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A model for stability of the semi-implicit backward differentiation formulas

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Abstract: A model is presented for stability for an extension of linear multistep methods for stiff ordinary differential equations. The method is based on a prediction followed by a fixed number of corrections obtained by a Newton scheme with inexact Jacobian matrix. The impact on stability of error in the matrix over a broad range of linear, constant coefficient equations is modeled. The model provides practical guidance for implementation of software for stiff equations.

Keywords: BDF, stability, stiff ODE, SIBDF.

1. Introduction

The Backward Differentiation Formulas (BDF) are effective for solving wide classes of stiff ordinary differential equations (ODEs). A major cost for these implicit methods is the requirement of some Newton-like iteration at each time step. Klopfenstein [8] first investigated a class of explicit P(EC)^m algorithms related to the BDFs involving a predictor (P) followed by m applications of a derivative evaluation (E) and a Newton-like process to compute the BDF correction (C) for the model test *system*,

$$y' = Jy, \quad y \in \mathbb{R}^s.$$

The method explored in this paper is closely related to Klopfenstein's and is called the *Semi-Implicit Backward Differentiation Formula* (SIBDF). This extension of linear, multistep methods was presented by Krogh and Stewart [9], is applicable to stiff ODEs and has been implemented in a code, STRUT [15].

Klopfenstein analyzed the stability of his method by examining the limit case $h = \infty$. Due to the continuous dependence of the roots of a polynomial on its coefficients, this produces a stability model applicable to methods with a sufficiently large stepsize. He called this model *Asymptotic* ($h \to \infty$) *Absolute Stability* (AAS). The difference equation for AAS is more involved than that for the BDF. Study of the AAS difference equation allowed statements to be made relating predictor-corrector order to relative matrix error in the Newton-like process under the assumption of stability.

Krogh and Stewart presented a simplified derivation of a related system of difference equations. This system of difference equations encompasses both the standard stability model for the BDF (which assumes the corrector is solved exactly) and AAS (where the corrector is not solved exactly and $h = \infty$ is assumed). This paper extends the work of Klopfenstein [8] and Krogh and Stewart [9] to handle the case of finite h with inexact solution of the corrector equation due to matrix error. The analysis can be done in general only for the scalar test equation, $y' = \lambda y$ but this provides valuable guidelines for practical codes. A technique is developed to enable the examination of families of λ values.

Section 2 presents the notation for the vector system of the SIBDF. Section 3 develops the system of difference equations used to model stability. Sections 3.1 (BDF) and 3.2 (AAS) briefly summarize the two cases for which the vector system of difference equations for stability can be solved. Section 4 presents new analysis for finite stepsize and inexact Jacobian for the SIBDF. Section 4.1 focusses on error in the coefficient of the correction matrix and is related to the work of Addison and Hanson [1] for the Semi-Implicit Blended Formulae. Section 4.2 focusses on error in the approximation of the ODE Jacobian and is related to the work of Bader and Deuflhard [2] for the Semi-Implicit Midpoint Rule. Section 5 concludes with the implications for implementation of codes based on the stability analysis of the SIBDF.

2. The SIBDF

The formulas of a SIBDF method solving

$$y' = f(x, y), \quad y(a) = y_a,$$

are briefly developed in this section and related to the more familiar BDF. Both are effective techniques for stiff ODEs. More detail is contained in [9,11]. Following Shampine and Gear [10], a problem is said to be stiff if the stepsize is limited more severely by stability than by accuracy when using one of the classical methods such as Adams. Methods more appropriate for solving stiff ODEs require a set of nonlinear equations be solved to some fixed accuracy at each time step.

The case for fixed order and constant stepsize is analyzed here and provides guidance for the case of variable order and stepsize. Thus, let the stepsize, h, and step number, k, be fixed. A fixed number of corrections, m, is performed at each time step. In [9], which analyzes the case for large h, it is shown that use of $m = 2$ and a predictor formula of order one lower than corrector formula is preferred from considerations of effectiveness of technique and enhanced stability properties.

The predicted k-step solution (of order $k-1$) at x_n is obtained by extrapolating the polynomial,

$$\mathscr{P}_{k,n-1}(x) = y_{n-1} + \frac{x - x_{n-1}}{h} \nabla y_{n-1} + \frac{(x - x_{n-1})(x - x_{n-2})}{h^2 2!} \nabla^2 y_{n-1} + \cdots + \frac{(x - x_{n-1}) \cdots (x - x_{n-k+1})}{h^{k-1}(k-1)!} \nabla^{k-1} y_{n-1},$$

which passes through the k previous equally spaced points, $x_{n-1}, \ldots, x_{n-k}$ to yield

$$p_n = \mathscr{P}_{k,n-1}(x_n) = \sum_{r=0}^{k-1} \nabla^r y_{n-1}. \tag{1}$$

Differentiating $\mathscr{P}_{k,n-1}$ and evaluating at $x = x_n$, we have the predicted derivative given by

$$p_n' = \frac{\mathrm{d}}{\mathrm{d}x}\mathscr{P}_{k,n-1}(x)|_{x=x_n} = \frac{1}{h}\sum_{r=1}^{k-1}\delta_r \nabla^r y_{n-1} \tag{2}$$

where

$$\frac{\delta_r}{h} = \frac{1}{h}\sum_{i=1}^{r}\frac{1}{i} = \frac{1}{h}\sum_{i=1}^{r}\delta_i^*.$$

The coefficient, $\delta_r^* = 1/r$, is from the backward difference form of the BDF [5].

