Stability regions for one-step multiderivative methods.
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## 0. ABSTRACT

Stability regions are plotted for certain members of a family of one-step multiderivative predictor-corrector methods developed by the authors in an earlier paper.

The methods discussed are tested on a linear system where the matrix of coefficients has constant complex eigenvalues and on a stiff non-linear system arising in reactor kinetics.

## 1. INTRODUCTION

In a recent publication by the authors [6], one-step multiderivative methods were used in PECE mode to solve the initial value problem

$$
\begin{equation*}
{\underset{\sim}{y}}^{\prime} \underset{\sim}{f}(\mathrm{x}, \underset{\sim}{\mathrm{y}}) \text { or }{\underset{\sim}{y}}_{\mathrm{y}^{\prime}}=\underset{\sim}{f}(\underset{\sim}{\mathrm{y}}), \underset{\sim}{\mathrm{y}} \in \mathrm{E}^{\mathrm{N}} \quad ; \underset{\sim}{\mathrm{y}}\left(\mathrm{x}_{0}\right)={\underset{\sim}{y}}_{0} . \tag{0}
\end{equation*}
$$

Intervals of absolute stability were calculated for the single test equation

$$
\begin{equation*}
\mathrm{y}^{\prime}=\lambda \mathrm{y} \quad ; \quad \mathrm{y}(0)=\mathrm{y}_{0} \tag{1}
\end{equation*}
$$

in which $\lambda<0$ was assumed to be real.

The multiderivative formulas used as predictors and correctors are found by making approximations to $\mathrm{e}^{\lambda \mathrm{h}}$ in the recurrence relation

$$
\begin{equation*}
\mathrm{y}(\mathrm{x}+\mathrm{h})=\mathrm{e}^{\lambda \mathrm{h}} \mathrm{y}(\mathrm{x}) \tag{2}
\end{equation*}
$$

which the solution $y(x)$ of (1) is seen to satisfy. In equation (2), $h$ is the constant increment in the independent variable $x$ and the solution $y_{n+1} \quad(\mathrm{n}=0,1,2, \ldots, \mathrm{~J}-1)$ is determined at the points $\mathrm{x}_{\mathrm{s}}=\mathrm{sh}$ ( $\mathrm{s}=1,2, ., ., \mathrm{J}$ ) by replacing (2) with

$$
\begin{equation*}
\mathrm{y}_{\mathrm{n}+1}=\mathrm{R}_{\mathrm{m}, \mathrm{k}}{ }^{(\lambda \mathrm{h})} \mathrm{y}_{\mathrm{n}}+0\left(\mathrm{~h}^{\mathrm{mk}+1}\right), \tag{3}
\end{equation*}
$$

where $R_{m, k}(\lambda h)$ is the $(m, k)$ Pade approximant to $e^{\lambda h}$.

In $[6,7], \mathrm{m}, \mathrm{k}=0,1,2,3,4$ were used (except the case $\mathrm{m}=\mathrm{k}=0$ ), equation (3) giving a family of one-step multiderivative methods which are explicit for $\mathrm{m}=0$ (the Taylor series of order k ) and implicit for $\mathrm{m} \neq 0$; it is assumed that $\mathrm{y}(\mathrm{x})$ is sufficiently often differentiable on $[0, \mathrm{Jh}]$. The methods are listed in the Appendix.

It is noted that the formulas based on the $(0,1),(1,1)$ and $(3,3)$ Pade approximants are respectively the Euler predictor, the Euler corrector or trapezoidal rule, and Milne's starting procedure [5]. The methods based on the $(k, k)$ Padé approximants $(k \geq 1)$ are one-step Obrechkoff methods (see Lambert [2;p.47] and Lambert and Mitchell [3;Table I]).

## 2. STABILITY REGIONS

In $[6,7], \lambda<0$ was assumed to be real. In this section of the present paper $\lambda$ will be assumed to be complex and the stability regions associated with a number of the predictor-corrector methods in $[6,7]$ will be plotted.

