-Kutta methods (SDIRKS).

2. DIMSIMs

DIMSIMs are formed by abscissa vector $c = (c_1, c_2, \cdots, c_s)^T$ and the coefficient matrices $[A, B, U, V]$ where

$$A = (a_{ij}) \in \mathbb{R}^{s\times s}, U = (u_{ij}) \in \mathbb{R}^{s\times r}, B = (b_{ij}) \in \mathbb{R}^{r\times s}, V = (v_{ij}) \in \mathbb{R}^{r\times r}.$$

The coefficient matrix A shows the implementation cost as same as assumed in RK methods [13]. Therefore, the phrases such as *singly-implicit* and *diagonally-implicit* can be directly borrowed from RK methods.

To lower the high cost of implementation of DIMSIMs, then the coefficient matrix A is considered as in [3] to being a very lower triangular as similar the case for the diagonally implicit RK methods. Moreover, if this coefficient being lower triangular with all equal of its diagonal elements, then in this case we can evaluate $Y_1, Y_2, \cdots, Y_s$ separately by using modified Newton iterations.

The system of DIMSIMs are defined on the uniformly grid as follows

$$x_{(n)} = x_{(0)} + nh, \quad n = (0, 1, \cdots, N), \quad NH = x - x_{(0)},$$

given by the following

$$Y_i = h\sum_{j=1}^{s} a_{ij} f(Y_j) + \sum_{j=1}^{r} u_{ij} y_i^{[n-1]}, \quad i = 1, 2, 3, \cdots, s, \tag{2.1}$$

$$y_i^{(n)} = h\sum_{j=1}^{s} b_{ij} f(Y_j) + \sum_{j=1}^{r} v_{ij} y_i^{[n-1]}, \quad i = 1, 2, 3, \cdots, s, \tag{2.2}$$

where $n = (1, 2, 3, \cdots, N)$, Y_i denotes internal stages are approximation of stage-order q according to [3],

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

where $y_i^{[(n)]}$ denotes external stages of order condition p and are approximate by

$$y_i^{[(n)]} = \sum_{k=0}^{p} q_{(ik)} h^k y^{(k)}(x_n) + O(h^{(p+1)}), \quad i = 1, 2, 3, \cdots, r.$$

To guarantee the zero stability of DIMSIMs, then coefficient matrix V is assumed as a rank one matrix, which is given by

$$V = eV^T \in \mathbb{R}^s, \quad V^T e = 1,$$

where

$$v = [v_1 v_2 \cdots v_s]^{(T)}, \quad e = [1, 1, \cdots, 1]^T \in \mathbb{R}^s.$$

Such methods in this case will be automatically zero-stable.

As we mentioned before, the coefficient matrix A is considered by a very lower triangular which is defined by

$$\begin{bmatrix} \lambda & & & \\ a_{(21)} & \lambda & & \\ \vdots & \vdots & \ddots & \\ a_{(s1)} & a_{(s2)} & \cdots & \lambda \end{bmatrix},$$

where $\lambda \geq 0$. If $(\lambda = 0)$ the methods are known as explicit methods, as considered in [13] which is known as type one DIMSIMs. However, if $(\lambda > 0)$ the methods are known as implicit methods, which are known as type two DIMSIMs. This article only focuses on type two DIMSIMs.

3. EXTRAPOLATION

Extrapolation for explicit DIMSIMs have been proven to improve the accuracy in solving nonstiff problems. This article extended the extrapolation technique for implicit DIMSIMs for solving stiff problems. Extrapolation is a technique to increase the accuracy of the method as considered by L.F. Richardson in [15]. This technique is also called as Richardson extrapolation given in the following the form

$$T_{i,j} = T_{i,(j-1)} + \frac{T_{i,(j-1)} - T_{(i-1),(j-1)}}{(\frac{m_i}{m_{i-(j+1)}})^p - 1}, \tag{3.1}$$

where $i = j = 2, \cdots, n$. Extrapolation can be carried out in two efficient ways. Active extrapolation happens when the determined value of extrapolation utilized to propagate the next computation whereas the passive extrapolation is not utilized in any subsequent computations.

