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NEW COMPUTATIONAL METHOD FOR SOLVING ORDINARY DIFFERENTIAL EQUATIONS

(Kaedah Pengiraan Baharu bagi Menyelesaikan Persamaan Pembezaan Biasa)

HUE CHI SAN, ZANARIAH ABDUL MAJID, MOHAMED OTHMAN & MOHAMED SULEIMAN

ABSTRACT

In this paper we present a developed couple block method for solving first order ordinary differential equations (ODEs). The coupled block method consists of two proposed block methods i.e the two point two step block method of order five and three point two step block method of order six. Therefore, these methods will estimate the numerical solutions at two and three points simultaneously within a block. The proposed block method is derived using Lagrange interpolation polynomial and is presented as in the simple form of the Adams Moulton type. The developed code is implemented using variable step size and order. The stability of the methods is also studied. Numerical results are presented to compare the performance of the developed code to the existence block method.

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

ABSTRAK

Dalam makalah ini dikemukan suatu kaedah blok gandingan yang telah dibangunkan untuk menyelesaikan persamaan pembezaan biasa peringkat pertama. Kaedah blok gandingan terdiri daripada dua kaedah blok yang dicadangkan, iaitu kaedah blok dua titik dua langkah peringkat lima dan kaedah blok tiga titik dua langkah peringkat enam. Oleh itu, kaedah ini akan menghampiri penyelesaian berangka pada dua dan tiga titik secara serentak dalam blok. Kaedah blok yang dicadangkan telah diterbitkan dengan menggunakan interpolasi polinomial Lagrange dan dipersembahkan dari jenis Adams Moulton yang ringkas. Kod yang dibangunkan telah dilaksanakan menggunakan panjang langkah dan peringkat yang berubah. Kestabilan kaedah ini juga dikaji. Hasil berangka diberikan untuk membandingkan prestasi kod yang dibangunkan dengan kaedah blok yang sedia ada.

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

1. Introduction

This paper considers the development of the codes for solving first order ODEs of the form

$$y' = f(x, y), \qquad y(x_0) = y_0, \qquad x \in [a, b]. \tag{1}$$

Mathematical models of problems in many physical science, social science, ecology as well as economics situations often involve the change of some variable with respect to another. The problems of the decay of radioactive material, population growth, chemical reactions the motion of a rotating mass around another body, and so forth may be modelled by Eq. (1).

Block method for numerical solution had been proposed by several researchers such as Milne (1953), Rosser (1967), Sommeijer *et al.* (1992), Burrage (1993) and Rao and Mouney (1997). They pointed out that application of block method can provide a faster solution to the problem since this method can simultaneously produces several numerical approximations within a block.

Gear and Watanabe (1974), Suleiman (1985), Shampine (1987), Lambert (1991) and Omar (1999) developed the variable step size and order multistep method for solving ODEs. However, the current multistep method using variable step size and order strategy as described by the researchers above involved tedious computations of divided difference and recurrence relation in computing the integration coefficients in the code. This will affect the execution times during the implementation of the code.

In the literature, Omar (1999) developed a variable step size and order two point block method for solving ODEs which the order k is restricted in the range $1 \le k \le 12$ as the integration progressed. A variable step size and order two point block methods of order five, seven and nine in the simple form of the Adams Moulton type has been proposed by Majid (2008) for solving ODEs.

In this paper, we introduce a coupled block method of order k and p where $k < p$ for solving Eq. (1) using variable step size and order. The couple block method is consist of two block methods i.e. *m*-point block method of order k and *n*-point block method of order p where $m \neq n$ and $k \neq p$. These methods are presented as in the simple form of the Adams Moulton type and all the coefficients involved in the code are stored in the proposed methods.

The aim of this paper is to develop a variable step size and order coupled block method of order five and six. The code is a combination of two point two step block method of order five which has been proposed by Majid (2008) and the new developed three point two step block method of order six. The proposed coupled block method will move two points or three points simultaneously within a block in order to reach the end of the interval. Hence, the developed code is expected to improve the total number of steps and achieve computational times faster compared to the code in Omar (1999).

2. Formulation of the Block Method

2.1. *Two point two step block method*

In Figure 1, the solutions of y_{n+1} and y_{n+2} with step size h are simultaneously computed in a block using three back values at the point $\{x_{n-j}\}_{j=0}^{2}$, of the previous two steps with step size rh.