Setting $y_n^{(0)} = p_n$, m corrections are computed by solving the sequence of linear systems

$$\hat{G}\,\Delta y_n^{(i)} = -r_n^{(i)}, \quad y_n^{(i+1)} = y_n^{(i)} + \Delta y_n^{(i)}, \qquad i = 0, \ldots, m-1, \tag{3}$$

where the *residual* $r_n^{(i)}$ of the corrector (k-step BDF of order k) formula is given by

$$r_n^{(i)} = f\big(x_n, y_n^{(i)}\big) - p_n' - \frac{\delta_k}{h}\big(y_n^{(i)} - p_n\big). \tag{4}$$

The *correction matrix,* $\hat{G}$ is a parameterized approximation to a Newton matrix, G

$$G = \frac{\partial r_n^{(i)}}{\partial y_n^{(i)}} = \frac{\partial f\big(x_n, y_n^{(i)}\big)}{\partial y_n} - \frac{\delta_k}{h}I = J - \alpha I.$$

$\hat{G}$ is called the correction matrix rather than iteration matrix to emphasize the *fixed* number of corrections to be computed.

In [9], $\hat{G}$ had the form $\hat{G}(c, \hat{\alpha}) = c(\hat{J} - \hat{\alpha}I)$, where the parameter $\hat{\alpha}$ is an approximation to $\alpha = \delta_k/h$; the matrix $\hat{J}$ is an approximation to J, the Jacobian of the differential equation; and the parameter c is a scalar which is manipulated to help reduce the error when $\hat{\alpha}$ differs from α due to changes in h or k. The parameter c is advantageous in implementing an effective variable order, variable stepsize method and this was addressed in [9]. Its value is 1.0 perturbed by a small amount depending on estimates of the extreme eigenvalues of $\hat{J}$. For the analysis below, c is taken to be 1.0, giving correction matrix

$$\hat{G}(\hat{\alpha}) = \hat{J} - \hat{\alpha}I. \tag{5}$$

This explicit correction scheme can be considered to be an iterative method taking $i = 0, 1, 2, \ldots,$ until convergence. Convergence would be controlled by the eigenvalues of the *relative error matrix*

$$B = I - \hat{G}^{-1}G. \tag{6}$$

For the model system, $y' = Jy$, this is the standard convergence matrix for the BDF. It is zero if $\hat{G} = G$. For $\hat{G} \neq G$, the convergence of the BDF requires the spectral radius of B be less than one, implying a condition on the approximation of J by $\hat{J}$ and α by $\hat{\alpha}$.

3. The Vector Generalized Difference Equation

Krogh and Stewart [9] presented an algebraic derivation of the SIBDF difference equations for the model system, $y' = Jy$. This is highlighted in this section.

Using the relative error matrix B, above, and labeling,

$$C_m = [I - B^m]G^{-1}$$

the solution, after m corrections, to the *Vector Generalized Difference Equation (VGDE)* is given by

$$y_n = \sum_{r=0}^{k-1} \left[B^m + \left(\frac{\delta_r}{h} - \frac{\delta_k}{h} \right) C_m \right] \nabla^r y_{n-1}, \tag{7}$$

with $\delta_0 = 0$. The VGDE will not be generally diagonalizable unless there is some special relationship between J and $\hat{J}$.

3.1. Zero matrix error (stability for the BDF)

One case where the VGDE can be diagonalized and easily analyzed is when $\hat{J} = J$ and $\hat{\alpha} = \delta_k/h$ $(= \alpha)$, giving an exact correction matrix and $B = 0$. This yields stability results identical to the standard stability results for the BDF which assumes the collocation equation [5, equation (5-45)]

$$f(y_n) = \mathscr{P}_{k+1,n}(x_n)$$

is solved exactly at each time step. Substituting $C_m = G^{-1}$ and $B = 0$ in (7) yields

$$\left(J - \frac{\delta_k}{h} I \right) y_n = \frac{1}{h} \left[\sum_{r=1}^{k-1} \delta_r \nabla^r y_{n-1} - \delta_k \sum_{r=0}^{k-1} \nabla^r y_{n-1} \right].$$

Rewriting yields,

$$\begin{aligned} Jy_n &= \frac{1}{h} \left[\sum_{r=1}^{k-1} \delta_r \nabla^r y_{n-1} + \delta_k \left(y_n - \sum_{r=0}^{k-1} \nabla^r y_{n-1} \right) \right] \\ &= \frac{1}{h} \left[\sum_{r=1}^{k-1} \delta_r \nabla^r y_{n-1} + \delta_k \nabla^k y_n \right] \\ &= \frac{1}{h} \left[\sum_{r=1}^{k-1} \delta_r \left[\nabla^r y_n - \nabla^{r+1} y_n \right] + \delta_k \nabla^k y_n \right] \\ &= \frac{1}{h} \sum_{r=1}^{k} \delta_r^* \nabla^r y_n \end{aligned}$$

using $\delta_r^* = \delta_r - \delta_{r-1}$. This is the k-step BDF (of order k) in backward difference form. In ordinate form we have

$$(I - \beta_0 hJ) y_n = \sum_{r=1}^{k} \alpha_r y_{n-r}$$

yielding the stability polynomial of the BDF

$$\pi(\zeta;\, h\lambda) = (\beta_0 h\lambda - 1)\zeta^k + \sum_{r=1}^{k} \alpha_r \zeta^{k-r} = \rho(\zeta) + h\lambda\beta_0\sigma(\zeta). \tag{8}$$

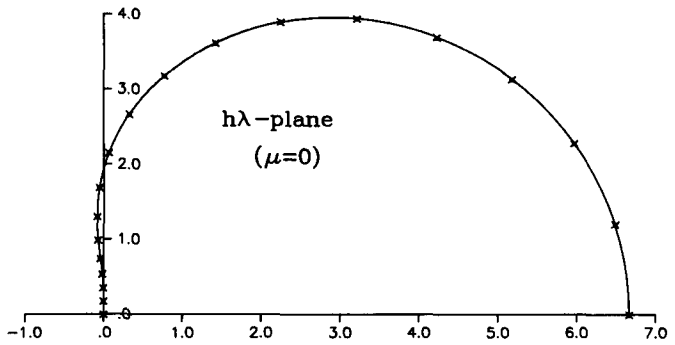

Fig. 1. Absolute stability region for three-step (third-order) BDF (stability in the interior of closed curve).

