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SOLUTIONS OF GENERAL SECOND ORDER ODES USING DIRECT BLOCK METHOD OF RUNGE-KUTTA TYPE

(Penyelesaian bagi Persamaan Pembezaan Biasa Umum Peringkat Kedua dengan Kaedah Blok Langsung Jenis Runge-Kutta)

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ABSTRACT

This paper presents a three point block variable step size method of Runge-Kutta type for solving general second order ordinary differential equations (ODEs). The block method is formulated using Lagrange interpolation polynomial. Most of the mathematical problems which involve higher order ODEs could be reduced to system of first order equations. The proposed method obtains the numerical solutions directly without reducing to first order systems of ODEs. The method is used to compute the solutions at three points simultaneously by integrating the coefficients over the closest point in the block. The stability region of the block method is also studied. The numerical results obtained shows that the proposed method is more efficient compared to existing block methods in terms of total steps and execution time.

Keywords: Block method; variable step size; ordinary differential equations

ABSTRAK

Dalam makalah ini diperkenalkan kaedah blok tiga titik jenis Runge-Kutta untuk penyelesaian peringkat kedua persamaan pembezaan biasa (PBB) umum menggunakan panjang langkah berubah. Kaedah blok ini dirumus menggunakan polinomial interpolasi Lagrange. Kebanyakan masalah matematik yang melibatkan peringkat tinggi PBB akan menurunkan masalah kepada sistem peringkat pertama PBB. Kaedah yang dicadangkan ini menentukan penyelesaian berangka secara langsung tanpa perlu diturunkan kepada sistem peringkat pertama PBB. Kaedah ini digunakan untuk mengira penyelesaian pada tiga titik secara serentak dengan mengamirkan pekali-pekali pada titik terdekat di dalam satu blok. Kestabilan kaedah blok ini juga turut dikaji. Keputusan berangka yang diperoleh menunjukkan kaedah yang dicadangkan adalah lebih cekap berbanding dengan kaedah blok sedia ada dari segi jumlah langkah dan masa pelaksanaan.

Kata kunci: Kaedah blok; panjang langkah berubah; persamaan pembezaan biasa

1. Introduction

This study is intended to solve second order non-stiff initial value problems (IVPs) of ordinary differential equations in the following form

$$y'' = f(x, y, y'), \qquad y(a) = y_0,\ y'(a) = y'_0, \qquad x \in [a, b] \tag{1}$$

The second order ODEs can be formed from many real problems in a wide variety of applications especially in science and engineering such as fluid dynamic, electrical circuit and other area of applications. The approach here is to solve Eq. (1) using block implicit one-step method. This block method of Runge-Kutta type has been studied by Rosser (1967), Shampine and Watts (1969) and Majid *et al.* (2003). Rosser (1967) introduced a block with a new approximation values simultaneously based on Newton-Cotes type while Majid *et al.*

(2003) presented a two point implicit block one-step method based on integration formula using Newton backward divided difference formula.

In the literature, there were a few researchers suggested to solve higher order ODEs directly such as Chakravarti and Worland (1971), Fatunla (1991), Suleiman (1989), and Omar and Suleiman (2005). The higher order ODEs can be reduced to a system of first order equations and then solved using first order ODEs. Consequently, this approach will enlarge the system of first order ODEs.

The idea in this paper is to derive the formulae of the three point block method based on the Lagrange interpolation polynomial and estimate the solutions of second order ODEs at three points simultaneously. Majid *et al.* (2006) has presented a three point implicit block method for solving system of first order ODEs. The numerical results in Majid *et al.* (2003, 2006) were compared to Rosser (1967). Both methods were implemented to solve the system of first order ODEs. Thus, this method inspired our research to solve the system of second order ODEs directly and compared the performance of the proposed method with Majid *et al.* (2006).

2. Formulation of the Method

In Figure 1, the proposed method will compute the three approximation values of y_{n+1}, y_{n+2} and y_{n+3} simultaneously. The interval $[a,b]$ is divided into a series of blocks with each block containing three points and the computed block has the step size 3*h*. The solution at the point x_n is used to start the *k* th block while the solution at the point x_{n+3} is the last point in the *k* th block will be used to start the (*k*+1) th block and the process continues for the next block.