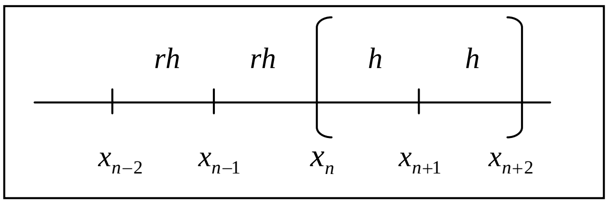

Figure 1: Two point two step block method

The two point two step block method is the combination of predictor of order four and the corrector of order five. The derivation and implementation of the method can be referred in Majid (2008). The following is the corrector formula in terms of r.

The 1st point

$$y(x_{n+1}) = y(x_n) + \frac{h}{240(r+1)(r+2)(2r+1)r^2}\Big[-(2r+1)r^2(3+15r+20r^2)\,f_{n+2}$$
$$+4r^2(r+2)(18+75r+80r^2)\,f_{n+1} + (r+1)(r+2)(2r+1)(7+45r+100r^2)\,f_n$$
$$-4(2r+1)(7+30r)\,f_{n-1} + (r+2)(7+15r)\,f_{n-2}\Big].$$

The 2nd point

$$y(x_{n+2}) = y(x_n) + \frac{h}{15r^2(2r+1)(r+2)(r+1)}\Big[r^2(2r+1)(5r^2+15r+9)\,f_{n+2}$$
$$+4r^2(r+2)(10r^2+15r+6)\,f_{n+1} + (r+2)(r+1)(2r+1)(5r^2-1)\,f_n$$
$$+4(2r+1)\,f_{n-1} - (r+2)\,f_{n-2}\Big].$$

2.2. *Three point two step block method*

In Figure 2, the three point two step block method will compute three points simultaneously in a block by using three back values at the points $\{x_{n-j}\}_{j=0}^{2}$, of the previous two steps with step size rh.

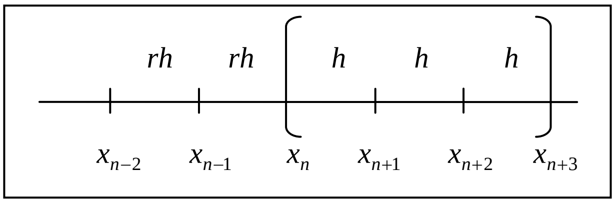

Figure 2: Three point two step block method

The corrector formula of the three point two step block method was derived using Lagrange interpolation polynomial and the interpolation points involved are $(x_{n-2}, f_{n-2}), \ldots, (x_{n+3}, f_{n+3})$. The three values of y_{n+1}, y_{n+2} and y_{n+3} can be obtained by integrating over the interval $[x_n, x_{n+1}], [x_n, x_{n+2}]$ and $[x_n, x_{n+3}]$ respectively using **MAPLE** and the following corrector formula in terms of r can be obtained:

The 1st point

$$y(x_{n+1}) = y(x_n) + \frac{h}{60}\Bigg[\frac{(4+21r+30r^2)}{6(2r+3)(r+3)}\,f_{n+3} - \frac{(7+36r+50r^2)}{4(r+1)(r+2)}\,f_{n+2}$$
$$+\frac{(40+171r+190r^2)}{2(2r+1)(r+1)}\,f_{n+1} + \frac{(17+114r+270r^2)}{12r^2}\,f_n$$
$$-\frac{(17+76r)}{r^2(r+1)(r+2)(r+3)}\,f_{n-1} + \frac{(17+38r)}{4r^2(2r+1)(r+1)(2r+3)}\,f_{n-2}\Bigg]. \qquad (2)$$

The 2nd point

$$y(x_{n+2}) = y(x_n) + \frac{h}{15}\left[-\frac{(8+12r)}{6(2r+3)(r+3)} f_{n+3} + \frac{(44+72r+20r^2)}{4(r+1)(r+2)} f_{n+2} \right.$$
$$+ \frac{(40+108r+80r^2)}{2(2r+1)(r+1)} f_{n+1} + \frac{(-4+12r+60r^2)}{12r^2} f_n$$
$$\left. - \frac{(-4+8r)}{r^2(r+1)(r+2)(r+3)} f_{n-1} + \frac{(-4+4r)}{4r^2(2r+1)(r+1)(2r+3)} f_{n-2} \right]. \tag{3}$$