The ( $\mathrm{m}, \mathrm{k}$ ) Padé approximant to $\mathrm{e}^{\mathrm{t}}$ is given by

$$
{ }^{\mathrm{R}} \mathrm{~m}, \mathrm{k}^{(\mathrm{t})}=\mathrm{p}_{\mathrm{k}}(\mathrm{t}) / \mathrm{Q}_{\mathrm{m}}(\mathrm{t})
$$

where $P_{k}, Q_{m}$ are polynomials defined by

$$
\mathrm{p}_{\mathrm{k}}(\mathrm{t})=1+\mathrm{p}_{1, \mathrm{k}} \mathrm{t}+\mathrm{p}_{2, \mathrm{k}} \mathrm{t}^{2}+\ldots \ldots+\mathrm{p} \mathrm{k}, \mathrm{k}^{\mathrm{t}^{\mathrm{k}}} ; \mathrm{p}_{0}(\mathrm{t}) \equiv 1
$$

and

$$
\mathrm{Q}_{\mathrm{m}}(\mathrm{t})=1-\mathrm{q}_{1, \mathrm{~m}} \mathrm{t}+\mathrm{q}_{2 \mathrm{~m} \mathrm{t}^{2}-\ldots \ldots+(-1)^{\mathrm{m}} \mathrm{q}_{\mathrm{m}, \mathrm{~m}} \mathrm{t}^{\mathrm{m}} ; \mathrm{Q}_{0}(\mathrm{t}) \equiv 1, ~}^{1}
$$

with $\mathrm{p}_{1, \mathrm{k}}>\mathrm{p}_{2, \mathrm{k}}>\ldots \ldots \mathrm{p}_{\mathrm{k}, \mathrm{k}}>0$ and $\mathrm{q}_{1, \mathrm{~m} \cdot}>\mathrm{q}_{2, \mathrm{~m}}>\ldots \ldots .>\mathrm{q}_{\mathrm{m}, \mathrm{m}}>0$ depending on the chosen Padé approximant. It was shown in [6,7] that a multiderivative method arising from (3) may be written in the form

$$
\begin{equation*}
y_{n+1}-y_{n}=\sum_{i=1}^{k} P_{i}, k^{h^{i}} y_{n}^{(i)}+\sum_{j=1}^{m}(-1)^{j+1} h^{j} y_{n+j}^{(j)} . \tag{4}
\end{equation*}
$$

Using the general $\left(0, \mathrm{k}^{*}\right)$ Pade approximant, it is clear that an explicit predictor formula is generated by the characteristic polynomials

$$
\begin{equation*}
\rho^{*}(\mathrm{r})=\mathrm{r}-1, \sigma_{\mathrm{i}}^{*}, \mathrm{k}^{*}(\mathrm{r})=\mathrm{p}_{\mathrm{i}, \mathrm{k}}{ }^{*} \tag{5}
\end{equation*}
$$

where the convention of using an asterisk with the predictor has been adopted. Using the general ( $\mathrm{m}, \mathrm{k}$ ) Padé approximant in (3) an implicit corrector formula is generated by the characteristic polynomials

$$
\begin{equation*}
\mathrm{p}(\mathrm{r})=\mathrm{r}-1 \quad, \quad \sigma_{\mathrm{i}, \mathrm{k}}(\mathrm{r})=\mathrm{p}_{\mathrm{i}, \mathrm{k}} \quad, \quad \gamma_{\mathrm{i}, \mathrm{~m}}(\mathrm{r})=(-1)^{\mathrm{j}+1}, \mathrm{q}_{\mathrm{i}, \mathrm{~m}}{ }^{\mathrm{r}} . \tag{6}
\end{equation*}
$$

In (5) and (6) $\mathrm{i}=1, \ldots, \mathrm{k}$ and $\mathrm{j}=1, \ldots, \mathrm{~m}$. This predictor-corrector combination is denoted by $\left(0, \mathrm{k}^{*}\right) ;(\mathrm{m}, \mathrm{k})$.