In another meaning, with possible conditions for the error $T_{i,1} - y(x_{(0)} + H)$ have an approximation expansion in power of H^2. However, the highly orders approximation of quantities $T_{(i,k)}$ to $y(x_0 + H)$ are formed from $T_{(i,1)}$ via the extrapolation formula. In this article, we will focus on the implicit methods using passive extrapolation to solve the stiff equations. We consider polynomial extrapolation rather than rational extrapolation since according to [7], rational extrapolation has more restrictions on the stepsize and it also lose its translation invariance while the polynomial extrapolation is more stable and therefore is more preferable.

4. IMPLICIT DIMSIMs

In this section, the formulation of implicit methods is reviewed, which will be efficient for stiff problems especially in a conventional environment. Implicit methods were considered by Butcher [4] for solving the stiff problems and also for differential-algebraic problems of RK methods. However, these methods are proven to have high implementation cost and more complicated to carried out as the stage value which required to be located by an iterative computation [5]. Despite these disadvantages, implicit methods was considered better than other methods like explicit methods to solve the stiff problems, because it gives better stability and it is computed by fewer stages with the same order [5]. The implicit methods of DIMSIMs (type two) which are poses stability considered exactly same the stability of the singly diagonally implicit Runge-Kutta methods.

In this paper, it is assumed the order condition p is equal to stage order q of DIMSIMs. Then, the internal stage values in this case satisfied by

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

The other two integers s, r are known as: the number of internal sages of DIMSIMs, the number of incoming and outgoing respectively. These integers assumed as $r = s = p + 1$. Therefor, the quantities moved step to another step have the following forms

$$\begin{aligned} y_i^{[n-1]} &= \sum_{k=0}^{p} a_{(ik)} y^{(k)}(x_{(n-1)}) + O(h^{(p+1)}), \\ y_i^{[n]} &= \sum_{k=0}^{p} a_{(ik)} y^{(k)}(x_{(n)}) + O(h^{(p+1)}). \end{aligned}$$

In order to make the implementation more easier since the way of change the step-size to a straightforward rescaled by the quantities of external-approximations, then these methods represents in the Nordsieck representation. Nordsieck vectors were defined by Nordsieck in 1962 [10] with Adams methods. DIMSIMs using the above representations will be considered as zero-stable for all selecting of variable mesh [6]. Therefore, the DIMSIMs represents in Nordsieck representation is given as follows:

$$\begin{aligned} Y^{[n]} &= h_n (A \otimes I_m) F(Y^{[n]}) + (PD(\delta_n) \otimes I_m) z^{[n-1]}, \\ z^{[n]} &= h_n (G \otimes I_m) F(Y^{[n]}) + (QD(\delta_n) \otimes I_m) z^{[n-1]}, \end{aligned}$$

where $h_{n-1} = x_{n-1} - x_{n-2}$, $n = 1, 2, 3, \cdots, N$, and $z_i^{[n]} = h_n^{i-1} y^{i-1}(x_n) + O(h_n^{p+1})$, $i = 1, 2, \cdots, r$, A, P, G and Q are defined as coefficient matrices with the following dimension $s \times s, s \times r, r \times s$ and $r \times r$, respectively.

Now, in order to construct the implicit DIMSIMs (type two), we have the stability matrix assumed as

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

$$= V + \frac{z}{1-\lambda z} B(I - \frac{z}{1-\lambda z}(A - \lambda I)^{-1},$$

and substituting $\hat{z} = \frac{z}{1-\lambda z}$ and $\hat{A} = A - \lambda I$ in the stability matrix. Then, it tends the following

$$\hat{M}(\hat{z}) = V + \hat{z}B(I - \hat{z}\hat{A})^{-1}.$$

Construction these methods depend on the assumption of the stability polynomial $\hat{p}(w, \hat{z})$ as referred in [[9],[3]] satisfying the following