The 3rd point

$$y(x_{n+3}) = y(x_n) + \frac{h}{20}\left[\frac{(324+351r+90r^2)}{6(2r+3)(r+3)} f_{n+3} + \frac{(243+324r+90r^2)}{4(r+1)(r+2)} f_{n+2} \right.$$
$$+ \frac{(81r+90r^2)}{2(2r+1)(r+1)} f_{n+1} + \frac{(27+54r+90r^2)}{12r^2} f_n - \frac{(27+36r)}{r^2(r+1)(r+2)(r+3)} f_{n-1}$$
$$\left. + \frac{(27+18r)}{4r^2(2r+1)(r+1)(2r+3)} f_{n-2} \right]. \tag{4}$$

During the implementation of the method, the choices for the next step size will be limited to half, double or the same as the current step size. In case of successful step size, the ratio r for the next constant step size is 1.0. Whenever the step size is double, the ratio r is 0.5. In case of step size failure, r is 2.0. The corrector formula in Eq. (2), Eq. (3) and Eq. (4) will be simplified by substituting the value of r.

The three point two step block method is the combination of predictor of order five and the corrector of order six. The interpolation points involved for obtaining the predictor formula for y_{n+1}, y_{n+2} and y_{n+3} are $(x_{n-4}, f_{n-4}), \ldots, (x_n, f_n)$.

3. Implementation

Firstly, the code will start with two point two step block method of order five. It is implemented in *PE(CE)^s* mode where *P* and *C* denote the application of predictor and corrector respectively while *E* denotes the evaluation of function f for the first two blocks. The *s* indicates the number of iteration that is needed for the two point two step block method corrector formula to be converges using the convergence test:

$$\left| y_{n+2}^{(s+1)} - y_{n+2}^{(s)} \right| < 0.1 \times \text{TOL}.$$

The convergence test for three point two step block method is $\left| y_{n+3}^{(s+1)} - y_{n+3}^{(s)} \right| < 0.1 \times \text{TOL}.$

After the successful convergence test, local error for two point and three point block methods will be calculated to control the integration step. The local error for two point block method at x_{n+2} can be estimated as $E_{k-1} = y_{n+2}(k) - y_{n+2}(k-1)$ where $y_{n+2}(k)$ is the corrector formula of order k and $y_{n+2}(k-1)$ is a similar corrector formula of order $k-1$.

Similarly, local error for three point block method at x_{n+3} can be calculated as $E_k = y_{n+3}(k+1) - y_{n+3}(k)$.

Suppose that the local error test $E \le \mathrm{TOL}$ is accepted in the integration step, the next order and step size have to be determined. We choose the order for which the estimates step size on the next step is the maximum. Therefore, one of the methods of orders k and $k+1$ can be used as the next order. Having available E_{k-1} and E_k, the maximum step size are as follows:

$$h_{k-1} = h_{old} \times \left(\frac{TOL}{2.0 \times E_{k-1}} \right)^{\frac{1}{k}}, \qquad h_k = h_{old} \times \left(\frac{TOL}{2.0 \times E_k} \right)^{\frac{1}{k+1}} \tag{5}$$

where h_{old} is the step size from the previous block and let $h_{\max}$ be the maximum step size in Eq. (5). The order which give the $h_{\max}$ will be the order on the next block. Therefore, the approximation of values y can be simultaneously computed using two point or three point block methods on the next block. In our code, to consider raising the order only can be done after having enough points for the higher order method to be used in the next step.

In our code, the $h_{\max}$ in Eq. (5) is not the final new step size for next block. The final step size after a successful step is given by

$$\begin{aligned} & h_{new} = C \times h_{\max} \\ & \text{if } \left(h_{new} \ge 2 \times h_{old} \right) \text{ then } h_{new} = 2 \times h_{old} \\ & \text{else } h_{new} = h_{old} \end{aligned} \tag{6}$$

where $C = 0.8$ is a safety factor. The purpose of having the safety factor is to give a more conservative estimate of the new step size. The algorithm when the step failure occurs is

$$h_{new} = \frac{1}{2} \times h_{old}. \tag{7}$$

The test in Eq. (6) and Eq. (7) will allow the new step size to vary only by constant, doubling or halving.