The stability polynomial for the $\left(0, \mathrm{k}^{*}\right) ;(\mathrm{m}, \mathrm{k})$ combination in PECE mode is given by

$$
\begin{align*}
\pi \operatorname{PECE}(\mathrm{r}, \tilde{\mathrm{~h}})=\mathrm{r}-1 & -\sum_{\mathrm{i}=1}^{\mathrm{k}} \mathrm{Pi}, \mathrm{k} \\
& +\sum_{\mathrm{j}=1}^{\mathrm{m}}(-1)^{\mathrm{j}} \mathrm{q}_{\mathrm{j}, \mathrm{~m}} \mathrm{~h}^{-\mathrm{j}}\left[1+\sum_{\mathrm{i}=1}^{\mathrm{k}^{*}} \mathrm{P}_{\mathrm{i}, \mathrm{k}} \mathrm{~h}^{-\mathrm{i}}\right] \tag{7}
\end{align*}
$$

where $\overline{\mathrm{h}}-\lambda h$ is complex. The stability region for the $\left(0, \mathrm{k}^{*}\right) ;(\mathrm{m}, \mathrm{k})$ combination in PECE mode is the region in the complex plane determined by solving the stability equation

$$
\begin{equation*}
{ }^{\pi} P E C E^{(\mathrm{r}, \overline{\mathrm{~h}})}=0 \tag{8}
\end{equation*}
$$

for r . Writing $\overline{\mathrm{h}}=\mathrm{u}+\mathrm{iv}(\mathrm{i}=+\sqrt{ }-1)$ and $\mathrm{r}=\cos \mathrm{A}+\mathrm{i} \sin \mathrm{A} \quad$ (so that $|\mathrm{r}|=1$ ), equation (8) takes the form

$$
\begin{equation*}
\mathrm{f}_{\mathrm{k}^{*}, \mathrm{~m}, \mathrm{k}}(\mathrm{u}, \mathrm{v})-\cos \mathrm{A}+\mathrm{i}\left\{\mathrm{~g}_{\mathrm{k}^{*}, \mathrm{~m}, \mathrm{k}}(\mathrm{u}, \mathrm{v})-\sin \mathrm{A}\right\}=0 \tag{9}
\end{equation*}
$$

where $A, u, v$ are real ; f,g are real valued functions and clearly change for each predictor-corrector combination. The stability region for the $\left(0, \mathrm{k}^{*}\right) ;(\mathrm{m}, \mathrm{k})$ combination is found by solving the non-linear system

$$
\left.\begin{array}{l}
\mathrm{f}_{\mathrm{k}^{*}, \mathrm{~m}, \mathrm{k}}(\mathrm{u}, \mathrm{v})-\cos \mathrm{A}=0  \tag{10}\\
\mathrm{~g}_{\mathrm{k}^{*}, \mathrm{~m}, \mathrm{k}}(\mathrm{u}, \mathrm{v})-\sin \mathrm{A}=0
\end{array}\right\}
$$

for each of a series of values of A in the interval $0 \leq \mathrm{A}<360^{\circ}$. It was found in $[6,7]$ that, for $k^{*}=1,2,3,4$, the $\left(0, k^{*}\right) ;\left(k^{*}, 0\right)$ combination gives the smallest interval of absolute stability when $\lambda<0$ in (1) is real, and that the $\left(0, \mathrm{k}^{*}\right) ;(\mathrm{m}, \mathrm{k})$ combination gives the biggest stability interval when $\mathrm{m}=1$ and $\mathrm{k}=4$.

The stability regions, for $\lambda$ complex, of these eight combinations will now be determined :

1. (a) the $(0,1)$; $(1,0)$ combination :

$$
\text { here, } \quad \mathrm{r}=1+\overline{\mathrm{h}}+\overline{\mathrm{h}}^{2},
$$

$$
\begin{aligned}
& \mathrm{f}_{1,1,0}(\mathrm{u}, \mathrm{v})=1 \rightarrow \mathrm{u}+\mathrm{u}^{2}-\mathrm{v}^{2}, \\
& \mathrm{~g}_{1,1,0}^{(\mathrm{u}, \mathrm{v})}=\mathrm{v}+2 \mathrm{uv}
\end{aligned}
$$