$$\hat{p}(w, \hat{z}) = w^{s-1}(w - \hat{R}(\hat{z})),$$

where $\hat{R}(\hat{z})$ known here as the stable function which is has same structure as in SDIRK method. This function considered as

$$R(z) = \hat{R}(\frac{z}{1-\lambda z}) = \frac{P(z)}{(1-\lambda z)^s},$$

where

$$P(z) = (-1)^s \sum_{j=0}^{s} L_s^{(s-j)}(\frac{1}{\lambda})(\lambda z)^j,$$

and L_s is Laguerre polynomial given by

$$L_s(x) = \sum_{j=0}^{s} (-1)^j \binom{s}{j} \frac{x^j}{j!}.$$

The order condition very important to construct the exist methods, So the following lemma which proved by [2] explains this case.

Lemma 4.1. *A general linear methods formed in Nordsieck representation with coefficient matrices A, U, B and V, of order conditions p as same as stage order q iff*

$$\exp(cz) = zA\exp(cz) + UZ + O(z^{p+1}),$$
$$\exp(z)Z = zB\exp(cz) + VZ + O(z^{p+1}),$$

$\exp(cz)$ *denotes here as a vector of components given by*

$$\begin{bmatrix} \exp(c_1 z) \\ \exp(c_2 z) \\ \vdots \\ \exp(c_s z) \end{bmatrix}.$$

The implementation of the existing methods given by the Matlab code `dim13xtrap.m` based on applying the extrapolation technique (3.1) with implicit DIMSIMs, where this code starts by order one $p_1 = 1$ and initial stepsize h_1 is given by $h_1 = \sqrt{2/\|d_2\|_{\text{sc}}}$ where

$$d_2 = \left(f\left(y_0 + h_0 f\left(y_0\right)\right) - f\left(y_0\right)\right)/h_0,$$

where

$$h_0 = 1/\left\|f\left(y_0\right)\right\|_{\text{sc}},$$

denotes the stepsize of methods of order zero. Besides, the standard step changing strategy is computed as similar as for explicit DIMSIMs and Runge-Kutta methods. The estimation of the local discretization error of implicit methods is computed by

$$\mathrm{err} = \left\| \mathrm{est}^* \left(x_n, p_n\right) \right\|_{\mathrm{sc}},$$

with

$$\mathbf{sc}_j = \mathrm{Atol}_j + \max\left\{ \left| z_{1,j}^{[n-1]} \right|, \left| z_{1,j}^{[n]} \right| \right\} \mathrm{Rtol}_j .$$

This consideration bring us to know the decision about the new order which is relied on the following ratio

$$\text{ratio } = \frac{\left\| \mathrm{est}^* \left(x_n, p_n\right) \right\|_{\mathrm{sc}}}{\left\| \mathrm{est}^* \left(x_n, p_n - 1\right) \right\|_{\mathrm{sc}}}.$$

This ratio is important also to know the step is rejected or accepted when applying the existing methods on the test problems which is given in the next.

5. NUMERICAL EXPERIMENTS

In this section, the numerical experiments are given for two well-known problems such as Van der Pol (VDP) and Hires problems. The first problem considered in [1] as the following

$$\begin{aligned} y_1' &= y_2, \\ y_2' &= (1 - y_1^2) y_2 - y_1, \end{aligned}$$

with initial values given by $y_2(0) = 2$ and $y_2(0) = 0$, $[0, 3]$.
The notations used in all the plots is given in Table 5.1.

Table 5.1: Notations for the plots given in numerical results.

Notations	**Definitions**
dim12s	implicit DIMSIM method of order-2
dim12xtrap	implicit DIMSIM method of order-2 with extrapolation
dim13s	implicit DIMSIM method of order-3
dim13xtrap	implicit DIMSIM method of order-3 with extrapolation
ode23s	modified Rosenbrock formula of order 2
ode23t	trapezoidal rule using a "free" interpolant
ode23tb	implicit trapezoidal formula (first stage) together with backward differentiation formula (second stage) of order-2

In Figure 1, it can be shown that implicit DIMSIM of order-2 and order-3 with extrapolation is more accurate than the implicit DIMSIM without extrapolation. Furthermore, the error of dim13s corresponding to $tol = 10^{-6}$ is larger than dim13xtrap.