4. Absolute Stability

In the development of the numerical methods, it is of practical importance to study the absolute stability region for those methods. All the stability regions in this paper were obtained using Mathematica programming.

The absolute stability of two point and three point block methods were derived in the previous section on a linear first order problem when those methods are applied to the test equation

$$y' = f = \lambda y. \tag{8}$$

The stability region is investigated when the step size is constant, double and halved for each of the method. For example, the following equation represent the formula of the three point two step block method at r=1.0,

$$
\begin{aligned}
y(x_{n+1}) &= y(x_n) + \frac{h}{1440}\left(11 f_{n+3} - 93 f_{n+2} + 802 f_{n+1} + 802 f_n - 93 f_{n-1} + 11 f_{n-2}\right)\\
y(x_{n+2}) &= y(x_n) + \frac{h}{90}\left(- f_{n+3} + 34 f_{n+2} + 114 f_{n+1} + 34 f_n - f_{n-1}\right)\\
y(x_{n+3}) &= y(x_n) + \frac{h}{160}\left(51 f_{n+3} + 219 f_{n+2} + 114 f_{n+1} + 114 f_n - 21 f_{n-1} + 3 f_{n-2}\right).
\end{aligned} \tag{9}
$$

Now, substituting Eq. (8) in Eq. (9) and form a matrix equivalent to

$$AY_m - (B + Ch)Y_{m-1} = 0 \tag{10}$$

where,

$$
A = \begin{bmatrix} 1 - \frac{802}{1440}h\lambda & \frac{93}{1440}h\lambda & -\frac{11}{1440}h\lambda \\ -\frac{114}{90}h\lambda & 1 - \frac{34}{90}h\lambda & \frac{1}{90}h\lambda \\ -\frac{114}{160}h\lambda & -\frac{219}{160}h\lambda & 1 - \frac{51}{160}h\lambda \end{bmatrix}, \; B = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix},
$$

$$
C = \begin{bmatrix} \frac{11}{1440}\lambda & -\frac{93}{1440}\lambda & \frac{802}{1440}\lambda \\ 0\lambda & -\frac{1}{90}\lambda & \frac{34}{90}\lambda \\ \frac{3}{160}\lambda & -\frac{21}{160}\lambda & \frac{114}{160}\lambda \end{bmatrix}, \; Y_m = \begin{bmatrix} y_{n+1} \\ y_{n+2} \\ y_{n+3} \end{bmatrix}, \; Y_{m-1} = \begin{bmatrix} y_{n-2} \\ y_{n-1} \\ y_n \end{bmatrix}. \tag{11}
$$

The stability polynomial of three point two step block method at *r*=1.0 is obtained by solving $\det\left|tA - (B + Ch)\right| = 0$ as follow:

$$
\begin{aligned}
&t^3\left(1 - \frac{361}{288}\bar{h} - \frac{77749}{129600}\bar{h}^2 - \frac{979}{8640}\bar{h}^3\right) + t^2\left(-1 - \frac{167}{90}\bar{h} - \frac{48409}{43200}\bar{h}^2 - \frac{32059}{43200}\bar{h}^3\right)\\
&t\left(\frac{157}{1440}\bar{h} + \frac{4669}{43200}\bar{h}^2 + \frac{1313}{43200}\bar{h}^3\right) + \frac{11}{129600}\bar{h}^2 + \frac{1}{43200}\bar{h}^3 = 0
\end{aligned} \tag{12}
$$

where $\bar{h} = h\lambda$ and the stability region is in Figure 4. The stability regions for two point two step block method is shown in Figure 3.