(b) the $(0,1) ;(1,4)$ combination :

$$
\begin{aligned}
& \text { here, } r=1+\bar{h}+\frac{1}{2} h^{-2}+\frac{1}{15} h^{-3}+\frac{1}{120} h^{-4}, \\
& f_{1,1,4}(u, v)=1+u+\frac{1}{2}\left(u^{2}-v^{2}\right)+\frac{1}{15}\left(u^{3}-3 u v^{2}\right)+\frac{1}{120}\left(u^{4}-6 u^{2} v^{2}+v^{4}\right), \\
& g_{1,1,4}(u, v)=v+u v+\frac{1}{15}\left(3 u v^{2}-v^{3}\right)+\frac{1}{30}\left(u^{3} v-u v^{3}\right) .
\end{aligned}
$$

The stability regions for these two combinations, in the second quarter-plane, are shown in Figure 1. The stability region for the Euler predictor-corrector combination in PECE mode is also shown in Figure 1. The error constants of all these combinations are of the same order [6,7 $]^{*}$
2. (a) the $(0,2)$; $(2,0)$ combination ;

$$
\begin{aligned}
& \text { here, } \mathrm{r}=1+\overline{\mathrm{h}}+\frac{1}{2} \bar{h}^{2}-+\frac{1}{4} \bar{h}^{3}, \\
& f_{2,2,0}(\mathrm{u}, \mathrm{v})=1+\mathrm{u}+\frac{1}{2}\left(\mathrm{u}^{2}-\mathrm{v}^{2}\right)-\frac{1}{4}\left(\mathrm{u}^{4}-6 u^{2} v^{2}+v^{4}\right), \\
& \mathrm{g}_{2,2,0} \quad(\mathrm{u}, \mathrm{v})=\mathrm{v}+\mathrm{uv}-\mathrm{u}^{3} v+\mathrm{u} v^{3} ;
\end{aligned}
$$

(b) the $(0,2)$; $(1,4)$ combination :

$$
\begin{aligned}
& \text { here, } r=1+\bar{h}+\frac{1}{2} \bar{h}^{2}+\frac{1}{6} \bar{h}^{-3}+\frac{1}{120} h^{-4} \\
& f_{2,1,4}(u, v)=1+u+\frac{1}{2}\left(u^{2}-v^{2}\right)+\frac{1}{6}\left(u^{3}-3 u v^{2}\right)+\frac{1}{120}\left(u^{4}-6 u^{2} v^{2}+v^{4}\right), \\
& g_{2,1,4}(u, v)=v+u v+\frac{1}{6}\left(3 u^{2} v-v^{3}\right)+\frac{1}{30}\left(u^{3} v-u v^{3}\right) .
\end{aligned}
$$

The stability regions for these two combinations are shown in Figure 2.
(a) the $(0,3)$; $(3,0)$ combination :
here, $\mathrm{r}=1+\overline{\mathrm{h}}+\frac{1}{2} \overline{\mathrm{~h}}^{2}+\frac{1}{6} \overline{\mathrm{~h}}^{3}+\frac{1}{12} \overline{\mathrm{~h}}^{4}+\frac{1}{36} \overline{\mathrm{~h}}^{6}$,
$f_{3,3,0}(u, v)=1+u+\frac{1}{2}\left(u^{2}-v^{2}\right)+\frac{1}{6}\left(u^{3}-3 u v^{2}\right)+\frac{1}{2}\left(u^{4}-6 u^{2} v^{2}+v^{4}\right)$, $+\frac{1}{36}\left(u^{6}-15 u^{4} v^{2}+15 u^{2} v^{4}-v^{6}\right)$
$g_{3,3,0}(u, v)=v+u v-\frac{1}{6}\left(3 u^{2} v-v^{3}\right)+\frac{1}{3}\left(u^{3} v-u v^{3}\right) ;$

$$
+\frac{1}{18}\left(3 u^{5} v-10 u^{3} v^{3}+3 u v^{5}\right)
$$

(b) the $(0,3) ;(1,4)$ combination :
here, $\mathrm{r}=1+\overline{\mathrm{h}}+\frac{1}{2} \overline{\mathrm{~h}}^{2}+\frac{1}{6} \overline{\mathrm{~h}}^{3}+\frac{1}{24} \mathrm{~h}^{4}$,
$f_{3,1,4}(u, v)=1+u+\frac{1}{2}\left(u^{2}-v^{2}\right)+\frac{1}{6}\left(u^{3}-3 u v^{2}\right)+\frac{1}{24}\left(u^{4}-6 u^{2} v^{2}+v^{4}\right)$,
$g_{3,1,4}(u, v)=v+u v+u v+\frac{1}{6}\left(3 u^{2} v-v^{3}\right)+\frac{1}{6}\left(u^{3} v-u v^{3}\right)$.