In the second part of Figure 1, the global error against step size h is plotted. Both methods examined with two and three orders which agrees totally with the predicted order of using accuracy and extrapolation of implicit DIMSIMs is more accurate for the same step size than implicit DIMSIMs without extrapolation.

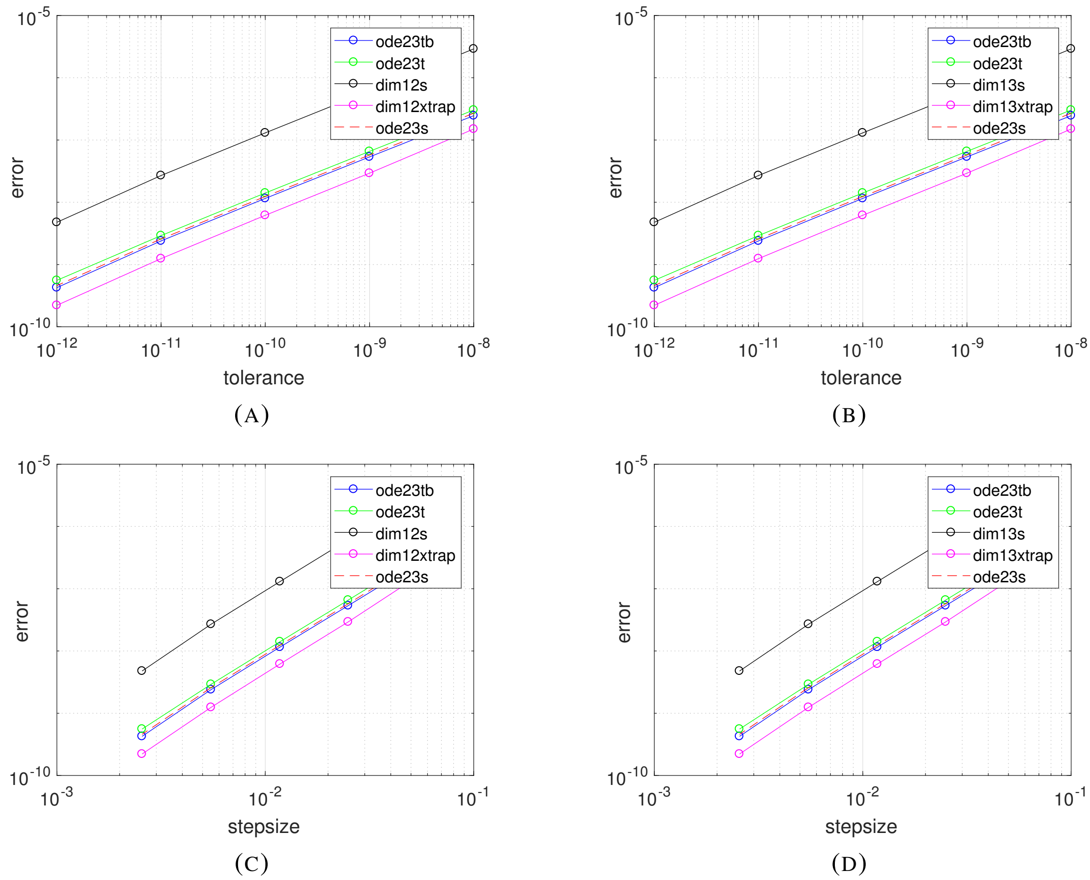


Figure 1: Numerical results for VDP problem, error via tolerance & step-size.

