PARALLEL ONE-BLOCK SECOND DERIVATIVE BACKWARD DIFFERENTIATION TYPE FORMULAE FOR ORDINARY DIFFERENTIAL EQUATIONS

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ABSTRACT

The second derivative parallel block backward differentiation type formulas suffer zero instability for block size greater than six. This paper seeks to restructure the second derivative parallel block backward differentiation type formulas so as to develop a family of methods that overcomes zero instability. Condition upon which the new methods are zero-stable *apiori* is given. Methods developed in this paper are A-stable for block sizes up to four.

INTRODUCTION

The numerical integration of stiff Initial Value Problems (IVPs) in Ordinary Differential Equations (ODEs) of the form

$$y' = f(y), y(a) = y_0, a \le x \le b, y: R \to R^N, f: R \times R^N \to R^N, \tag{1}$$

is still a very active field of research as shown by the plethora contributions in recent years; some of which are documented in several books such as Burrage (1995), Butcher (2008), Fatunla, (1988), Lambert (1991), Hairer and Wanner (2002). The demand for new methods well-suited for integration of stiff IVPs in ode on parallel computers is still relevant in exploitation of computational high speed of modern day computers.

Exploitation of computation speedup is done via: (i) parallelism across the method; (ii) parallelism across the step, and (iii) parallelism across the system, Ikhile and Muka (2015), Burrage (1995). Classes of methods that parallelism across methods has been achieved include block methods. Block methods are generalization of classical Linear Multistep Methods (LMMs), Sommeijer *et al* (1989), Muka (2011). Numerous block methods have been proposed, these include block methods of Shampine and Watt (1969), Sommeijer *et al* (1989),Chu and Halmiton (1987), Chartier (1993), Muka and Ikhile (2009a, 2009b), Akpodamure and Muka (2016).

Muka and Ikhile (2009a) designed block methods which are direct generalization of the Second Derivative Backward Differentiation Formulas (SDBDF), (Hairer and Wanner (2002). These methods called the second derivative parallel block backward differentiation type formulas, are zero unstable for block sizes greater than six unlike the SDBDF which are zero unstable for step sizes greater than ten. This paper is devoted to restructuring of the second derivative parallel block backward differentiation type formulas in Muka and Ikhile (2009a); so as to develop a family of methods that is zero stable *apriori*. This is done using the idea of Chartier (1993).

METHODOLOGY

Chartier (1993) generalized the well known backward differentiation formulae (BDF), to design methods with the structure

$$Y_m = A_1 Y_{m-1} + hB_0 F(Y_m) \tag{2}$$

Where Y_m, and $F(Y_m)$ are k dimensional vectors given as:

$Y_m = (y_{n+1}, y_{n+2}, \cdots, y_{n+k})^T$, and $F(Y_m) = (f(y_{n+1}), f(y_{n+2}), \cdots, f(y_{n+k}))^T$ (for $n = mk,\ m = 0,1$). The y_n is the numerical approximation of the solution $y(x_n)$ of (1) at the point x_n. A_1 and B_0 are $k \times k$ matrices whose entries are real constants to be determined.

Zero-stability requires that the eigenvalues λ of matrix A_1 in (2) are all less than or equal to unity, and the eigenvalue λ equal to unity must be simple Muka and Ikhile (2009a), Lambert (1991). The method (2) is zero unstable for block size greater than three. The method (2) is reformulated in Chartier (1993), as follows:
Set

$$B_0 = \frac{1}{\gamma}(I + diag(c)), \tag{3}$$

where γ a nonzero real is constant, I is the $k \times k$ unit matrix and $diag(c)$ is $k \times k$ diagonal matrix with component $c = (1,2,\cdots,k)^T$. This is to ensure that the reformulated method with matrix B_0 in (3) is zero stable by design.
Inserting (3) into (2), we have

$$Y_m = A_1 Y_{m-1} + h\frac{1}{\gamma}(I + diag(c))F(Y_m). \tag{4}$$

We shall call (4) Backward Differentiation Type Block Formulae (BDTBF). The eigenvalues of matrix A_1 in (4) are known *apriori* and are given as

$$\lambda(\gamma) = 1 - \frac{j}{\gamma}, \quad j = 0,1,\cdots,k-1, \quad \gamma > 0. \tag{5}$$