The tability regions for hese two combinations are shown in
Figure 3. The stability region for the fourth order Adams-BashforthMoulton combination in PECE mode, which has the same order error constant as the $(0,3)$; $(1,4)$ combination $[6,7]$, is also shown in Figure 3.
4. (a) the $(0,4)$; $(4,0)$ combination :

$$
\begin{aligned}
& \text { here, } r=1+\bar{h}+\frac{1}{2} \bar{h}^{2}+\frac{1}{6} \bar{h}^{3}+\frac{1}{24} \bar{h}^{4}-\frac{1}{72} \bar{h}^{6}-\frac{1}{576} \bar{h}^{8} \\
& f_{4,4,0}(u, v)= 1+u+\frac{1}{2}\left(u^{2}-v^{2}\right)+\frac{1}{6}\left(u^{3}-3 u v^{2}\right)+\frac{1}{24}\left(u^{4}-6 u^{2} v^{2}+v^{4}\right) \\
&-\frac{1}{72}\left(u^{6}-15 u^{4} v^{2}+15 u^{2} v^{4}-v^{6}\right) \\
&-\frac{1}{576}\left(u^{8}-28 u^{6} v^{2}+70 u^{4} v^{4}-28 u^{2} v^{6}+v^{8}\right) \\
& g_{4,4,0}(u, v)= v+u v+\frac{1}{6}\left(3 u^{2} v-v^{3}\right)+\frac{1}{6}\left(u^{3} v-u v^{3}\right)
\end{aligned}
$$

$$
\begin{aligned}
& -\frac{1}{36}\left(3 u^{5} v-10 u^{3} v^{3}+3 u v^{5}\right) \\
& -\frac{1}{72}\left(u^{7} v-7 u^{5} v^{3}+7 u^{3} v^{5}-u v^{7}\right)
\end{aligned}
$$

(b) the $(0,4) ;(1,4)$ combination :

$$
\begin{aligned}
\text { here, } r=1+\overline{\mathrm{h}} & +\frac{1}{2} \overline{\mathrm{~h}}^{2}+\frac{1}{6} \bar{h}^{3}+\frac{1}{24} \overline{\mathrm{~h}}^{4}+\frac{1}{120} \bar{h}^{5} \\
\mathrm{f}_{4,1,4}(\mathrm{u}, \mathrm{v})= & 1+\mathrm{u}+\frac{1}{2}\left(\mathrm{u}^{2}-\mathrm{v}^{2}\right)+\frac{1}{6}\left(\mathrm{u}^{3}-3 \mathrm{u} v^{2}\right) \\
& +\frac{1}{24}\left(\mathrm{u}^{4}-6 \mathrm{u}^{2} v^{2}+v^{4}\right)+\frac{1}{120}\left(u^{5}-10 \mathrm{u}^{3} v^{2}+5 u v^{4}\right) \\
\mathrm{g}_{4,1,4}(\mathrm{u}, \mathrm{v})= & \mathrm{v}+\mathrm{uv}+\frac{1}{6}\left(3 \mathrm{u}^{2} v-v^{3}\right)+\frac{1}{6}\left(u^{3} v-\mathrm{uv}^{3}\right) \\
& +\frac{1}{120}\left(5 u^{4} v-10 u^{2} v^{3}+v^{5}\right)
\end{aligned}
$$

The stability regions for these two combinations are shown in Figure 4. The stability region of the fourth order Adams-Bashforth-Moulton combination, which has the same order error constant in PECE mode as the $(0,4) ;(4,0)$ combination, is also shown in Figure 4.