The second problem which is the HIRES problem as in [12] is given by

$$
\begin{aligned}
y_1' &= -1.71 \cdot y_1 + 0.43 \cdot y_2 + 8.32 \cdot y_3 + 0.0007,\\
y_2' &= 1.71 \cdot y_1 - 8.75 \cdot y_2,\\
y_3' &= -10.03 \cdot y_3 + 0.43 \cdot y_4 + 0.035 \cdot y_5,\\
y_4' &= 8.32 \cdot y_2 + 1.71 \cdot y_3 - 1.12 \cdot y_4,\\
y_5' &= 1.745 \cdot y_5 + 0.43 \cdot y_6 + 0.43 \cdot y_7,\\
y_6' &= -280 \cdot y_6 y_8 + 0.69 \cdot y_4 + 1.71 \cdot y_5 - 0.43 \cdot y_6 + 0.69 \cdot y_7,\\
y_7' &= -y_7'.
\end{aligned}
$$

Similarly, we can also see in Figure 2, that dim13xtrap and dim12xtrap are more accurate than dim12s and dim13s and others for most the tolerances. Furthermore, the error of dim12s and dim13s corresponding to $tol = 10^{-6}$ is also larger than dim12xtrap and dim12xtrap. In the second part of Figure 2, the global error against step size h for HIRES problem is plotted. We can also see clearly the extrapolation of implicit DIMSIMs is more accurate for the same step size than implicit DIMSIMs without extrapolation.

Furthermore, Figure 3 and Figure 4 denote the results of global error versus cputime for VDP and HIRES test problems. The cputime is measured using *tic* and *toc* build-in functions in Matlab. The results show that implicit DIMSIMs with extrapolation is more efficient than methods without extrapolation.

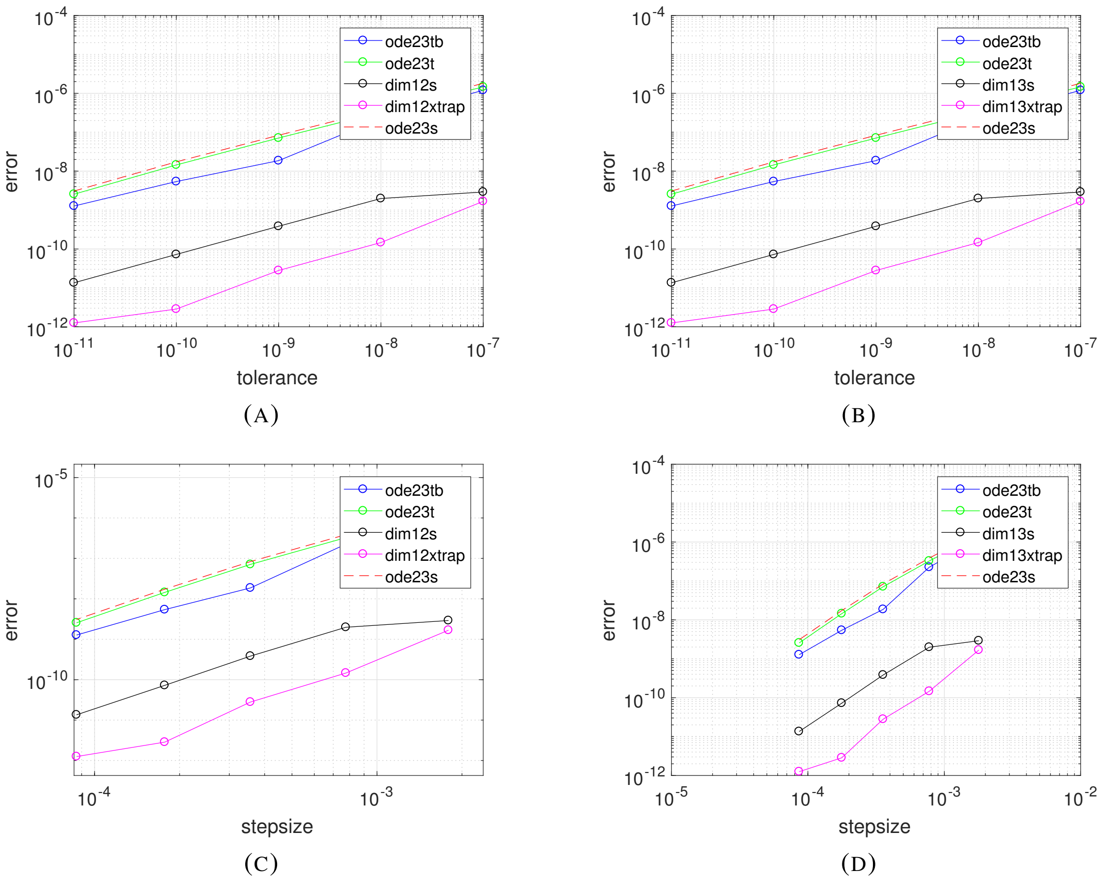


Figure 2: Numerical results for HIRES problem, error via tolerance & step-size.