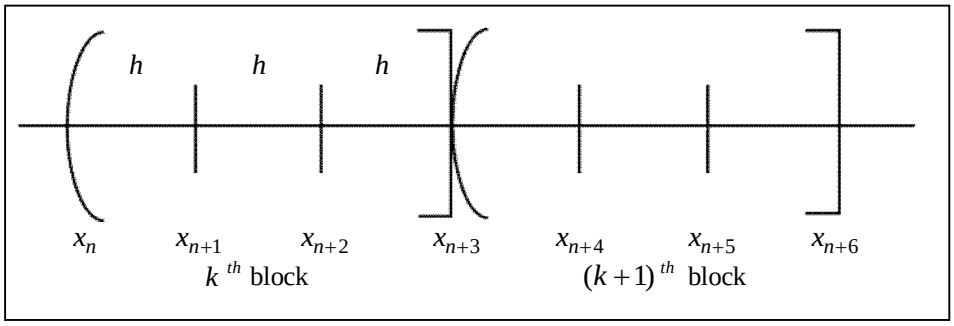

Figure 1: Three point block method

The predictor formula involved the Euler method, while the corrector formula of the block method in Figure 1 was derived using Lagrange interpolation polynomial. The first point, y_{n+1} and y'_{n+1} can be obtaining by integrating Eq. (1) once and twice over the interval $[x_n, x_{n+1}]$,

$$\begin{aligned} \int_{x_n}^{x_{n+1}} y''(x)\,dx &= \int_{x_n}^{x_{n+1}} f(x,y,y')\,dx \\ \int_{x_n}^{x_{n+1}} \int_{x_n}^{x} y''(x)\,dx\,dx &= \int_{x_n}^{x_{n+1}} \int_{x_n}^{x} f(x,y,y')\,dx\,dx \end{aligned} \tag{2}$$

Taking $x_{n+1} = x_n + h$, gives

$$\begin{aligned} y'(x_{n+1}) - y'(x_n) &= \int_{x_n}^{x_{n+1}} f(x, y, y')\ dx \\ y(x_{n+1}) - y(x_n) - hy'(x_n) &= \int_{x_n}^{x_{n+1}} (x_{n+1} - x) f(x, y, y')\ dx \end{aligned} \tag{3}$$

The Lagrange interpolation polynomial will replace the $f(x, y, y')$ in Eq. (3). The interpolation points in the block will involve (x_n, f_n), (x_{n+1}, f_{n+1}), (x_{n+2}, f_{n+2}) and (x_{n+3}, f_{n+3}).

Taking $s = \dfrac{x - x_{n+3}}{h}$ and $dx = h\ ds$; then replace into Eq. (3) and changing the limit of integration from -1 to 0. The formulae of y_{n+1} and y'_{n+1} will be obtained by using MATHEMATICA,

$$\begin{aligned} y'_{n+1} &= y'_n + \frac{h}{24}(9 f_n + 19 f_{n+1} - 5 f_{n+2} + f_{n+3}), \\ y_{n+1} &= y_n + hy'_n + \frac{h^2}{360}(97 f_n + 114 f_{n+1} - 39 f_{n+2} + 8 f_{n+3}). \end{aligned} \tag{4}$$

To approximate the value of y_{n+2} and y'_{n+2}, let $x_{n+2} = x_n + 2h$ and integrate Eq. (1) once and twice over the interval $[x_{n+1}, x_{n+2}]$,

$$\begin{aligned} y'_{n+2} &= y'_{n+1} + \frac{h}{24}(-f_n + 13 f_{n+1} + 13 f_{n+2} - f_{n+3}), \\ y_{n+2} &= y_{n+1} + hy'_{n+1} + \frac{h^2}{360}(-8 f_n + 129 f_{n+1} + 66 f_{n+2} - 7 f_{n+3}). \end{aligned} \tag{5}$$

Taking $x_{n+3} = x_n + 3h$, the value of y_{n+3} and y'_{n+3} can be obtained by integrating once and twice of Eq. (1) over the interval $[x_{n+2}, x_{n+3}]$. Then, we obtain the following corrector formulae,

$$\begin{aligned} y'_{n+3} &= y'_{n+2} + \frac{h}{24}(f_n - 5 f_{n+1} + 19 f_{n+2} + 9 f_{n+3}) \\ y_{n+3} &= y_{n+2} + hy'_{n+2} + \frac{h^2}{360}(7 f_n - 36 f_{n+1} + 171 f_{n+2} + 38 f_{n+3}) \end{aligned} \tag{6}$$

In order to determine the order and error constant of the method, we had referred to Lambert (1981) and Fatunla (1991). Thus, the formula in Eq. (4), (5) and (6) are order of $p = 4$ and the error constant is $C_{p+2} = C_6 = \begin{bmatrix} -\frac{19}{160} & -\frac{7}{480} & \frac{11}{720} & \frac{11}{1440} & -\frac{19}{720} & -\frac{17}{1440} \end{bmatrix}^T \neq 0$.