It is noted that the $(0,3) ;(1,4)$ and $(0,4) ;(1,4)$ combinations have the same stability regions as the fourth and fifth order Taylor series methods, respectively. The axes of all four figures are drawn to the same scale.

The results of numeri cal experiments for real negative values of $\lambda$ using the multiderivative method discussed in this paper, are reported in $[6,7$.$] .$

The stability regions are, of course, applicable to systems of linear differential equations of the form

$$
\begin{equation*}
\underset{\sim}{\mathrm{y}^{\prime}(\mathrm{x})}=\mathrm{A} \underset{\sim}{\mathrm{y}}(\mathrm{x}) \quad ; \underset{\sim}{\mathrm{x}}(0)=\underset{\sim}{\mathrm{y}} \underset{\sim}{\mathrm{y}} \tag{11}
\end{equation*}
$$

where A is a square matrix of order N with constant coefficients ; the real parts of the eigenvalues $\lambda_{j} . \quad(j=1, ., N)$ of $A$ must be nonpositive. For non-linear systems of the form (0) the eigenvalues $\lambda_{j} .(j=1, \ldots, N)$ are those of the Jacobian matrix $\partial \mathrm{f} / \partial \mathrm{y}$; these eigenvalues are calculated at each point $\mathrm{x}_{\mathrm{n}}$.

## 3. NUMERICAL EXAMPLES

The $\left(0, \mathrm{k}^{*}\right) ;\left(\mathrm{k}^{*}, 0\right)$ and $\left(0, \mathrm{k}^{*}\right) ;(1,4)$ combinations $(\mathrm{k}=1,2,3,4)$ are tested on two problems, the first a system of the form (11) with complex eigenvalues, the second a system of the form (10) with negative real eigenvalues but a large stiffness ratio.

Problem 1 (Lambert [2; p.229])

$$
\begin{aligned}
& y_{1}^{\prime}=-21 y_{1}+19 y_{2}-20 y_{3}, \\
& y_{2}^{\prime}=19 y_{1}-21 y_{2}+20 y_{3}, \\
& y_{3}^{\prime}=40 y_{1}-40 y_{2}-40 y_{3},
\end{aligned}
$$

with initial conditions $\mathrm{y}(0)=(1,0,-1)^{\mathrm{T}}$. The matrix of coefficients has eigenvalues $\lambda_{1}=-2, \quad \lambda_{2}=-40+40 \mathrm{i}, \quad \lambda_{3}=-40-40 \mathrm{i}$ giving a moderate stiffness ratio of 20 . The maximum steplength for each method is found by drawing the line $\operatorname{Im}(\overline{\mathrm{h}})=-\operatorname{Re}(\overline{\mathrm{h}})$ in Figures 1,2,3,4 and estimating the point of intersection with the boundary of the stability region. The maximum steplengths for each of the predictorcorrector combinations follows in an obvious manner and are given in Table 1, truncated to three decimal places, together with the maximum steplengths which may be used with the Euler-modified Euler and Adams-Bashforth-Moulton combinations.

It was noted by Lambert [2; p.229] that the theoretical solution of the problem given by

$$
\begin{aligned}
& \mathrm{y}_{1}=\frac{1}{2} \mathrm{e}^{-2 \mathrm{x}}+\frac{1}{2} \mathrm{e}^{-40 \mathrm{x}}(\cos 40 \mathrm{x}+\sin 40 \mathrm{x}) \\
& \mathrm{y}_{2}=\frac{1}{2} \mathrm{e}^{-2 \mathrm{x}}-\frac{1}{2} \mathrm{e}^{-40 \mathrm{x}}(\cos 40 \mathrm{x}+\sin 40 \mathrm{x}) \\
& \mathrm{y}_{3}=-\mathrm{e}^{-40 \mathrm{x}}(\cos 40 \mathrm{x}+\sin 40 \mathrm{x})
\end{aligned}
$$

behaves as $\underline{y}=\left(\frac{1}{2} e^{-2 x}, \frac{1}{2} e^{-2 x}, 0\right)^{T} \quad$ for $\mathrm{x}>0.1 \quad$ (approximately).
The solution vector was therefore computed only for $x$ in the interval $0 \leq \mathrm{x} \leq 0.09$ using the step lengths $\mathrm{h}=0.01,0.015,0.03$.