In order to obtain zero-stable methods, the choice of parameter γ must satisfy the inequality

$$\gamma \geq \frac{k-1}{2}. \tag{6}$$

The second derivative parallel block backward differentiation type formulas developed in Muka and Ikhile (2009a) has the structure

$$Y_m = A_1 Y_{m-1} + hB_0 F(Y_m) + h^2 D_0 F'(Y_m) \tag{7}$$

with $F'(Y_m) = (f'(y_{n+1}), f'(y_{n+2}), \cdots, f'(y_{n+k}))^T$ and D_0 a $k \times k$ matrix with constant entries to be determined.
The method (7) is zero unstable for block sizes greater than six. Using the idea in Chartier (1993), we set matrices B_0 in (7) as defined in (3) and set D_0 as

$$D_0 = \frac{1}{\delta}(I + diag(c) + diag(c^2)). \tag{8}$$

where I ,and $diag(c)$ are as previously specified, δ a real constant and $diag(c^2)$ is $k \times k$ diagonal matrix with component $c^2 = (1, 2^2, \cdots, k^2)^T$.
Inserting (3) and (8) into (7) yields

$$Y_m = A_1 Y_{m-1} + \frac{h}{\gamma}(I + diag(c))F(Y_m) + \frac{h^2}{\delta}(I + diag(c) + diag(c^2))F'(Y_m) \tag{9}$$

Hereafter, we shall refer to (9) as Second Derivative Backward Differentiation Type Block Formulae (SDBDTBF).

Let $e = (1,1,\cdots,1)^T$, the elements of matrix A_1 in (9) can be determined using the following order conditions

$$C_0 = e - A_1 e$$
$$C_1 = c - A_1(c - ke) - \frac{1}{\gamma}(I + diag(c))e$$
$$C_2 = c^2 - A_1(c - ke)^2 - \frac{2}{\gamma}(I + diag(c))c - -\frac{2}{\delta}(I + diag(c) + diag(c^2))e$$
$$\vdots$$
$$C_j = c^j - A_1(c - ke)^j - \frac{j}{\gamma}(I + diag(c))c^{j-1} - -\frac{j(j-1)}{\delta}(I + diag(c) + diag(c^2))c^{j-2}, \quad j =,3,4,\dots \tag{10}$$

Lemma 1

SDBDTBF is of order p if for $j = 1,2,\cdots, p; \quad C_j = 0$ *and* $C_{p+1} \neq 0$.

Proof

The lemma can easily be proofed by Taylor's expansion of the linear difference operator (see Lambert (1991)) of the SDBDTBF (9).

By specifying matrices B_0 and D_0 as in equations (3) and (8), the free parameter space is reduced; so that for a k-point method the SDBDTBF will be of order $p = k - 1$.

Hence,

$$0 = c^j - A_1(c - ke)^j - \frac{j}{\gamma}(I + diag(c))c^{j-1} - \frac{j(j-1)}{\delta}(I + diag(c) + diag(c^2))c^{j-2}, \ j = 0,1,\dots,k-1 \tag{11}$$

holds. The binomial expansion of (11) yields

$$A_1 c^j = (1 - \frac{j}{\gamma} - \frac{j(j-1)}{\delta})c^j - (\frac{j}{\gamma} + \frac{j(j-1)}{\delta})c^{j-1} - \frac{j(j-1)}{\delta}c^{j-2} - \sum_{s=0}^{j-1} C_s^j c^s (-k)^{j-s}, \quad j = 0,1,\dots,k-1 \tag{12}$$

Since components of c are pair wise distinct, it therefore implies that the linear combination of the vectors $e, c, c^2, \dots c^j$ are linearly independent.