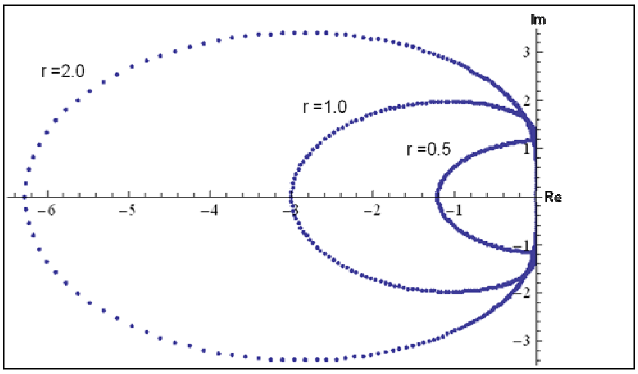

Figure 3: Stability region for two point two step block method
when r=1.0, r=2.0 and r=0.5

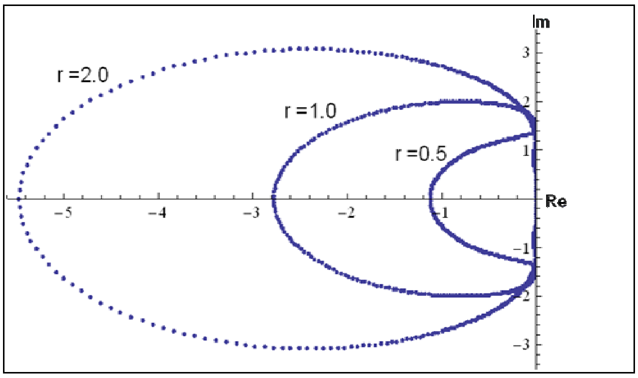

Figure 4: Stability region for three point two step block method
when r=1.0, r=2.0 and r=0.5

The stability region is bounded by the dotted points. Figures 3-4 clearly showed that the stability region is getting smaller when the step size being constant (r=1.0) or double (r=0.5) for both proposed methods. In addition, the stability region is the largest when the step size is halved (r=2.0) for all the methods. We also observed that the stability regions for higher order method are smaller compared to the stability regions for lower order method.

5. Results and Discussions

The efficiency of the developed codes in the previous sections are tested using the following problems:

Problem 1: Nonlinear Krogh's problem (Non stiff)

$$y_i' = -\beta_i y_i + y_i^2, \quad i = 1,2,3,4$$

$$y_i(0) = -1, \qquad [0,20]$$

$$\beta_1 = 0.2, \quad \beta_2 = 0.2, \quad \beta_3 = 0.3, \quad \beta_4 = 0.4$$

Solution: $$y(x) = \frac{\beta_i}{1 + c_i e^{\beta_i x}}, \quad c_i = -(1 + \beta_i)$$

Source: Johnson & Barney (1976)

Problem 2: A two-body orbit problem (Mildly stiff)

$$y_1' = y_3,\ \ y_2' = y_4,\ \ y_3' = -\frac{y_1}{r^3},\ \ y_4' = -\frac{y_2}{r^3},\ \ r = \sqrt{y_1^2 + y_2^2}$$

$$y_1(0) = 1,\ \ y_2(0) = 0,\ \ y_3(0) = 0,\ \ y_4(0) = 1,\qquad [0,20]$$

Solution: $y_1(x) = \cos(x),\ \ y_2(x) = \sin(x),$

$y_3(x) = -\sin(x),\ \ y_4(x) = \cos(x),$

Source: Hairer *et al*. (1993)

Problem 3:

$$y_1' = 1 + y_1 + 2y_2,$$

$$y_2' = -1 + 4y_1 + 3y_2,$$

$$y_1(0) = 1,\ \ y_2(0) = 2,\qquad [0,100]$$

Solution: $y_1(x) = e^{5x} - e^{-x} + 1,$

$y_2(x) = 2e^{5x} + e^{-x} - 1,$

Source: Bronson (1973)

The notations used in the tables are as follows:

TOL	Tolerance
MTD	Method employed
TS	Total steps taken
FS	Total failure steps
MAXE	Magnitude of the maximum error
AVEERR	Magnitude of the average error
FCN	Total function calls
Time	The execution time taken in microseconds
CB(5,6)	Implementation of coupled block method (two and three points) of order five and six
2PBVSO	Implementation of two point block method of variable step size and order in Omar(1999)

The errors calculated are defined as:

$$(e_i)_t = \left| \frac{(y_i)_t - \left(y(x_i)_t\right)}{A + B\left(y(x_i)_t\right)} \right|$$

where $(y)_t$ is the t-th component of the approximate y. A=1, B=0 correspond to the absolute error test. A=0, B=1 correspond to the relative error test and finally A=1, B=1 correspond to mixed error test. The relative error test is used for Problem 1 and Problem 3 while the mixed error test is utilised for Problem 2. The maximum error and average error are defined as follow:

MAXE = $\max_{1 \le i \le SSTEP} \left(\max_{1 \le i \le N} (e_i)_t \right)$ and

$$\text{AVEERR} = \frac{\sum_{i=1}^{SSTEP} \sum_{i=1}^{N} (e_i)_t}{(P)(N)(SSTEP)}$$

where P is the number of point, N is the number of equations in the system and $SSTEP$ is the number of successful steps.

The performance of the codes were written and executed in C language. The following tables showed the numerical results for the tested problems.

Table 1: Comparison between CB(5,6) and 2PBVSO for Solving Problem 1

TOL	MTD	TS	FS	MAXE	AVEERR	FCN	TIME(ms)
10^{-4}	CB(5,6)	32	0	3.25632(-6)	9.29801(-7)	222	767
	2PBVSO	36	0	1.52382(-4)	1.27857(-5)	109	1239
10^{-6}	CB(5,6)	44	0	2.04522(-8)	4.15156(-9)	420	1266
	2PBVSO	53	0	8.43893(-7)	3.18774(-7)	160	1673
10^{-8}	CB(5,6)	76	0	1.88864(-10)	7.87324(-11)	747	2159
	2PBVSO	118	0	1.81094(-8)	9.31300(-9)	355	3350
10^{-10}	CB(5,6)	143	0	2.73984(-12)	1.22357(-12)	1422	4079
	2PBVSO	264	0	2.01525(-10)	1.10543(-10)	793	7399

Table 2: Comparison between CB(5,6) and 2PBVSO for Solving Problem 2

TOL	MTD	TS	FS	MAXE	AVEERR	FCN	TIME(ms)
10^{-4}	CB(5,6)	46	0	9.02471(-5)	1.40442(-5)	541	1428
	2PBVSO	52	0	5.02384(-2)	6.30896(-3)	157	1682
10^{-6}	CB(5,6)	97	0	6.59849(-7)	1.87380(-7)	1043	2747
	2PBVSO	102	0	3.59812(-3)	4.94070(-4)	307	3216
10^{-8}	CB(5,6)	123	0	1.69570(-8)	2.83364(-9)	1616	3858
	2PBVSO	228	0	8.47692(-5)	1.22402(-5)	685	7115
10^{-10}	CB(5,6)	275	0	2.80919(-11)	4.58084(-12)	3144	8026
	2PBVSO	537	0	1.06158(-6)	1.60873(-7)	1612	16805

Table 3: Comparison between CB(5,6) and 2PBVSO for Solving Problem 3

TOL	MTD	TS	FS	MAXE	AVEERR	FCN	TIME(ms)
10^{-4}	CB(5,6)	989	0	1.02050(-4)	5.00269(-5)	11767	16205
	2PBVSO	511	0	2.25449(-1)	1.04599(-1)	3690	10598
10^{-6}	CB(5,6)	1237	0	9.45001(-6)	4.65692(-6)	18377	22139
	2PBVSO	1543	0	5.23500(-4)	2.58489(-4)	11264	29129
10^{-8}	CB(5,6)	3070	0	2.64591(-8)	1.31565(-8)	36703	50258
	2PBVSO	5945	0	8.03553(-6)	4.00485(-6)	43624	102028
10^{-10}	CB(5,6)	7650	0	2.92513(-10)	1.14954(-10)	91641	125499
	2PBVSO	14550	0	1.01089(-7)	5.04638(-8)	115674	249808

The numerical results in Table 1-3 showed the advantage of using CB(5,6) method over the 2PBVSO method in terms of accuracy. It is obvious that the proposed method has better maximum error and average error at all tolerances. It can be observed that generally the total number of steps taken by CB(5,6) method is less than the total number of steps taken by 2PBVSO method in all the tested problems. The proposed method shows greater reduction in the total number of steps at smaller tolerances.

Based on the numerical results, we observed that in most cases the execution times of CB(5,6) is faster than 2PBVSO for solving the given problems at all tolerances; even though the function calls in CB(5,6)is more than the function calls in 2PBVSO.