3. Implementation of the Method

The approximation values of $y_{n+1}, y'_{n+1}, y_{n+2}, y'_{n+2}, y_{n+3}$ and y'_{n+3} in Eq. (4), (5) and (6) will be approximated using the predictor-corrector schemes. If r corrections are needed, then the

sequence of computations at any mesh point is $(PE)(C_0E)...(C_rE)$ where P , E and C indicate the predictor, evaluation of the function f and the corrector respectively.

The predictor equations:

$$P: \quad y'^{p}_{n+i,0} = y'_{n+(i-1),0} + hf_{n+(i-1),0}$$

$$y'^{p}_{n+i,0} = y_{n+(i-1),0} + hy'_{n+(i-1),0} + \frac{h^2}{2!} f_{n+(i-1),0}$$

$$E: \quad f^{p}_{n+i,0} = f(x_{n+i}, y^{p}_{n+i,0}, y'^{p}_{n+i,0}) \qquad i = 1,2,3. \tag{7}$$

The corrector equations:

For $r = 0$;

$$C: \quad y'^{c}_{n+i,1} = y'^{c}_{n+(i-1),1} + h\sum_{j=0}^{3} \alpha_{j,i}\ f^{p}_{n+j,0}$$

$$y^{c}_{n+i,1} = y^{c}_{n+(i-1),1} + hy'^{c}_{n+(i-1),1} + h^2 \sum_{j=0}^{3} \beta_{j,i}\ f^{p}_{n+j,0}$$

$$E: \quad f^{c}_{n+i,1} = f(x_{n+i}, y^{c}_{n+i,1}, y'^{c}_{n+i,1}) \qquad i = 1,2,3. \tag{8}$$

For $r = 1,2,3...$;

$$C: \quad y'^{c}_{n+i,r+1} = y'^{c}_{n+(i-1),r+1} + h\sum_{j=0}^{3} \alpha_{j,i}\ f^{c}_{n+j,r}$$

$$y^{c}_{n+i,r+1} = y^{c}_{n+(i-1),r+1} + hy'^{c}_{n+(i-1),r+1} + h^2 \sum_{j=0}^{3} \beta_{j,i}\ f^{c}_{n+j,r}$$

$$E: \quad f^{c}_{n+i,r+1} = f(x_{n+i}, y^{c}_{n+i,r+1}, y'^{c}_{n+i,r+1}) \qquad i = 1,2,3. \tag{9}$$

In the code, the convergence test will iterate the corrector to converge as follows:

$$\left| y_{n+3,s+1} - y_{n+3,s} \right| < 0.1 \times \mathrm{TOL},$$

where s is the number of iterations. After the successful convergence test, the error for the block will be performed. Then, the maximum error is defined as follow;

$$\mathrm{MAXE} = \max_{1 \le i \le TS} \left(\max_{1 \le i \le N} (E_i)_t \right),$$

where TS is the number of successful steps, $(E_i)_t$ is the error and N is the number of equation. The selection of the next step size will be similar as in Majid *et al.* (2003). The choices for the next step size will be constant or double. The step size will be restricted to half if the step size failure.

4. Stability Region

The main concern in this section is to discuss the stability of the proposed method derived in the previous section on a linear second order problem when the method is applied to the test equation

$$y'' = \theta y' + \lambda y \,. \tag{10}$$

The formulae of the three point implicit block method were given by Eq. (4), (5) and (6). Hence for r = 0, the test equation in Eq. (10) is substituting into Eq. (7) and (8). Then, transforming into a matrix form and we obtain the stability polynomial as follows:

r = 0:

$$\begin{aligned}
&\Bigg(1+\frac{77H_1}{24}+\frac{383H_1^{\,2}}{72}+\frac{337H_1^{\,3}}{72}+\frac{25H_1^{\,4}}{9}+\frac{5H_1^{\,5}}{6}+\frac{H_1^{\,6}}{4}+\frac{49H_2}{180}-\frac{11H_1H_2}{30}-\\
&\frac{289H_1^{\,2}H_2}{720}-\frac{13H_1^{\,3}H_2}{24}+\frac{H_1^{\,4}H_2}{10}-\frac{3H_1^{\,5}H_2}{40}-\frac{467H_2^{\,2}}{1080}-\frac{863H_1H_2^{\,2}}{2160}-\frac{517H_1^{\,2}H_2^{\,2}}{864}-\\
&\frac{193H_1^{\,3}H_2^{\,2}}{720}-\frac{H_1^{\,4}H_2^{\,2}}{8}-\frac{397H_2^{\,3}}{8640}+\frac{3989H_1H_2^{\,3}}{8640}-\frac{49H_1^{\,2}H_2^{\,3}}{720}+\frac{9H_1^{\,3}H_2^{\,3}}{160}+\\
&\frac{1607H_2^{\,4}}{8640}-\frac{61H_1H_2^{\,4}}{2880}-\frac{3H_1^{\,2}H_2^{\,4}}{320}-\frac{7H_2^{\,5}}{960}-\frac{7H_1H_2^{\,5}}{160}-\frac{7H_2^{\,6}}{640}\Bigg)t^4+\Bigg(-2-\frac{41H_1}{12}-\\
&\frac{397H_1^{\,2}}{72}-\frac{335H_1^{\,3}}{72}-\frac{199H_1^{\,4}}{72}-\frac{5H_1^{\,5}}{6}-\frac{H_1^{\,6}}{4}-\frac{859H2}{90}-\frac{1211H_1H_2}{80}-\frac{1967H_1^{\,2}H_2}{144}-\\
&\frac{937H_1^{\,3}H_2}{120}-\frac{13H_1^{\,4}H_2}{5}-\frac{27H_1^{\,5}H_2}{40}-\frac{18949H_2^{\,2}}{2160}-\frac{23999H_1H_2^{\,2}}{2160}-\frac{16789H_1^{\,2}H_2^{\,2}}{2160}-\\
&\frac{2183H_1^{\,3}H_2^{\,2}}{720}-\frac{31H_1^{\,4}H_2^{\,2}}{40}-\frac{12563H_2^{\,3}}{4320}-\frac{3539H_1H_2^{\,3}}{1080}-\frac{247H_1^{\,2}H_2^{\,3}}{144}-\frac{39H_1^{\,3}H_2^{\,3}}{80}-\\
&\frac{1723H_2^{\,4}}{3456}-\frac{277H_1H_2^{\,4}}{576}-\frac{57H_1^{\,2}H_2^{\,4}}{320}-\frac{13H_2^{\,5}}{240}-\frac{23H_1H_2^{\,5}}{640}-\frac{H_2^{\,6}}{320}\Bigg)t^5+\Bigg(1+\frac{5H_1}{24}+\\
&\frac{7H_2^{\,2}}{36}-\frac{H_1^{\,3}}{36}-\frac{H_1^{\,4}}{72}+\frac{49H_2}{180}+\frac{31H_1H_2}{240}-\frac{23H_1^{\,2}H_2}{360}-\frac{H_1^{\,3}H_2}{40}+\frac{11H_2^{\,2}}{2160}-\frac{43H_1H_2^{\,2}}{1080}-\\
&\frac{71H_1^{\,2}H_2^{\,2}}{4320}-\frac{H_2^{\,3}}{135}-\frac{H_1H_2^{\,3}}{216}-\frac{H_2^{\,4}}{2160}\Bigg)t^6=0,
\end{aligned} \tag{11}$$

where $H_1 = h\theta$ and $H_2 = h^2\lambda$.

For the case r = 1, we substitute C and E in Eq. (8) into the right hand side of C in Eq. (9) and we obtain the stability polynomial and plot the stability region as in Figure 3. Figures 2 and 3 show the stability region of the three point implicit block one step method when r = 0 and r = 1,