The coefficients of vectors $e, c, c^2, \dots c^j$ in (12) must all be necessarily equal to zero. This implies

$$\left| A_1 - (1 - \frac{j}{\gamma} - \frac{j(j-1)}{\delta})I \right| = 0. \tag{13}$$

Equation (13) is characteristics polynomial equation with distinct roots

$$(1 - \frac{j}{\gamma} - \frac{j(j-1)}{\delta}), \qquad j = 0,1,\cdots,k-1. \tag{14}$$

These roots are the eigenvalues of matrix A_1 in (9). Zero stability of the SDBDTBF requires that

$$\left| 1 - \frac{j}{\gamma} - \frac{j(j-1)}{\delta} \right| \leq 1, \quad j = 0,1,\dots,k. \tag{15}$$

Lemma 2

The SDBDTBF is zero stable if $\gamma \geq 0$ and satisfies

$$-\frac{(k-2)}{\delta} < \gamma < \frac{2\delta - (k-1)(k-2)}{\delta(k-1)}, \quad k \geq 2, \delta < 0 \tag{16}$$

Proof

Set $j = k-1$ in (15) and express γ in terms of δ.

Parameters γ and δ will be selected in a way as to ensure that $C_k = 0$ in (10), is satisfied and that γ is within the range of values in (16).

This choice of γ only exist if δ is a vector value which depends on γ. Therefore, we let $G = diag(\delta(k))$ be a $k \times k$ matrix with $\delta(\gamma) = (\delta_1(\gamma), \delta_2(\gamma), \cdots, \delta_k(\gamma))^T$. The matrix D_0 in (8) will now be

$$D_0 = G^{-1}(I + diag\,(c) + diag\,(c^2)) \tag{17}$$

while (16) becomes

$$-\frac{(k-2)}{\delta_i} < \gamma < \frac{2\delta_i - (k-1)(k-2)}{\delta_i(k-1)}, \quad k \geq 2,\ \delta_i(\gamma) < 0, \quad i = 1,2,\ldots,k. \tag{18}$$

The matrix coefficient A_1 of SDBDTBF are given for block sizes two, three and four with scalar parameter γ and the corresponding vector parameter δ.

Two Point Block Method

$$\gamma = \frac{19}{10},\ \delta(\gamma) = \left(\frac{3\gamma}{-3+\gamma}, \frac{14\gamma}{3(-5+2\gamma)}\right)^T$$

$$A_1 = \begin{pmatrix} \frac{2-\gamma}{\gamma} & \frac{2(-1+\gamma)}{\gamma} \\ \frac{3-2\gamma}{\gamma} & \frac{3(-1+\gamma)}{\gamma} \end{pmatrix},\ Y_{m-1} = \begin{pmatrix} y_{n-1} \\ y_n \end{pmatrix}, Y_m = \begin{pmatrix} y_{n+1} \\ y_{n+2} \end{pmatrix}$$

$$F(Y_{m-1}) = \begin{pmatrix} f_{n-1} \\ f_n \end{pmatrix}, F(Y_m) = \begin{pmatrix} f_{n+1} \\ f_{n+2} \end{pmatrix}, F'(Y_{m-1}) = \begin{pmatrix} f'_{n-1} \\ f'_n \end{pmatrix}, F'(Y_m) = \begin{pmatrix} f'_{n+1} \\ f'_{n+2} \end{pmatrix} \tag{19}$$

$$C_3 = \left[\frac{7-3\gamma}{3\gamma}, \frac{3}{7} - \frac{33}{8\gamma} + \frac{14\gamma}{15-6\gamma}\right]$$

Three Point Block Method

$$\gamma = \frac{1489}{705},\ \delta(\gamma) = \left(\frac{18\gamma}{-11+3\gamma}, -\frac{21\gamma}{-13+4\gamma}, \frac{78\gamma}{-47+15\gamma}\right)^T$$

$$A_1 = \begin{pmatrix} 1 - \frac{3}{\gamma} - \frac{3}{\delta_1} & \frac{6\gamma + 8\delta_1 - 3\gamma\delta_1}{\gamma\delta_1} & 3 - \frac{5}{\gamma} - \frac{3}{\delta_1} \\ 3 - \frac{15}{2\gamma} - \frac{7}{\delta_2} & -\frac{2(-7\gamma - 9\delta_2 + 4\gamma\delta_2)}{\gamma\delta_2} & 6 - \frac{21}{2\gamma} - \frac{7}{\delta_2} \\ 6 - \frac{14}{\gamma} - \frac{13}{\delta_3} & \frac{26\gamma + 32\delta_3 - 15\gamma\delta_3}{\gamma\delta_3} & 10 - \frac{18}{2\gamma} - \frac{13}{\delta_3} \end{pmatrix},\ Y_{m-1} = \begin{pmatrix} y_{n-2} \\ y_{n-1} \\ y_n \end{pmatrix}, Y_m = \begin{pmatrix} y_{n+1} \\ y_{n+2} \\ y_{n+3} \end{pmatrix}$$

