Third Order Backward Difference Formula for a First Order Stiff System in Piecewise Uniform Mesh

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ABSTRACT: Stiff system of Ordinary Differential Equations can be exemplified by problems in chemical kinetics, fluid dynamics, quantum mechanics, electrical networks, etc. In this paper, a third order Backward Differentiation Formula (BDF-3) is suggested on a piecewise uniform mesh(PUM) to solve a system of first order stiff Ordinary Differential Equations(ODEs). It is proved that the numerical approximations generated by this method with PUM produce numerical solutions with less computational effort and less error as compared to the method without PUM. Numerical results are presented in support of the theory.

Keywords: System of stiff differential equations, Initial value problem, BDF-3, Piecewise uniform mesh.

I. INTRODUCTION

In this paper, we are concerned with the numerical solution of the linear system of first order equations

$$\begin{pmatrix} \frac{du(t)}{dt} \\ \frac{dv(t)}{dt} \end{pmatrix} = \begin{pmatrix} f_1(t,u,v) \\ f_2(t,u,v) \end{pmatrix}, \text{.......(1.1)}$$

where $\begin{pmatrix} f_1(t,u,v) \\ f_2(t,u,v) \end{pmatrix} = A\begin{pmatrix} u(t) \\ v(t) \end{pmatrix} + \begin{pmatrix} g_1(t) \\ g_2(t) \end{pmatrix}$

where $A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$,

a constant matrix and $g_1(t), g_2(t)$

are continuous functions of t, where $t \in (0,1]$ with initial values

$$u(0) = \alpha \;,\; v(0) = \beta, \text{.............(1.2)}$$

and here

$$|a_{ij}| >> 1, \text{for } i, j = 1,2.$$

The linear system (1.1) - (1.2) is said to be stiff if

(i) $Re(\lambda_i) < 0, \quad i = 1,...,n$ and

(ii) $max_i |Re(\lambda_i)| >> min_i |Re(\lambda_i)|$ where λ_i are the eigenvalues of stiff ODEs,

n is the number of equations in the system and the ratio

(1.1)

$$SR = \frac{max_i |real \;\; part\; of \;\; \lambda_i|}{min_i |real \;\; part\; of \;\; \lambda_i|}, i = 1,2,....,n$$

(1.3)

is called the stiffness ratio or stiffness index. In [24], [25] and [26] Trapezoidal method, Backward euler method and second order Backward difference formula with the PUM was implemented for stiff system of ODEs for all $a_{ij} >> 1$. In this paper we apply the work for another method BDF-3 in PUM for all $a_{ij} >> 1$.

For a detailed discussion on stiff nature, application, implicit methods and BDF-3 with UM of stiff system of ODEs, one may refer to [1, 2, 5, 6, 7, 9, 10, 11, 12, 15, 17, 18, 21, 22, 23] and the thesis [3], to name a few. PUM are discussed by several researchers such as C. Clavero, J. L. Gracia and F. Lisbona [4], Kailash C. Patidar [13], J. J. H. Miller, E. O' Riordan and G. I. Shishkin [16], Natalia Kopteva and Eugene O' Riordan [19].

2 BDF-3 Scheme

Approximating the equations (1.1) and (1.2) by applying the BDF-3 method we have

$$\begin{cases} u_{j+1} = \frac{2}{11}u_{j-2} - \frac{9}{11}u_{j-1} + \frac{18}{11}u_j + \frac{6\,h}{11}[\,f_1(t_{j+1}, u_{j+1}, v_{j+1})] \\ v_{j+1} = \frac{2}{11}v_{j-2} - \frac{9}{11}v_{j-1} + \frac{18}{11}v_j + \frac{6\,h}{11}[\,f_2(t_{j+1}, u_{j+1}, v_{j+1})] \end{cases}$$

……………………………….(2.1)

where $j = 1\text{to}(N-1)$ and N is the number of mesh point.