Figure 1 presents the plot of the absolute stability region for the third-order BDF for later discussions.

3.2. Limit for sufficiently large h (AAS)

The second case where stability of the system in (7) can be analyzed is the limit as $h \to \infty$. Examining the difference equation (7), $h \to \infty$ will cause the coefficient of C_m to vanish. The solution of a difference equation can be expressed in terms of the eigenvalues of the associated companion matrix. Since the eigenvalues of a matrix are continuous functions of the elements of that matrix [7, Theorem 4-2], the limit matrix resulting from $h = \infty$ will have eigenvalues which are close to those when h is sufficiently large.

In solving stiff problems we are concerned with stability for large h. The limit case when $h = \infty$ is not of interest in itself but it is solvable and provides guidance. Experimentation [12,14] and the analysis in Section 4 for finite h provide guidance to determine how well the limit results pertain to the practical case of finite, but large h.

Klopfenstein's definition of AAS required a uniform bound on the solution of the difference equation. If all roots of the difference equation in the limit case are less than one, solution growth is bounded. If any root has magnitude larger than one, then some solution will be unbounded. For the purposes of this paper, all roots of the difference equation are required to be strictly less than one in modulus as $h \to \infty$. By continuous dependence of eigenvalues on the elements of the matrix, for h sufficiently large, the solution to the VGDE will be bounded if the method has AAS.

As $h \to \infty$, (7) becomes

$$y_n = B^m \sum_{r=0}^{k-1} \nabla^r y_{n-1} = B^m p_n. \tag{9}$$

This difference equation depends only on the step number k of the predictor and the relative error matrix B. This can be related back to the BDF by examining (8). As $h \to \infty$, $\pi(\zeta; h\lambda)$ is dominated by $\sigma(\zeta) = \zeta^k$. Since all roots of $\sigma(\zeta) = 0$ are zero, there is no inherited error, implying that the only error is that made in the current step by the predictor.

The solution of a difference equation is expressed in terms of the roots of the characteristic polynomial. For the BDF, these roots depend on $h\lambda$, where λ is an eigenvalue of J. Assuming

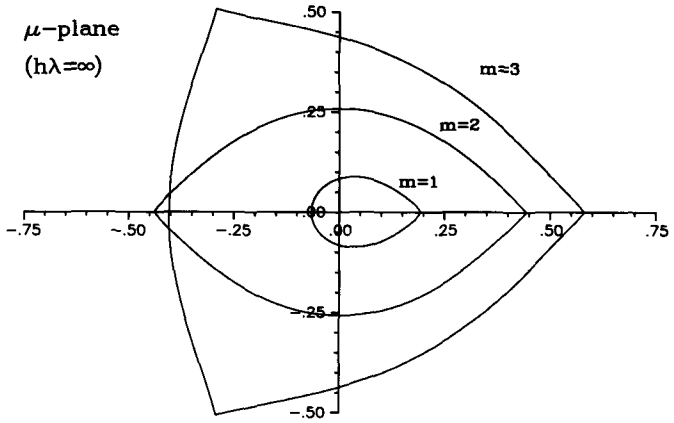

Fig. 2. Asymptotic ($h \to \infty$) absolute stability region for three-step predictor formula (stability in the interior of closed curve).

the matrix B can be diagonalized, we examine the stability of the diagonalized form of the difference equation in (9) in terms of the eigenvalues of B and the roots $z^n = y_n$ of the characteristic equation. The typical component is of the form

$$z^n = \mu^m \sum_{r=0}^{k-1} z^{n-1}\left(1 - \frac{1}{z}\right)^r, \tag{10}$$

since $\nabla^r z^j = z^j(1 - 1/z)^r$. For AAS, the roots, z, depend on the eigenvalues, μ, of the relative error matrix, B. These eigenvalues measure the accuracy of the approximation of G by $\hat{G}$. The requirement for stability is $|z| < 1$. As in [9], to obtain the limitation on μ corresponding to a stable root z, we solve (10) for μ^m using the geometric sum to yield

$$\mu^m = \frac{1}{1 - \left[1 - \frac{1}{z}\right]^k}.$$

The mapping, $z = e^{i\theta}$, $\theta = 0(10°)360°$, takes the unit circle in the z-plane into the boundary of the AAS stability region in the μ-plane. Figure 2 presents the AAS region for the three-step, second-order predictor with m corrections of the three-step third-order corrector to tie in with the three-step, third-order BDF in Fig. 1. The method is stable for μ in the interior of the closed curve which corresponds to number of corrections, m, equal to 1, 2, and 3.