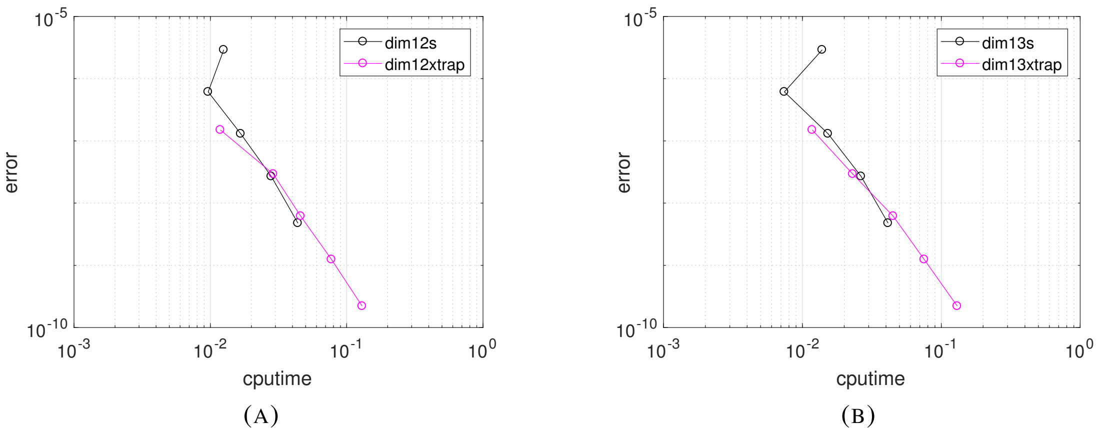
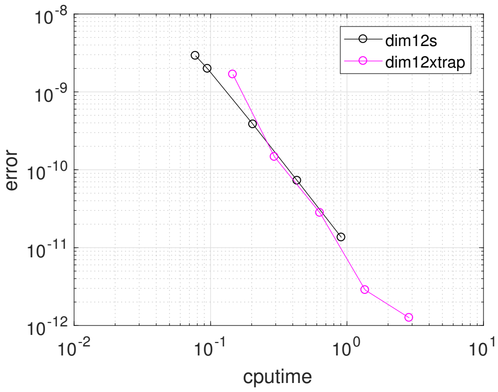


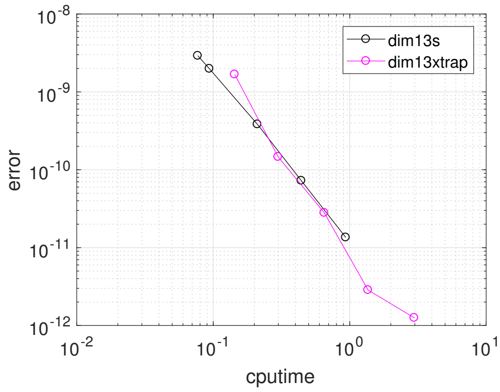
Figure 3: Numerical results for VDP problem, error via CPU times.

6. CONCLUSION

This paper discuss the issues related to the efficient development of solving the ordinary differential equation for the implicit DIMSIMs with extrapolation in solving stiff differential equations. These issues includes the implementation of extrapolation and the choice of initial step-size, order changing strategies and local error estimation. Future work will contains various implementation related to these methods of high order such as select of initial step-size, local



(A)



(B)

Figure 4: Numerical results for HIRES problem, error via CPU times.

error estimation, construction of starting procedures, as well as using variable stepsize variable order derived with these methods.

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