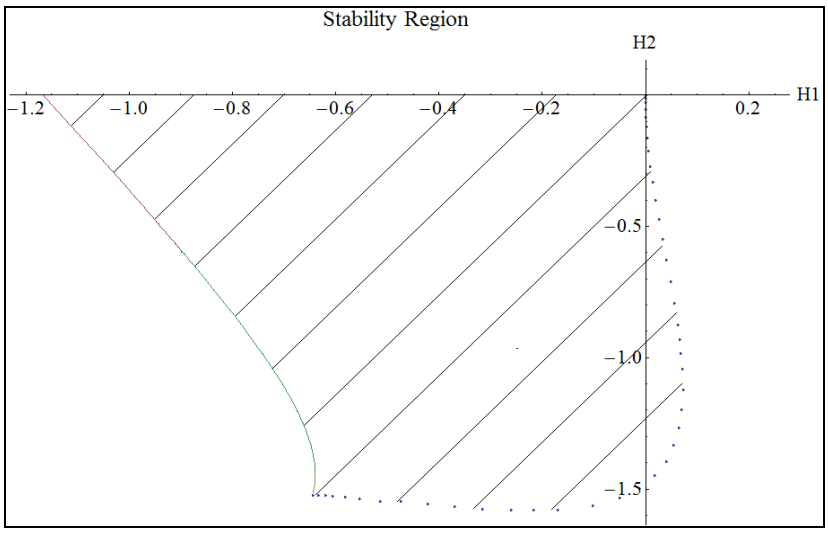

Figure 2 : Stability region for three point implicit block method at $r = 0$

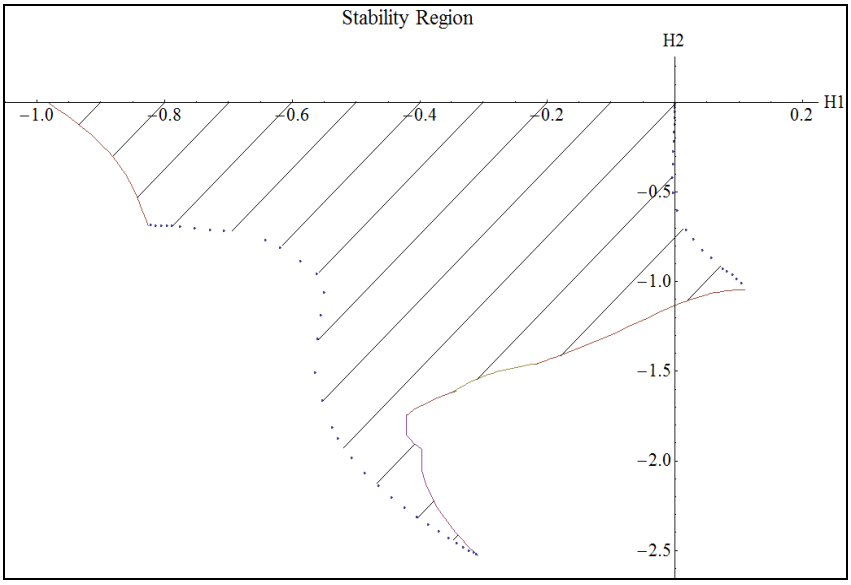

Figure 3 : Stability region for three point implicit block method at $r = 1$

The stability region is plotted using MATHEMATICA and the shaded region inside the boundary in Figures 2 and 3 demonstrate the stability region for the proposed method.

5. Numerical Results

The tables below show the numerical results for the three given problems when solved using the proposed method compared to the problems reduce to system of first order ODEs using the method in Majid *et al.* (2006).

The following notations are used in Tables 1-3:

TOL	Tolerance
MTD	Method employed
TS	Total steps taken

FS	Total failure steps
MAXE	Magnitude of the maximum error of the computed solution
AVERR	The average error
FCN	Total function calls
TIME	Execution time taken in microseconds
3PRED	Implementation of the three point implicit block one-step method in Majid *et al.* (2006) i.e. reducing to system of first order ODEs
3PDIR	Implementation of the direct three point block method proposed in this research

Tested problems :

Problem 1: $2yy'' - (y')^2 + 4y^2 = 0$

$$y\left(\frac{\pi}{6}\right) = \frac{1}{4}, \quad y'\left(\frac{\pi}{6}\right) = \frac{\sqrt{3}}{2}, \qquad x \in \left[\frac{\pi}{6}, 2\right]$$

Exact solution: $y(x) = (\sin x)^2$

Source: Jator & Li (2009)

Problem 2: $y_1'' = -y_2 + \sin \pi x$, $\quad y_1(0) = 0$, $\quad y_1'(0) = -1$

$y_2'' = y_1 + 1 - \pi^2 \sin \pi x$, $\quad y_2(0) = 1$, $\quad y_2'(0) = 1 + \pi \qquad [0,10]$