Additional plots and discussion of AAS regions are contained in [9]. The deviation of μ from zero measures the amount of relative error allowed in a stable computation. The size of the AAS

Table 1
Minimum $|\mu|$ for μ on the boundary of the region of AAS for a three-step P(EC)^m

m	1	2	3	...	∞
min $\|\mu\|$	0.067	0.258	0.405		1

region is easily summarized by computing the radius of the largest circle contained entirely within the appropriate AAS region. The results for a three-step predictor followed by m corrections are given in Table 1. As more corrections are performed, more error can be tolerated in the correction matrix and still yield a stable solution of the difference equation. The large gain in tolerated error from $m = 1$ to $m = 2$, with a reduced gain going to $m = 3$, motivated the choice of $m = 2$ to implement in a code. As presented in [9], this is true for all orders examined. Also in [9], as the order of predictor increases, the limitations on μ are uniformly more strict. This justified the choice of the predictor of order one lower than corrector.

4. The extended stability model

The matrices B and C_m appearing in the VGDE (7) will not, in general, be simultaneously diagonalizable. Section 3 examined two limiting cases that eliminate one of these matrices, either B is zero (corrector solved exactly, i.e., the BDF) or the scalar coefficient of C_m goes to zero (sufficiently large h, i.e., the AAS).

Another way to glean information from the stability model is to examine the scalar case with matrix error and finite $h\lambda$, $\lambda \in \mathbb{C}$. Let $\hat{\delta}_k \equiv h\hat{\alpha}$. Consider the scalar problem

$$y' = \lambda y, \quad \lambda \in \mathbb{C}.$$

The results using (7) when $\lambda = \hat{\lambda}$ and $\delta_k = \hat{\delta}_k$ constitute the case of BDF absolute stability which were presented in Fig. 1 for $k = 3$.

The effect of matrix error when the stepsize is finite is now examined. With one correction, $m = 1$,

$$B = I - \hat{G}^{-1}G = \frac{h\hat{\lambda} - \hat{\delta}_k - (h\lambda - \delta_k)}{h\hat{\lambda} - \hat{\delta}_k}, \qquad C_1 = (I - B)G^{-1} = \hat{G}^{-1} = \frac{1}{\lambda - \hat{\alpha}}.$$

When the substitution, $y_n = z^n$, is made in the scalar version of (7), the result is

$$z^n = \sum_{r=0}^{k-1} \left[\frac{(h\hat{\lambda} - h\lambda) - (\hat{\delta}_k - \delta_k)}{h\hat{\lambda} - \hat{\delta}_k} + \frac{\delta_r - \delta_k}{h\lambda - \hat{\delta}_k} \right] z^{n-1} \left(1 - \frac{1}{z}\right)^r. \tag{11}$$

Stability requires $|z| < 1$, with z depending continuously on the parameters $\hat{\delta}_k$, $h\lambda$, and $h\hat{\lambda}$. There are too many parameters to be tractable. Two case are easily examined.

(a) Let $\lambda = \hat{\lambda}$ (exact ODE Jacobian in $\hat{G}$). Then examine the effect of error in the coefficient, say due to stepsize and order changes.

(b) Let $\hat{\delta}_k = \delta_k$ (exact method coefficient in $\hat{G}$). Then examine the effect of error in the Jacobian approximation.

4.1. Error in the coefficient

Addison and Hanson [1] examined the scalar stability of the Semi-Implicit Blended Formulae using a fixed number of corrections with the assumption that $\hat{\lambda} = \lambda$. A major cost of the Blended Formulae is solving linear systems with an iteration matrix involving the square of the ODE Jacobian. Effective implementations use a perfect square factorization which introduces error

into the correction matrix. The analysis done by Addison and Hanson led them to propose an alternate form for the perfect square that enhanced stability.

4.1.1. One correction in the SIBDF

In the case of the SIBDF with $m = 1$, the assumption $\hat{\lambda} = \lambda$ in (11) yields

$$z = \sum_{r=0}^{k-1} \left[\frac{\delta_r - \hat{\delta}_k}{h\lambda - \hat{\delta}_k} \right] \left(1 - \frac{1}{z}\right)^r. \tag{12}$$

One can fix a value of $\hat{\delta}_k$ to yield a region of stability in the $h\lambda$-plane defining a class of problems which would be stable when $\hat{\delta}_k$ is used in the correction matrix instead of δ_k. Alternatively, the focus can be placed on a particular problem, by fixing $h\lambda$, and examining region in the $\hat{\delta}_k$-plane defining coefficients that could be used in the matrix and yield a stable computation.

First, focus on a fixed value of $h\lambda$ and the stability region in the $\hat{\delta}_k$-plane. We are interested in the behavior of the method for problems which are stable, i.e. λ is in the left half-plane. Even if $\hat{G} = G$, corresponding to the BDF, methods of order greater than two can be unstable. Examining the root equation for the third-order BDF

$$h\lambda\zeta^n = \sum_{r=1}^{3} \frac{1}{r} \nabla^r \zeta^n,$$

the greatest instability occurs for $h\lambda$ on the imaginary axis. Thus set $h\lambda = \mathrm{i}v$, allow v to vary and compute maximum of the three roots of the difference equation. This yields $\zeta = 1.0456$ occurring for $h\lambda = 1.149$ i. In our first examination, we analyze the stability in the $\hat{\delta}_k$-plane using the value of $h\lambda$ which leads to the greatest instability for the BDF.