From (2.1), u_{j+1} and v_{j+1} are determined implicitly. The new solution approximation needs to be computed iteratively, typically by a explict Euler method

$$\begin{cases} u_{j+1} = u_j + hf_1(t_j, u_j, v_j) \\ v_{j+1} = v_j + hf_2(t_j, u_j, v_j) \quad where \quad j = 0\text{to}(N-1) \end{cases}$$

(2.2)

BDF-2 is A-stable (damping out errors but not being too dissipative) but all higher order methods are not A-stable. Indeed, Dahlquist in 1963, proved that a multistep method that is A-stable cannot have an order greater than two and that the method of order two with the smallest error constant (0.5) is the trapezoidal rule. [7] Since the restriction on order for an A-stable method to solve stiff systems is a severe one, two less demanding stability definitions have been proposed:

(i) $A(\alpha)-$stable [14] if it is absolute stable for some (sufficiently small) $\alpha \in (0, \frac{\pi}{2})$ and

(ii) Stiffly stable [8, 14] if in the region R_1 $(Re(\lambda h) \le -a)$ it is absolutely stable, and in R_2 $(-a < Re(\lambda h) < b)$, $(|Im(\lambda h)| < c)$ it is accurate. BDfs are not necessarily A-stable but are $A(\alpha)-$ or stiffly stable.

BDF-3 is $A(\alpha)$ stable rather than A-stable; its stability region includes a wedge of angle α and this includes the eigenvalues of many problems such as those arising in fluid mechanics. BDF-3 method may not be pretty or easy to use, but it will handle rough country and will nearly always get you where you want to go.

In the next section, the description of PUM is presented.

3 Description of PUM

The point σ is called the transition point in the literature of SPPs. This point divide the given region $[0,1]$ into two regions $[0,\sigma]$ and $[\sigma,1]$; in one region the solution changes abruptly and in another it is smooth. To get a better picture of the solution in the first region, being a smaller one, we take $\frac{N}{4}$ points there.

Therefore the PUM is constructed by dividing $[0,\sigma]$ into $\frac{N}{4}$ equal mesh elements and $[\sigma,1]$ into $\frac{3N}{4}$ equal mesh elements. The piecewise uniform mesh is used with the following location of the transition point $\sigma = \min\{\frac{1}{4},(\frac{\varepsilon}{\alpha})\, lnN\}$. (3.1)

Choose the parameter ε as

$$\varepsilon < \frac{1}{M}, \tag{3.2}$$

where M is the greatest eigen value and α is the smallest eigen value of the matrix A.

Assume that $N = 2^m \ \ with \ \ m \geq 11 \ for \ all\, |a_{ij}(t)| >> 1$

for $j = 1,2$ where $t \in (0,1]$ and

$$\begin{cases} t_j = jh_1 \quad where \quad h_1 = \frac{4\sigma}{N}, \\ j = 0(1)\frac{N}{4}, \\ t_j = \sigma + (j - \frac{N}{4})h_2 \ where \ h_2 = \frac{4(1-\sigma)}{3N}, \\ j = (\frac{N}{4}+1)(1)N. \end{cases} \tag{3.3}$$

If $\sigma = \frac{1}{4}$ then $h_1 = N^{-1}$ and $h_2 = N^{-1}$.

In such a case the method can be analysed using the standard techniques. We therefore assume that

$$\sigma = \frac{\varepsilon}{\alpha} lnN. \tag{3.4}$$

The above scheme will give less error and less average error of the solution if the stiff ratio lies between 400 to 1000.