Exact solution: $y_1(x) = 1 - e^x$, $\quad y_2(x) = e^x + \sin \pi x$

Source: Bronson (1973)

Problem 3: $x^2 y'' + xy' + (x^2 - 0.25)y = 0$

$$y(1) = \sqrt{\frac{2}{\pi}} \sin 1, \quad y'(1) = \frac{(2\cos 1 - \sin 1)}{\sqrt{2\pi}}, \qquad x \in [1,8]$$

Exact solution: $y(x) = \sqrt{\frac{2}{\pi x}} \sin x$

Source: Jator & Li (2009)

Table 1: Comparison between 3PRED and 3PDIR for solving Problem 1

TOL	MTD	TS	FS	MAXE	AVERR	FCN	TIME (ms)
10^{-2}	3PRED	2	0	7.69304e-003	2.61683e-004	37	197
	3PDIR	2	0	9.97275e-004	5.83536e-004	28	180
10^{-4}	3PRED	8	1	1.06150e-005	2.91476e-006	148	325
	3PDIR	4	0	1.90443e-005	6.18695e-006	61	241
10^{-6}	3PRED	19	1	2.34728e-007	6.20481e-008	340	547
	3PDIR	9	0	2.32153e-007	1.34058e-007	136	291
10^{-8}	3PRED	49	1	4.72364e-009	1.22088e-009	841	1132
	3PDIR	23	0	1.07486e-008	2.94740e-009	343	432

Table 2: Comparison between 3PRED and 3PDIR for solving Problem 2

TOL	MTD	TS	FS	MAXE	AVERR	FCN	TIME (ms)
10^{-2}	3PRED	21	1	5.69787e-003	8.64637e-004	325	1470
	3PDIR	10	0	2.80809e-002	1.69345e-002	121	540
10^{-4}	3PRED	74	1	4.20700e-006	1.02946e-006	1015	3650
	3PDIR	25	0	5.85020e-004	2.95871e-004	298	931
10^{-6}	3PRED	219	2	4.16237e-007	4.21474e-008	3289	9170
	3PDIR	82	1	2.74912e-006	8.18396e-007	964	3654
10^{-8}	3PRED	665	2	3.38589e-010	3.38589e-010	9352	32901
	3PDIR	157	2	5.73548e-008	2.79436e-008	1810	5422

Table 3: Comparison between 3PRED and 3PDIR for solving Problem 3

TOL	MTD	TS	FS	MAXE	AVERR	FCN	TIME
10^{-2}	3PRED	7	0	8.14259e-004	3.07213e-004	124	329
	3PDIR	6	0	8.58857e-004	3.08802e-004	76	235
10^{-4}	3PRED	17	0	1.12729e-005	4.87629e-006	307	548
	3PDIR	10	0	2.56193e-005	9.57997e-006	145	303
10^{-6}	3PRED	43	0	2.51517e-007	1.17662e-007	772	1180
	3PDIR	24	0	9.25077e-007	3.17166e-007	334	443
10^{-8}	3PRED	179	1	9.70038e-010	4.37159e-010	2683	4897
	3PDIR	58	0	2.67589e-009	9.97129e-009	820	741

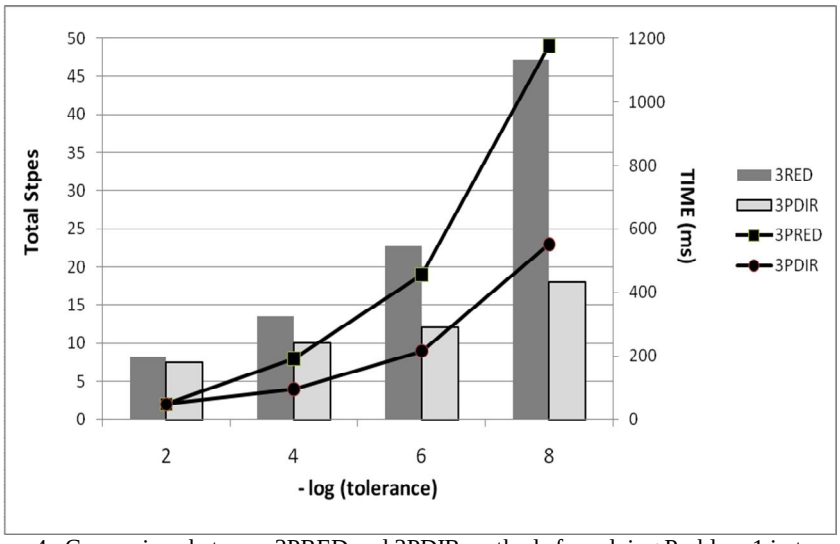

Figure 4 : Comparison between 3PRED and 3PDIR methods for solving Problem 1 in terms of – log (tolerance) versus number of total steps and time in microsecond