Figure 3 presents the boundary of stability in the $\hat{\delta}_3$-plane for the problem $h\lambda = 1.149$ i. This is obtained by solving (12) for $\hat{\delta}_k$ in terms of z and $h\lambda$,

$$\hat{\delta}_k = \frac{h\lambda - \frac{1}{z} \sum_{r=0}^{k-1} \delta_r \left(1 - \frac{1}{z}\right)^r}{\left(1 - \frac{1}{z}\right)^k}, \tag{13}$$

and then mapping the unit circle in the z-plane, $z = \mathrm{e}^{\mathrm{i}\theta}$ into the $\hat{\delta}_3$-plane. The interior of the closed curve defines the range of coefficients that will yield a stable computation. The BDF coefficient $\delta_3 = 1.8333$ (labelled 'Exact Coef' in Fig. 3) is outside the region of stability. Another value of $\hat{\delta}_3$, say 1.73, the nearest value on the stability boundary, yields stability at the cost of impaired accuracy from the corrector. Typically the predictor delivers accuracy and the correction process is used to enhance stability, so this seems a reasonable trade-off.

Now that there is a coefficient to use in the matrix that enhances stability on the imaginary axis, what range of values of $h\lambda$ can also expect to benefit from this stability induced error. Figure 4 presents the boundary of stability in the $h\lambda$-plane obtained by solving (13) for $h\lambda$ given this choice of $\hat{\delta}_3 = 1.73$,

$$h\lambda = \hat{\delta}_k \left(1 - \frac{1}{z}\right)^k + \frac{1}{z} \sum_{r=0}^{k-1} \delta_r \left(1 - \frac{1}{z}\right)^r,$$

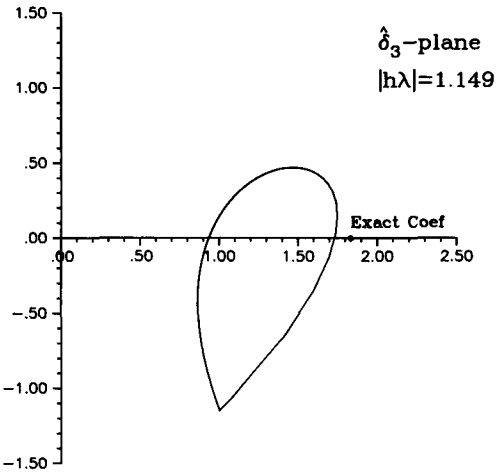

Fig. 3. Range of coefficients in $\hat{G}$ for stable three-step one-correction SIBDF for fixed problem $h\lambda = 1.149$ (stable inside the closed curve).

and plotting the image of the unit circle from the z-plane in the $h\lambda$-plane. This yields an A-stable method which can be compared to Fig. 3 for the BDF.

The value $\hat{\delta}_3 = 1.73$ is between $\delta_2 = 1.5$ and $\delta_3 = 1.833$. This is an indication that on change of order, it may not be beneficial to form a new matrix. This is certainly the case for problems with eigenvalues near the imaginary axis where the BDF have demonstrated poor performance due to stability limitations [3]. If we use $\hat{\delta}_3 = 1.5$, we have the second-order BDF which is A-stable and second order.

It is not convenient to examine in detail the results for each specific $h\lambda$ as above. A broad range of $h\lambda$ values is characterized by fixing the magnitude of $h\lambda$ and then specifying six equally spaced arguments in the upper quadrant of the left half-plane. The boundaries of the stability regions in the $\hat{\delta}_3$-plane were computed using (13) and are presented in Figs. 5 and 6 for moduli equal to one and five. The method is stable in the interior of the closed curves. From Fig. 5, $\hat{\delta}_3 = 1.73$ yields a stable method for all $h\lambda$ of magnitude one.

For a larger modulus of $h\lambda$, say $|h\lambda| = 5$, the third-order BDF is stable for all arguments of $h\lambda$ in the left half-plane (from Fig. 1). Figure 6 shows the region of stability for the SIBDF in the

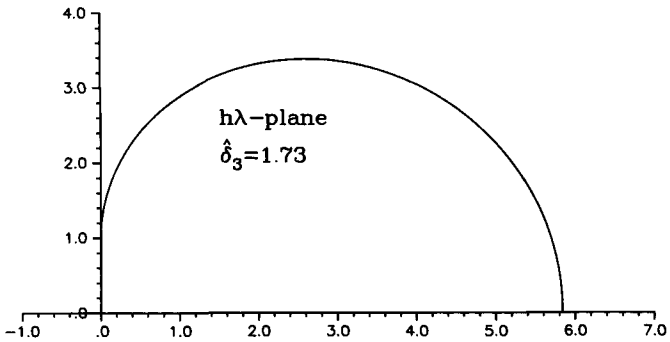

Fig. 4. A-stable three-step one-correction SIBDF with fixed coefficient $\hat{\delta}_3 = 1.73$ (stable inside the closed curve).

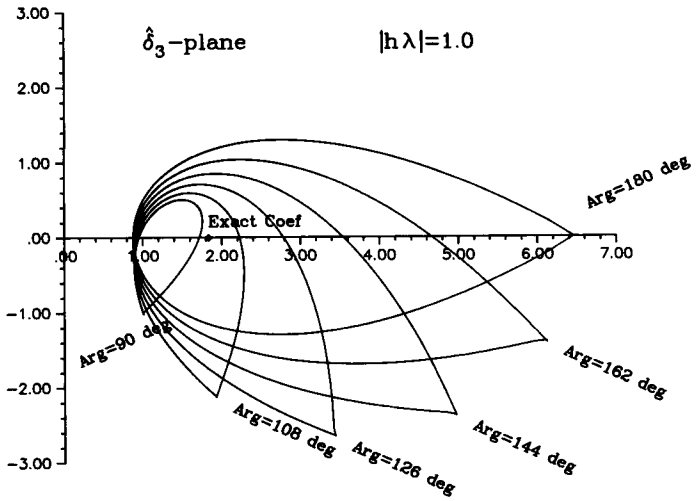

Fig. 5. Range of coefficient to use in $\hat{G}$ for stable three-step one-correction SIBDF for six problems with $|h\lambda| = 1$ (stable inside the closed curve).