4 Order of Convergence

In general, $u(t_{j+1})$ is the exact value and u_{j+1} is the approximate numerical value and the local truncation error at the point $t_{(j+1)}$ in the BDF-3 with UM is

$$T_{j+1} = u(t_{j+1}) - u_{j+1} \quad where j = 0,1 \ldots N-1$$

$$= u(t_{j+1}) - \frac{18}{11}u(t_j) + \frac{9}{11}u(t_{j-1}) - \frac{2}{11}u(t_{j-2})$$

$$-\frac{6h}{11}[f(t_{j+1}, u(t_{j+1}))]$$

$$= u(t_{j+1}) - \frac{18}{11}[u(t_{j+1}) - hu^{'}(t_{j+1}) + \frac{h^2}{2}u^{''}(t_{j+1})$$

$$-\frac{h^3}{3!}u^{'''}(t_{j+1}) + \frac{h^4}{4!}u^4(t_{j+1})]$$

$$+\frac{9}{11}[u(t_{j+1}) - 2hu^{'}(t_{j+1}) + \frac{4h^2}{2}u^{''}(t_{j+1}) - \frac{8h^3}{3!}u^{'''}(t_{j+1})$$

$$+\frac{16h^4}{4!}u^4(t_{j+1})]$$

$$-\frac{2}{11}[u(t_{j+1}) - 3hu^{'}(t_{j+1}) + \frac{9h^2}{2}u^{''}(t_{j+1}) - \frac{27h^3}{3!}u^{'''}(t_{j+1})$$

$$+\frac{81h^4}{4!}u^4(t_{j+1})] - \frac{6h}{11}u^{'}(t_{j+1})$$

where
$$u(t_j) = u(t_{j+1} - h); \quad f(t_{j+1}, u_{j+1}) = u^{'}(t_{j+1});$$
$$u(t_{j-1}) = u(t_{j+1} - 2h);$$
$$u(t_{j-2}) = u(t_{j+1} - 3h)$$

$$\Rightarrow T_{j+1} = Ch^4 u^4(t_{j+1})$$

Applying the BDF-3 with PUM, the truncation error for $0 \le j \le \frac{N}{4} - 1$ is

$$T_{j+1} = u(t_{j+1}) - u_{j+1} \quad \text{where} j = 0,1 \ldots N-1$$

$$= u(t_{j+1}) - \frac{18}{11}u(t_j) + \frac{9}{11}u(t_{j-1}) - \frac{2}{11}u(t_{j-2})$$

$$-\frac{6\,h_1}{11}[f(t_{j+1}, u(t_{j+1}))]$$

$$= u(t_{j+1}) - \frac{18}{11}[u(t_{j+1}) - h_1 u'(t_{j+1}) + \frac{h_1^2}{2}u''(t_{j+1})$$

$$-\frac{h_1^3}{3!}u'''(t_{j+1}) + \frac{h_1^4}{4!}u^4(t_{j+1})]$$

$$+\frac{9}{11}[u(t_{j+1}) - 2h_1 u'(t_{j+1}) + \frac{4h_1^2}{2}u''(t_{j+1}) - \frac{8h_1^3}{3!}u'''(t_{j+1})$$

$$+\frac{16h_1^4}{4!}u^4(t_{j+1})]$$

$$-\frac{2}{11}[u(t_{j+1}) - 3h_1 u'(t_{j+1}) + \frac{9h_1^2}{2}u''(t_{j+1}) - \frac{27h_1^3}{3!}u'''(t_{j+1})$$

$$+\frac{81h_1^4}{4!}u^4(t_{j+1})] - \frac{6h_1}{11}u'(t_{j+1})$$

where
$$u(t_j) = u(t_{j+1} - h_1);$$
$$f(t_{j+1}, u_{j+1}) = u'(t_{j+1});$$
$$u(t_{j-1}) = u(t_{j+1} - 2h_1);$$
$$u(t_{j-2}) = u(t_{j+1} - 3h_1)$$

$$\Rightarrow T_{j+1} = Ch_1^4 u^4(t_{j+1})$$

The truncation error for $\frac{N}{4} \le j \le N-1$ is

$$T_{j+1} = u(t_{j+1}) - u_{j+1} \quad \text{where} j = 0,1 \ldots N-1$$

$$= u(t_{j+1}) - \frac{18}{11}u(t_j) + \frac{9}{11}u(t_{j-1}) - \frac{2}{11}u(t_{j-2})$$