$$F(Y_{m-1}) = \begin{pmatrix} f_{n-2} \\ f_{n-1} \\ f_n \end{pmatrix}, F(Y_m) = \begin{pmatrix} f_{n+1} \\ f_{n+2} \\ f_{n+3} \end{pmatrix}, F'(Y_{m-1}) = \begin{pmatrix} f'_{n-2} \\ f'_{n-1} \\ f'_n \end{pmatrix}, F'(Y_m) = \begin{pmatrix} f'_{n+1} \\ f'_{n+2} \\ f'_{n+3} \end{pmatrix} \tag{20}$$

$$C_4 = \left(\frac{85-33\gamma}{72\gamma}, -\frac{26}{9} + \frac{115}{18\gamma}, -\frac{67}{8} + \frac{2429}{120\gamma}\right)^T$$

Four Point Block Method

$$\gamma=\frac{64171}{26796},\ \delta(\gamma)=\left(\frac{105\gamma}{2(-25+6\gamma)},\frac{497\gamma}{3(-77+20\gamma)},\frac{1547\gamma}{36(-19+5\gamma)},\frac{3759\gamma}{-319+84\gamma}\right)^{T}$$

$$A_1=\begin{pmatrix} -1+\frac{11}{3\gamma}+\frac{6}{\delta_1} & 4-\frac{14}{\gamma}-\frac{21}{\delta_1} & -6+\frac{19}{\gamma}+\frac{24}{\delta_1} & 4-\frac{26}{3\gamma}-\frac{9}{\delta_1} \\ -4+\frac{13}{\gamma}+\frac{21}{\delta_2} & 15-\frac{93}{2\gamma}-\frac{70}{\delta_2} & -20+\frac{57}{\gamma}+\frac{77}{\delta_2} & 10-\frac{47}{2\gamma}-\frac{28}{\delta_2} \\ -10+\frac{94}{3\gamma}+\frac{52}{\delta_3} & 36-\frac{108}{\gamma}-\frac{169}{\delta_3} & -45+\frac{126}{\gamma}+\frac{182}{\delta_3} & 20-\frac{148}{3\gamma}-\frac{65}{\delta_3} \\ -20+\frac{185}{3\gamma}+\frac{105}{\delta_4} & 70-\frac{415}{2\gamma}-\frac{336}{\delta_4} & -84+\frac{235}{\gamma}+\frac{357}{\delta_4} & 35-\frac{535}{6\gamma}-\frac{126}{\delta_4} \end{pmatrix} \quad (21)$$

$$C_5=\left(\frac{-2}{7}+\frac{83}{105\gamma},\frac{-154}{71}+\frac{3799}{710\gamma},-\frac{1026}{119}+\frac{12354}{595\gamma},-\frac{7406}{537}+\frac{131161}{3222\gamma}\right)^{T}$$

Stability Analysis of SDBDTBF.

The choices of γ *and* δ in (19) ensure that A_1 satisfies the root condition (*i.e.* zero stability). Applying SDBDTBF (9) to the test equation $y'=\lambda y$, yields the characteristic polynomial

$$\pi(\mathrm{R},z)=\det\left(-A_1+R-\frac{zR}{\gamma}(I+diag(c))-\frac{z^2R}{\delta}(I+diag(c)+diag(c^2))\right)=0. \quad (22)$$

The boundary locus for SDBDTBF for block sizes two, three and four are shown in Figures 1–3.