$\hat{\delta}_3$-plane has increased with $|h\lambda|$, i.e., a broader choice of the coefficient $\hat{\delta}_3$ can be used and yield stability. If $\hat{\delta}_3 = \delta_3$, third-order accuracy is obtained. Figure 6 shows stability is obtained by choosing method coefficient, $\hat{\delta}_3$ near δ_3, though the cases with dominant imaginary part for λ are more restrictive in the tolerable error. Still, $\hat{\delta}_3 = 1.73$ is stable for all arguments of $h\lambda$.

Since the choice of $m = 2$ and lower order predictor was made based on AAS ($h \to \infty$) results, the μ-plane plots for finite h will help clarify the applicability of the asymptotic results. Once $\hat{\delta}_k$ is found from (13), the value for the eigenvalue of the relative error matrix is

$$\mu = \frac{\delta_k - \hat{\delta}_k}{h\lambda - \hat{\delta}_k} \tag{14}$$

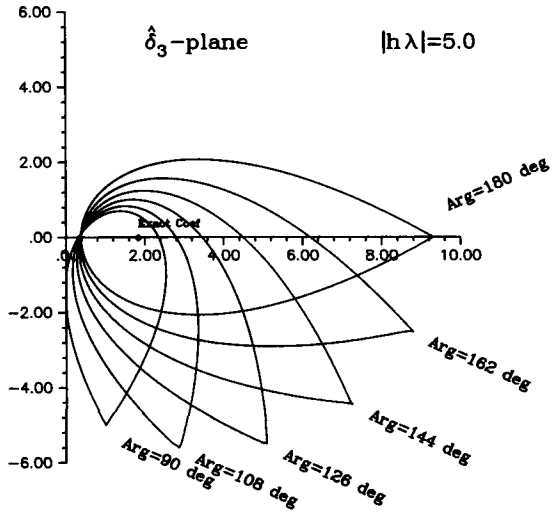

Fig. 6. Range of coefficient to use in $\hat{G}$ for stable three-step one-correction SIBDF for six problems with $|h\lambda| = 5$ (stable inside the closed curve).

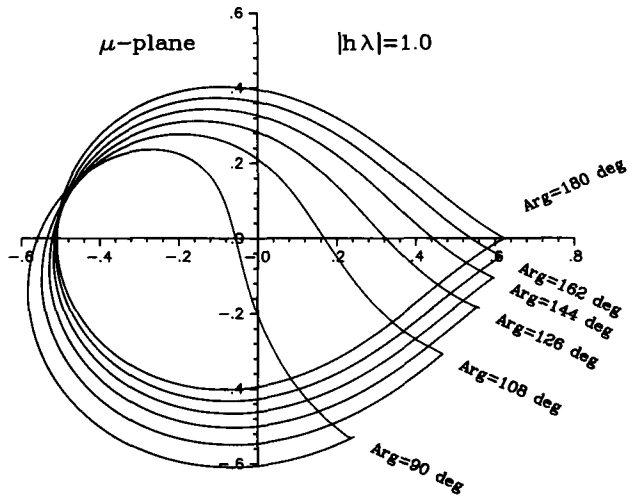

Fig. 7. Relative error tolerated by three-step one-correction SIBDF for six problems with $|h\lambda| = 1$ (stable inside the closed curve).

which is plotted in the μ-plane in Fig. 7 for the three-step predictor with three-step corrector. The region of absolute stability is the interior of the region since the origin, $\mu = 0$, corresponds to the BDF third-order corrector which is absolutely stable when $|h\lambda| = 1$ for all arguments of $h\lambda$ except on the imaginary axis.

Figures 7, 8, and 9 allow us to examine the amount of relative error tolerated by a stable method as $h\lambda$ grows. Figure 8 presents the μ-plane stability restriction when $|h\lambda| = 5$ for the full complement of $h\lambda$ values. Figure 9, for $|h\lambda| = 25$, reveals stability boundaries collapsing into a single curve very near the $m = 1$ case for AAS (Fig. 2).

Because the AAS bounds on μ are easily summarized as in Table 1, they were used as the basis of the code STRUT which has compared favorably with BDF codes [12,14]. The case of

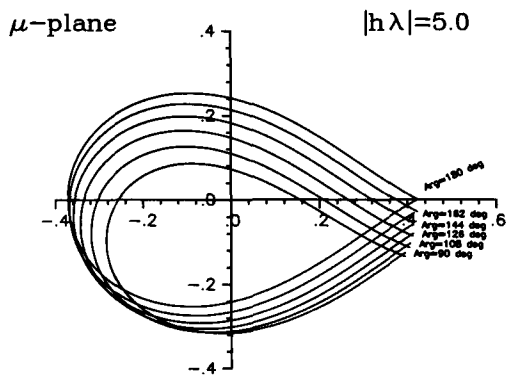

Fig. 8. Relative error tolerated by three-step one-correction SIBDF for six problems with $|h\lambda| = 5$ (stable inside the closed curve).