The numerical results obtained were in keeping with the theory, and are given for $x=0.09$ in Table 2. The results for the $(0,1) ;(1,0)$, (0.2) ; $(2,0)$ and $(0,3)$; $(3,0)$ combinations, for which $\mathrm{h}=0.03$ exceeds the maximum steplength, display evidence of instability. For all other combinations, using all three values of $h$, the error was found to decay with increasing x .

## Problem 2

$$
\begin{aligned}
& \mathrm{y}_{1}^{\prime}=0.01-\left(0.01+\mathrm{y}_{1}+\mathrm{y}_{2}\right)\left(\mathrm{y}_{1}^{2}+1001 \mathrm{y}_{1}+1001\right) \\
& \mathrm{y}_{2}^{\prime}=0.01-\left(0.01+\mathrm{y}_{1}+\mathrm{y}_{2}\right)\left(1+\mathrm{y}_{2}^{2}\right)
\end{aligned}
$$

with initial conditions $\mathrm{y}(0)=(0,0)^{\mathrm{T}}$. This problem arises in reactor kinetics and has been discussed by Liniger and Willoughby [4], Lambert [2], and Cash [1]. The Jacobian matrix $\partial \mathrm{f} / \partial \mathrm{y}$ has eigenvalues -1012 and -0.01 at $x=0$; it thus has an initial stiffness ratio $\simeq 105$ and may be classed initially as being very stiff. The maximum steplengths which may be used with the multiderivative predictor-corrector combinations are found by dividing the value of $\operatorname{Re}(\overline{\mathrm{h}})$, where the curves bounding the stability regions in Figures $1,2,3,4$ cut the real axis, by -1012 . These maximum values, truncated to five decimal places, are given in Table 1.

One of the main difficulties in the application of multiderivative methods to systems of non-linear equations is in the calculation of the higher order derivatives. These were easily obtained for the present problem and were evaluated at each step of the following computations. The theoretical solution of the problem is not known
and, following Cash [1], was found approximately using the fourth order Runge-Kutta process.

The numerical experiments of Cash [1; p.245] were repeated using the eight multiderivative predictor-corrector combinations discussed in Section 2. The steplength $h$ was given the values $0.001,0.0001$, $0.00001,0.000001$ and the solution was computed for ten steps in each case. Cash [1] also used the value 0.01 , but this value was greater than the maximum steplength for all eight predictor-corrector methods and was not used.

The numerical results obtained for Problem 2 using the ( $0, \mathrm{k}^{*}$ ) ; ( 1,4 ) combinations $\left(\mathrm{k}^{*}=1,2,3,4\right)$ are summarized in Table 3. Comparison with the numerical results obtained using the extended backward differentiation formula of Cash [1], show that the multiderivative methods developed by the authors in $[6,7]$ give smaller errors in PECE mode. For Problem 2 also, the numerical results were found to be in keeping with the theory.

Overall, the results obtained for the two problems indicate strongly that multiderivative methods in PECE mode give very good numerical results for linear system where the coefficient matrix has complex eigenvalues and for stiff systems of non-linear ordinary differential equations. They can readily be used to solve problems for which the higher derivatives can be obtained, or estimated, with reasonable ease .

Table 1 : Maximum steplengths which may be used each, predictor-corrector combination for Problem 1 and 2

|  | Maximum steplength |  |
| :---: | :---: | :---: |
| Combination | Problem 1 | Problem 2 |
| $(0,1) ;(1,0)$ | 0.025 | 0.00098 |
| $(0,1) ;(1,4)$ | 0.050 | 0.00257 |
| $(0,1) ;(1,1)$ <br> $($ Euler) | 0.037 | 0.00197 |
| $(0,2) ;(2,0)$ <br> $(0,2) ;(1,4)$ | 0.025 | 0.00159 |
| $(0,3) ;(3,0)$ |  |  |
| $(0,3) ;(1,4)$ | 0.031 | 0.00274 |
| $(0,4) ;(4,0)$ | 0.035 | 0.00157 |
| $(0,4) ;(1,4)$ | 0.055 | 0.00275 |
| A-B -M | 0.016 | 0.00317 |