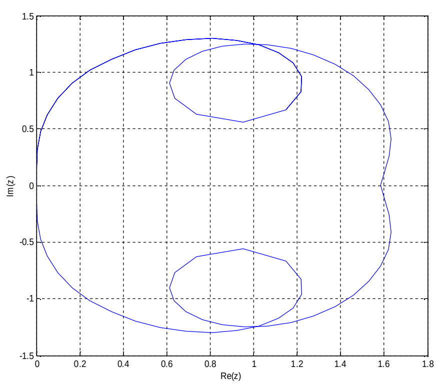

Fig. 1: Stability plot of SDBDTBF block size three

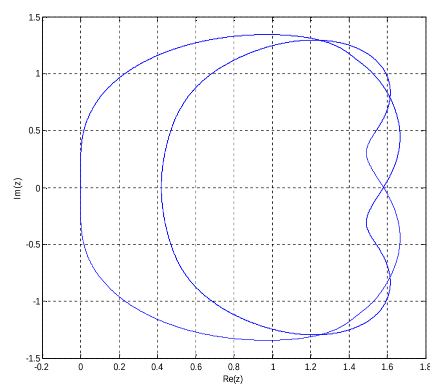

Fig. 2: Stability plot of SDBDTBF block size three

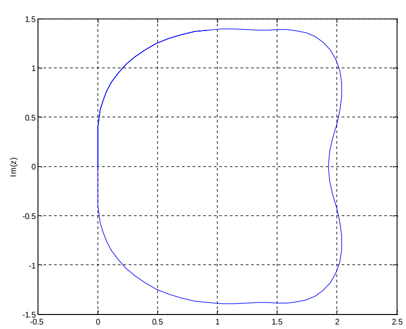

Fig. 3: stability plot of SDBDTBF size four

From the boundary locus plots in figures (1-3), the region of stabilities contain the entire left of the complex plane, therefore SDBDTBF are A–stable for block sizes two, three and four.

Numerical Experiments

In this section, the SDBDTBF of block size two is tested on the following problems:

Problem 1: Linear problem, (cf. Enright (1974))

$$y' = \begin{pmatrix} -0.1 & 0 & 0 & 0 \\ 0 & -10 & 0 & 0 \\ 0 & 0 & -100 & 0 \\ 0 & 0 & 0 & -1000 \end{pmatrix} y,\ y(0) = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix},\ y(x) = \begin{pmatrix} e^{-0.1x} \\ e^{-10x} \\ e^{-100x} \\ e^{-1000x} \end{pmatrix}, \quad 0 \le x \le 1$$

Problem 2: Nonlinear problem, Kaps (1981)

$$y_1' = -(2+\varepsilon^{-1})y_1 + \varepsilon^{-1} y_2^2$$

$$y_2' = y_1 - y_2(1+y_2), \qquad y_1(0) = y_2(0) = 1,\ y(x) = \begin{pmatrix} e^{-2x} \\ e^{-x} \end{pmatrix}, \quad 0 \le x \le 1;\ \varepsilon = 10^{-8},$$

Problem 3: Oscillatory problem, (Muka (2011))

$$y' = \begin{pmatrix} -10 & \alpha & 0 & 0 & 0 & 0 \\ -\alpha & -10 & 0 & 0 & 0 & 0 \\ 0 & 0 & -4 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & -0.1 \end{pmatrix} y,\ y(x) = \begin{pmatrix} e^{-10x}(\cos(\alpha x) + \sin(\alpha x)) \\ e^{-10x}(\cos(\alpha x) - \sin(\alpha x)) \\ e^{-4x} \\ e^{-x} \\ e^{-0.5x} \\ e^{-0.1x} \end{pmatrix}, \quad y(0) = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, 0 \le x \le 3.$$

In Figure 4 the approximate solution generated by SDBDTBF is compared with the exact solution, in Figure 5, approximate solutions of first component of problem 2 generated by SDBDTBF and BDTBF of Chartier (1993) are plotted against the exact solution. In Figure 6 approximate solutions of first component of problem 3 generated by SDBDTBF and BDTBF are compared.