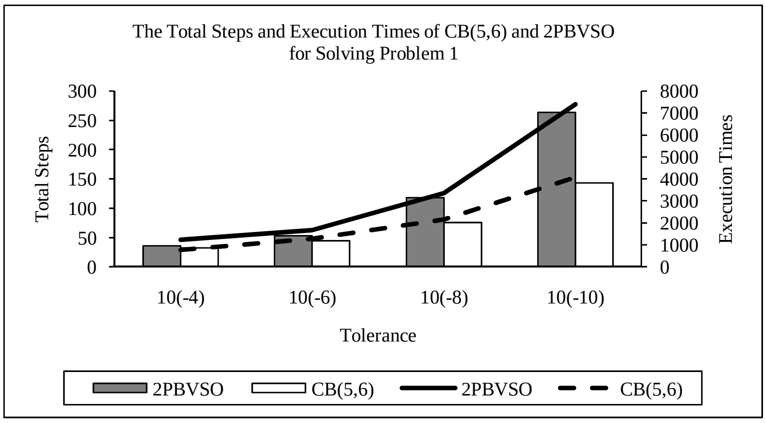

Figure 5: The total steps and execution times of CB(5,6) and 2PBVSO for solving Problem 1

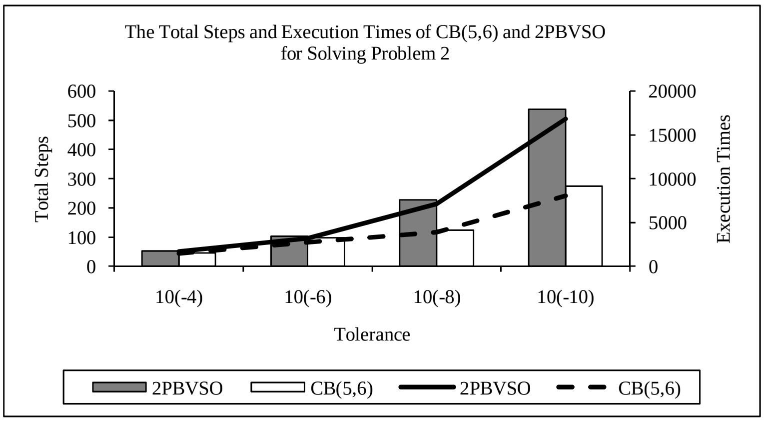

Figure 6: The total steps and execution times of CB(5,6) and 2PBVSO for solving Problem 2

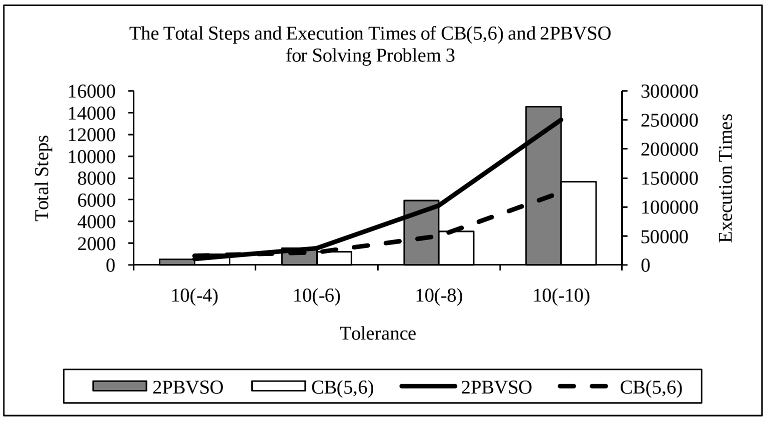

Figure 7: The total steps and execution times of CB(5,6) and 2PBVSO for solving Problem 3

The graphs in Figure 5-7 clearly showed that the CB(5,6) code reduced the total number of steps to almost one half at smaller tolerances. Generally, the gaps between the execution times line of both methods indicates that CB(5,6) is more efficient than 2PBVSO in the tested problems.

6. Conclusion

In this paper, we have considered the performance of the coupled block method that consist of two point two step and three point two step block methods for solving system of ODEs using variable step size and order. The developed coupled block method has shown the superiority in terms of total number of steps, maximum error, average error and execution times over the 2PBVSO method.

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