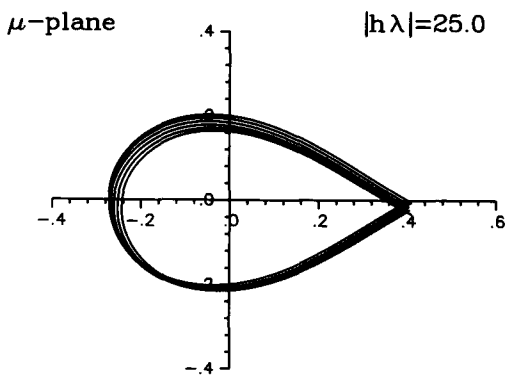

Fig. 9. Relative error tolerated by three-step one-correction SIBDF for six problems with $|h\lambda| = 25$ (stable inside the closed curve).

finite $h\lambda$ allows us to respond to the question, "When do the asymptotics apply?", i.e., for what finite value of h will the model results of AAS be applicable. Figures 7, 8, and 9 display the smooth emergence of the tear-drop shaped region characteristic of the AAS model for the three-step, second-order predictor with $m = 1$ correction in Fig. 2. P(EC)^m regions for predictors of orders zero through four were explored in [11] with similar results. The implication is that for $|h\lambda| = 25$, the region is sufficiently close to the asymptotic case.

4.1.2. Two corrections in the SIBDF

The BDF are iterated to convergence, which corresponds to infinitely many corrections in the SIBDF stability model. As more corrections are computed, the behavior (good and bad) of the BDF is expected to emerge. We have seen that a three-step A-stable method is possible if exactly one correction is performed. The question is: Can a stable two-correction method be formulated where the BDF are unstable? This could yield enhanced stability performance along the imaginary axis for BDF-related methods.

For $m = 2$, the scalar case of (7) has

$$B^2 = \mu^2 = \left[\frac{h\lambda - h\hat{\lambda} - (\delta_k - \hat{\delta}_k)}{h\hat{\lambda} - \hat{\delta}_k}\right]^2 \quad \text{and} \quad C_2 = \frac{1 - B^2}{\lambda - \delta_k/h}.$$

Stability is examined through (7) yielding

$$z^n = \sum_{r=0}^{k-1}\left[B^2 + C_2\left(\frac{\delta_r}{h} - \frac{\delta_k}{h}\right)\right] z^{n-1}\left(1 - \frac{1}{z}\right)^r. \tag{15}$$

If the error is placed in the coefficient, i.e., $\lambda = \hat{\lambda}$, then

$$B^2 = \left[\frac{-(\delta_k - \hat{\delta}_k)}{h\lambda - \hat{\delta}_k}\right]^2,$$

$$C_2 = \frac{1}{\lambda - \delta_k/h}\left[1 - \left(\frac{\delta_k - \hat{\delta}_k}{h\lambda - \hat{\delta}_k}\right)^2\right].$$

Substituting these values in (15), μ^2 can be solved for. Given $h\lambda$ and $z = e^{i\theta}$, the two values of μ are computed. Once μ is determined, $\hat{\delta}_k$ can be solved for from (14).

We begin by examining the worse case $h\lambda = 1.149\,i$ for BDF stability. Figure 10 gives the stability region in the $\hat{\delta}_3$-plane for this problem. Since the coefficient in the correction matrix must be real, we see in Fig. 10 there is no real value of the coefficient that can induce stability for $m = 2$. For this moderately small value of $h\lambda$, the instabilities of the BDF are inherited by the SIBDF after just two corrections.

The ability to examine in detail the scalar test problem reveals information valuable to the implementation of the SIBDF as well as BDF. There is no simple change in the third-order Backward Differentiation Formula that will induce stability for problems with eigenvalues near the imaginary axis once two corrections are computed. In the general case of nonlinear problems, error in the matrix is inevitable and two or more corrections is common.

A promising technique to allow the BDF and related methods to handle problems with eigenvalues near the imaginary axis is through proper order selection [13] using low-order

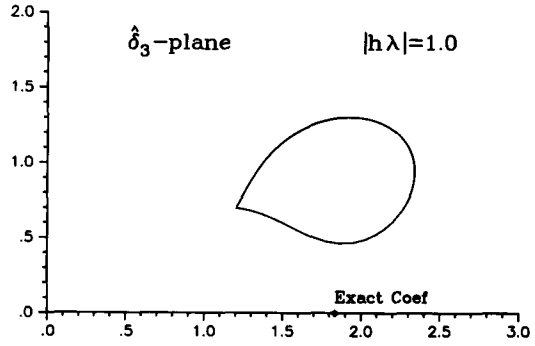

Fig. 10. Range of coefficients in $\hat{G}$ for stable three-step two-correction SIBDF for fixed problem $h\lambda = 1.149$ (stable inside the closed curve).

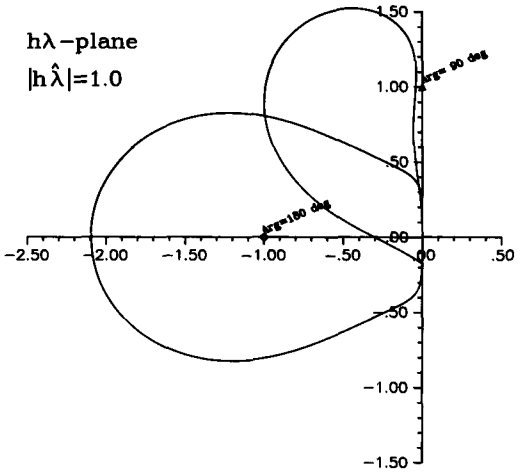

Fig. 11. Range of problems for stable three-step one-correction SIBDF with $|h\lambda| = 1$ (stable inside the closed curve).

formulas when h is small enough to cause $h\lambda$ to be in an unstable region of the higher-order methods.

4.2. *Error in the Jacobian*

Bader and Deuflhard [2] analyzed the stability for the scalar test problem solved with the Semi-Implicit Midpoint Rule under the assumption that the only error was due to an inexact Jacobian (in their Section 2.2 notation, $z_0 = hA \neq h\,\partial f/\partial y = z$, which in the current notation would have $h\hat{\lambda} = z_0$ and $h\lambda = z$).