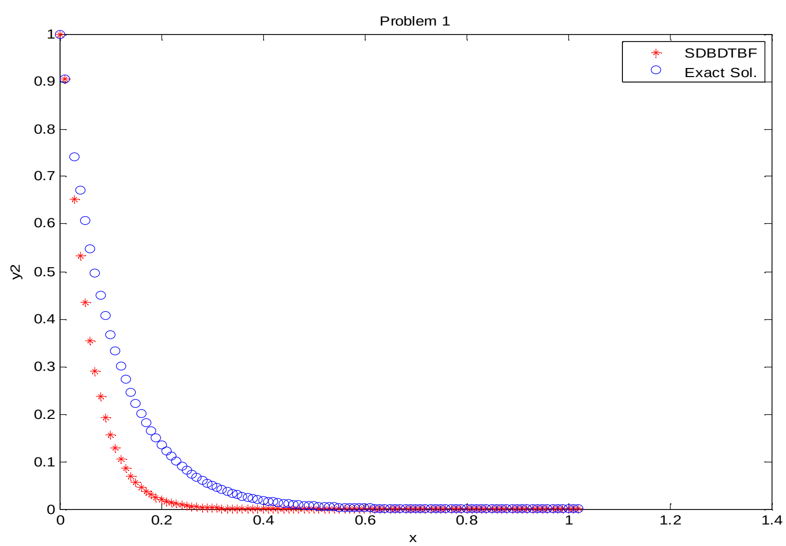

Fig. 4 SDBDTBF and Exact Sol. of Problem 1.

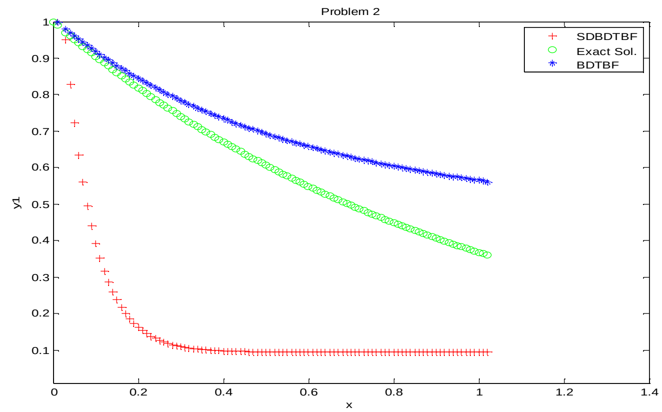

Fig.5. SDBDTBF, Exact Sol. and BDTBF Solution of Problem 2.

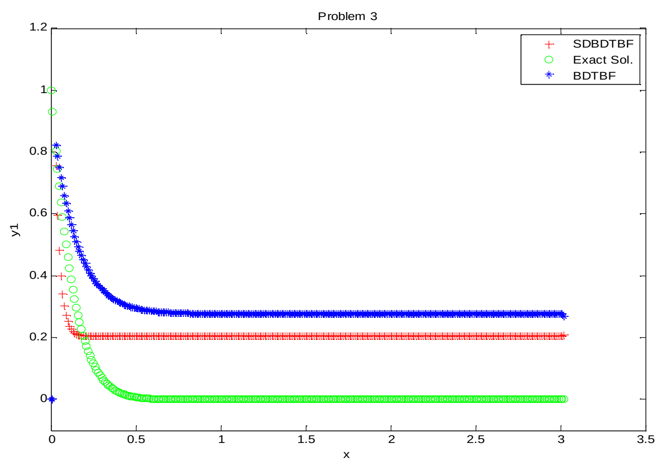

Fig.6 SDBDTBF, Exact Sol. and BDTBF Solution of Problem 3.

Figure 4 shows that SDBDTBF generates approximate solutions which mimic the exact solution of problem 1. The approximate solution of problem 2 using SDBDTBF shows that the numerical solution of SDBDTBF decay faster than that of BDTBF and so may not be good for integrating mildly stiff non-linear IVPs. The numerical solution of SDBDTBF in Figure 6 shows that SDBDTBF is applicable on stiff oscillatory IVPs. Indeed, Figures 4–6 show that SDBDTBF compares favourably with BDTBF of Chartier (1993).

CONCLUSION

In this paper, we restructured the block methods developed in Muka and Ikhile (2009a) and give conditions by which the new method SDBDTBF will be zero stable *apriori*. The SDBDTBF are A-stable for block sizes two, three and four, hence are well suited for parallel integration of stiff IVPs in ODEs.

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