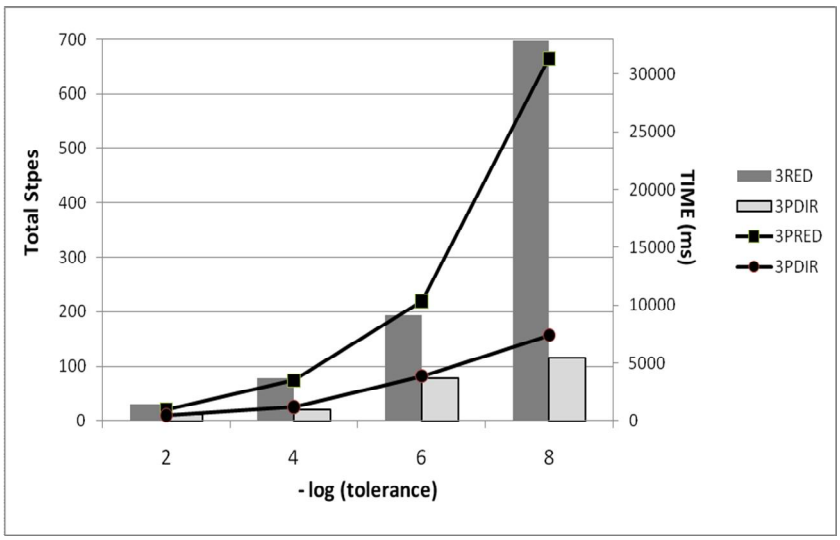

Figure 5 : Comparison between 3PRED and 3PDIR methods for solving Problem 2 in terms of – log (tolerance) versus number of total steps and time in microsecond

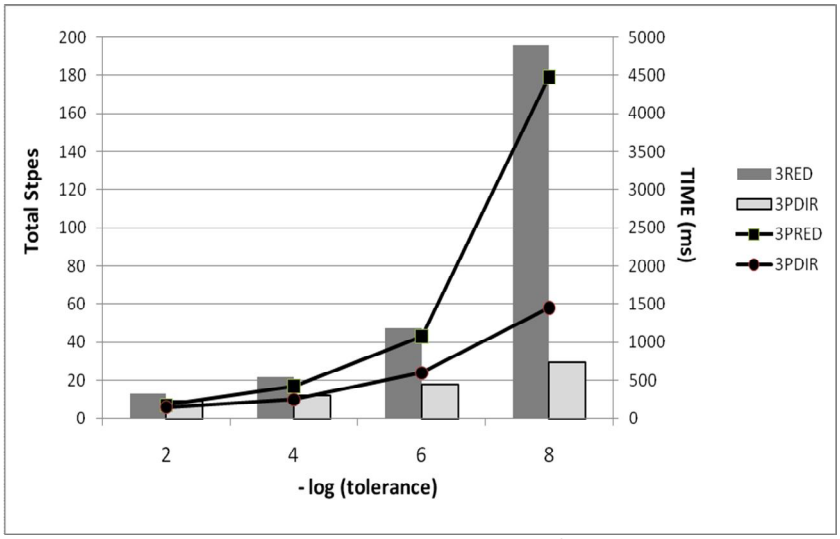

Figure 6 : Comparison between 3PRED and 3PDIR methods for solving Problem 3 in terms of – log (tolerance) versus number of total steps and time in microsecond

5. Discussions and Conclusions

From tables 1-3 and figures 4-6, the total number of steps taken by 3PDIR is comparable or less than 3PRED. It is also observed that 3PDIR required less number of function call compared to 3PRED at all given tolerances. In Problem 1 and 3, the maximum error of 3PDIR is comparable or one decimal place better than 3PRED method but vice versa at TOL=10^{-8}. The accuracy of 3PDIR in Problem 2 is one and two decimal places larger than 3PRED but it is still within the given tolerances. In terms of execution time, 3PDIR is faster than 3PRED when the problems were solved directly. Hence, we have shown the efficiency of the proposed method is suitable for solving general second order ODEs directly.

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