Due to the results of Section 4.1.2, only the case $m = 1$ will be discussed. When $\hat{\delta}_k = \delta_k$ in (7), a relationship between $h\lambda$ and $h\hat{\lambda}$ results. Fixing a value for $h\hat{\lambda}$, (7) can be solved for $h\lambda$. This is the appropriate model of stability to use when considering a code that uses sequences of fixed stepsizes and order and updates the matrix when order and stepsize are altered such as LSODE [6]. If the code is typically using only one iteration, then the analysis for the SIBDF with $m = 1$ is applicable.

Figure 11 presents the boundary of stability in the $h\lambda$-plane for the three-step method in the extreme cases of $h\hat{\lambda} = \mathrm{i}$ and $h\hat{\lambda} = -1$. Other arguments of $h\hat{\lambda}$ provide a smooth transition between these cases and were suppressed for clarity in the plot. If the value used in the correction matrix is $h\hat{\lambda} = \mathrm{i}$, then the method will not be stable on the problem $y' = \mathrm{i}\,y$. This corresponds to zero matrix error or the BDF, whose three-step formula is not stable for $h\lambda = \mathrm{i}$. For $h\hat{\lambda} = -1$, a wide range of problems, including $y' = -y$, can be solved in a stable manner using the three-step formula.

Figure 12 presents the case when $|h\hat{\lambda}| = 25$. The case when $h\lambda = h\hat{\lambda}$ is now stable for both cases displayed. As expected, plots in the $h\lambda$-plane revealed stability with zero matrix error for all $h\lambda$ once $|h\hat{\lambda}| \geqslant 2$, since this defines the upper limit of the unstable lobe of the three-step BDF from Fig. 1.

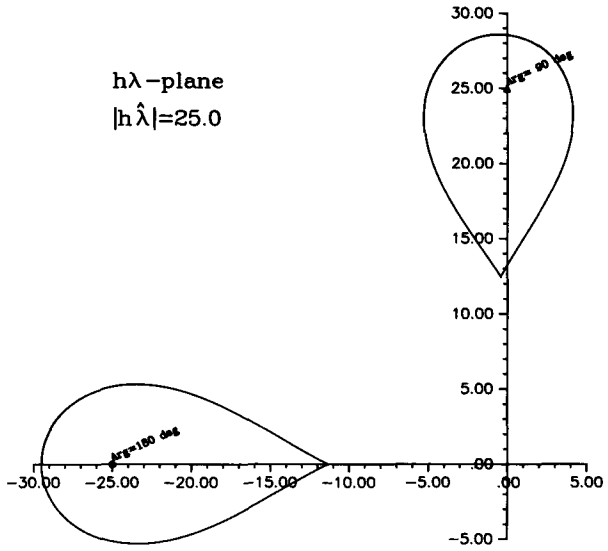

Fig. 12. Range of problems for stable three-step one-correction SIBDF with $|h\lambda| = 25$ (stable inside the closed curve).

5. Conclusions

Any linear problem $y' = Jy$ can be expected to encompass a variety of real or conjugate pair eigenvalues. The models of stability presented in this paper allow statements to be made that cover a broad range of $h\lambda$ as well as different strategies for evaluating the correction matrix.

The AAS model [8,9] has been used to characterize the magnitude of allowable relative matrix error with respect to the number of corrections computed and as the basis of a code which has performed well compared with BDF codes [12,14]. AAS uses the assumption $h = \infty$. From Section 4.1.2, this asymptotic case is appropriate when all $h\lambda$ have magnitude 25 or larger.

From the μ-plane plots we see that for small magnitudes of $h\lambda$, the method behavior is distinctly different depending on the argument of λ. For λ purely real, the more restrictive case for tolerated matrix error, $|\mu|$, is for large $h\lambda$. Small values of $|h\lambda|$ allow the method to tolerate more error in the correction matrix or use fewer corrections. For λ purely imaginary the opposite is true. For order three and above, the small $|h\lambda|$ case, with λ imaginary, is unstable when the correction matrix is exact, while increasing $|h\lambda|$ shifts the μ-plane region to include the origin. Once h is sufficiently large for some fixed λ, the region becomes that of the AAS and the method is stable for all $\text{Arg}(\lambda)$. Values of $h\lambda$ with both real and imaginary part exhibit a smooth transition from these two extreme cases.

The implication is that for h small and $\text{Re}(\lambda) \gg \text{Im}(\lambda)$, a SIBDF method is stable even with large relative error in the correction matrix. Therefore, few correction matrices need be computed as the order and stepsize change when $h\lambda$ is small and primarily real.

Altering the SIBDF to enhance stability near the imaginary axis by changing the coefficient in the correction matrix was not profitable. We have shown that enhanced stability is possible for the one-correction method related to the third-order BDF, but when two corrections would be required no stable scheme could be proposed for small $h\lambda$. The two-correction SIBDF is preferable to the one-correction scheme in most cases because of the sensitivity of the one-correc-

tion scheme to error in the iteration matrix. Thus the slight improvement obtained for the one-correction case is of primarily academic interest.

Proper order selection is a possible solution to allow BDF related methods to effectively solve problems with eigenvalues near the imaginary axis [13]. Lower-order formulas are used when h is small. Once h is sufficiently large, higher-order formulas, if accuracy dictates, can be effectively used. Another possibility is an investigation of the interplay between correction matrix error and the coefficient of the highest-order difference used in the method.

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