$$-\frac{6\,h_2}{11}[f(t_{j+1}, u(t_{j+1}))]$$

$$= u(t_{j+1}) - \frac{18}{11}[u(t_{j+1}) - h_2 u'(t_{j+1}) + \frac{h_2^2}{2}u''(t_{j+1})$$

$$-\frac{h_2^3}{3!}u'''(t_{j+1}) + \frac{h_2^4}{4!}u^4(t_{j+1})]$$

$$+\frac{9}{11}[u(t_{j+1}) - 2h_2 u'(t_{j+1}) + \frac{4h_2^2}{2}u''(t_{j+1})$$

$$-\frac{8h_2^3}{3!}u'''(t_{j+1}) + \frac{16h_2^4}{4!}u^4(t_{j+1})]$$

$$-\frac{2}{11}[u(t_{j+1}) - 3h_2 u'(t_{j+1}) + \frac{9h_2^2}{2}u''(t_{j+1})$$

$$-\frac{27h_2^3}{3!}u'''(t_{j+1}) + \frac{81h_2^4}{4!}u^4(t_{j+1})] - \frac{6h_2}{11}u'(t_{j+1})$$

where
$$u(t_j) = u(t_{j+1} - h_2); \quad f(t_{j+1}, u_{j+1}) = u'(t_{j+1});$$
$$u(t_{j-1}) = u(t_{j+1} - 2h_2); \quad u(t_{j-2}) = u(t_{j+1} - 3h_2)$$

$$\Rightarrow T_{j+1} = Ch_2^4 u^4(t_{j+1})$$

Therefore, the truncation error for BDF-3 with piecewise uniform mesh is

$$T_{j+1} = \begin{cases} C\,h_1^4\,u^4(t_{j+1}) & for \quad 0 \le j \le \frac{N}{4} - 1 \\ C\,h_2^4\,u^4(t_{j+1}) & for \quad \frac{N}{4} \le j \le N-1 \end{cases}$$

Similarly, the truncation error for the second component v can be easily derived.

$$we\ \ define\ \|Y\|_s = sup\{|u^{(s)}(t)|,|v^{(s)}(t)|\}$$
$$for\ all \quad t \in (0,1].$$

since $h_1 \le h_2$ then $h^4 = h_2{}^4$

Therefore $T_{j+1}(h) \le C\,h^4 \|Y\|_4$

$$where\ \|Y\|_4 = sup\{|u^4|,|v^4|\} \quad for\ all \quad t \in (0,1].$$

Hence, by the definition given as in [12], the order of convergence of BDF-3 with PUM is four.

5 Numerical example

In this section, we present two examples to illustrate the performance of our method. The numerical results of BDF-3 with PUM will be compared with uniform mesh(UM). The comparison is based in terms of maximum error and average error. The numerical results are recorded interms of the following quantities and tabulated. As the formula given in [20] for UM we have,

$h = \dfrac{(b-a)}{N}$, where b is the end value of t and a is the initial value of t.

The calculation of error (for PUM and UM) is given as,

$$error_j = |u(t_j)_{(exact\ solution)} - u_{j(approximate)}|.$$

For maximum error (MAXE) (for PUM and UM), we use the formula,

$$MAXE^N = \max(error_j)$$

The average error for BDF-3 with UM is defined as,

$$AVE = \frac{\sum_{j=1}^{N} error_j}{N}. \tag{4.1}$$

The average error(AVE) for BDF-3 with PUM is defined as,

$$AVE1 = \frac{\sum_{j=1}^{\frac{N}{4}} (error_j)}{\frac{N}{4}}$$

$$AVE2 = \frac{\sum_{j=\frac{N}{4}+1}^{N} (error_j)}{\frac{3N}{4}}$$

$$AVE = max\{AVE1, AVE2\}.$$

Examples 5.1 and 5.2 have stiffness ratio between 400 to 1000.

Example 5.1 $u'(t) = 998u(t) + 1998v(t)$

$$v'(t) = -999u(t) - 1999v(t) \quad \forall t \in [0,1],$$

$$u(0) = 1, v(0) = 1.$$

The exact solution is:

$$u(t) = 4e^{-t} - 3e^{-1000t}$$

$$v(t) = -2e^{-t} + 3e^{-1000t}.$$

The numerical results obtained by applying the PUM to the *example* 5.1 are given in Table 1.

Example 5.2 $u'(t) = 1195u(t) - 1995v(t)$

$$v'(t) = 1197u(t) - 1997v(t) \quad \forall t \in [0,1],$$

$$u(0) = 1, v(0) = 1.$$

Exact solution is:

$$u(t) = 10e^{-2t} - 8e^{-800t}$$

$$v(t) = -6e^{-2t} + 8e^{-800t}.$$

The numerical results obtained by applying the PUM to the *example* 5.2 are given in Table 2.

6 Conclusion

In this paper the BDF-3 have been presented and implemented with new mesh generation makes our method attractive for numerical solution of stiff problems having stiffness ratio from 400 to 1000 type problems. We have demonstrated the efficiency of our BDF-3 with PUM over the existing BDF-3 with UM as shown in the tables. Numerical example of differential equations has been used here to show the superiority of the proposed integration method, we conclude that when the number of subintervals N is increased we can obtain a very good accuracy. In general, for stiff equations when the mesh is refined with more number of points the stability will be lost. But on PUM eventhough the number of mesh points are increased the stability is not lost.

Table 1: *Value of* $MAXE(u), AVE(u), MAXE(v), AVE(v)$ *for the solution component* u *and* v *for the Example 5.1*

N	MESH	MAXE(u)	AVE(u)	MAXE(v)	AVE(v)
	PUM	0.1250e-004	0.1876e-006	0.6087e-005	0.9352e-007
	UM	0.4287e-001	0.1047e-004	0.2143e-001	0.5233e-005
	PUM	0.6545e-004	0.2777e-007	0.3275e-004	0.1387e-007
	UM	0.1267e-001	0.1546e-005	0.6333e-002	0.7731e-006
	PUM	0.4570e-004	0.4045e-008	0.2285e-004	0.2021e-008
	UM	0.3581e-002	0.2185e-006	0.1790e-002	0.1093e-006
	PUM	0.2590e-004	0.1054e-008	0.1295e-004	0.5270e-009
	UM	0.9572e-003	0.2921e-007	0.4785e-003	0.1461e-007
	PUM	0.1366e-004	0.2779e-009	0.6831e-005	0.1390e-009
	UM	0.2477e-003	0.3780e-008	0.1239e-003	0.1890e-008
	PUM	0.6986e-005	0.7107e-010	0.3493e-005	0.3554e-010
	UM	0.6303e-004	0.4809e-009	0.3151e-004	0.2404e-009

Table 2: *Value of* $MAXE(u), AVE(u), MAXE(v), AVE(v)$ *for the solution component* u *and* v *for the Example 5.2*

	Mesh	MAXE(u)	AVE(u)	MAXE(v)	AVE(v)
	PUM	0.7269e-002	0.2366e-005	0.4362e-002	0.1420e-005
	UM	0.4655e-001	0.1137e-004	0.2793e-001	0.6820e-005
	PUM	0.8184e-003	0.1332e-006	0.4912e-003	0.7994e-007
	UM	0.1429e-001	0.1744e-005	0.8571e-002	0.1046e-005
	PUM	0.1751e-003	0.1425e-007	0.1051e-003	0.8551e-008
	UM	0.4112e-002	0.2510e-006	0.2468e-002	0.1506e-006
	PUM	0. 5915e-004	0.2407e-008	0.3550e-004	0.1444e-008
	UM	0.1110e-002	0.3388e-007	0.6660e-003	0.2033e-007
	PUM	0.2633e-004	0.5356e-009	0.1580e-004	0.3214e-009
	UM	0.2887e-003	0.4405e-008	0.1732e-003	0.2643e-008
	PUM	0.1295e-004	0.1317e-009	0.7767e-005	0.7901e-010
	UM	0. 7364e-004	0.5619e-009	0.4418e-004	0.3371e-009

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