Table 2: Errors $e_{1}, e_{2}, e_{3}$ in $y_{1} y_{2}, y_{3}$ at $x=0.09$ for Problem 1 using the multiderivative predictorcorrector combinations with $\mathrm{h}=0.01,0.015,0.03$,

| Combination | Errors |  | $\begin{aligned} & \text { in } y_{1}, y_{2}, \\ & h=0.015 \end{aligned}$ | $\begin{gathered} \mathrm{y}_{3} \\ \mathrm{~h}=0.03 \end{gathered}$ |
| :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{h}=0.01$ |  |  |
| $(0,1) ;(1,0)$ | $\begin{aligned} & \mathrm{e}_{1} \\ & \mathrm{e}_{2} \\ & \mathrm{e}_{3} \end{aligned}$ | $\begin{gathered} -0.262(-1) \\ 0.246(-1) \\ 0.630(-2) \end{gathered}$ | $\begin{gathered} -0.164(-1) \\ 0.140(-1) \\ 0.167(-1) \end{gathered}$ | $\begin{gathered} -0.313(+1) \\ 0.313(+1) \\ -0.284(+1) \end{gathered}$ |
| $(0,1) ;(1,4)$ | $\begin{aligned} & \mathrm{e}_{1} \\ & \mathrm{e}_{2} \\ & \mathrm{e}_{3} \end{aligned}$ | $\begin{array}{r} -0,375(-2) \\ 0.375(-2) \\ -0.104(-2) \end{array}$ | $\begin{array}{r} -0.855(-2) \\ 0.853(-2) \\ 0.716(-3) \end{array}$ | $\begin{gathered} -0.183(-1) \\ 0.182(-1) \\ 0.124(-1) \end{gathered}$ |
| $(0,2) ;(2,0)$ | $\begin{aligned} & \mathrm{e}_{1} \\ & \mathrm{e}_{2} \\ & \mathrm{e}_{3} \end{aligned}$ | $\begin{array}{r} -0.275(-2) \\ 0.274(-2) \\ -0.103(-1) \end{array}$ | $\begin{gathered} -0.130(-1) \\ 0.129(-1) \\ -0.412(-1) \end{gathered}$ | $\begin{gathered} -0.189(+1) \\ 0.189(+1) \\ 0.878(+1) \end{gathered}$ |
| $(0,2) ;(1,4)$ | $\begin{aligned} & \mathrm{e}_{1} \\ & \mathrm{e}_{2} \\ & \mathrm{e}_{3} \end{aligned}$ | $\begin{array}{r} 0.656(-3) \\ -0.656(-3) \\ -0.968(-3) \end{array}$ | $\begin{gathered} 0.229(-2) \\ -0.229(-2) \\ -0.486(-2) \end{gathered}$ | $\begin{array}{r} 0.361(-2) \\ -0.361(-2) \\ 0.111(-1) \end{array}$ |
| $(0,3) ;(3,0)$ | $\begin{aligned} & \mathrm{e}_{1} \\ & \mathrm{e}_{2} \\ & \mathrm{e}_{3} \end{aligned}$ | $\begin{aligned} & -0.686(-3) \\ & 0.686(-3) \\ & 0.199(-2) \end{aligned}$ | $\begin{gathered} -0.147(-2) \\ 0.147(-2) \\ 0.104(-1) \end{gathered}$ | $\begin{aligned} & -0.125 \\ & 0.125 \\ & 0.163(+1) \end{aligned}$ |
| $(0,3) ;(1,4)$ | $\mathrm{e}_{1}$ $\mathrm{e}_{2}$ $\mathrm{e}_{3}$ | $\begin{gathered} -0.145(-4) \\ 0.145(-4) \\ 0.232(-3) \end{gathered}$ | $\begin{gathered} 0.2370(-4) \\ -0.237(-4) \\ 0.139(-2) \end{gathered}$ | $\begin{gathered} 0.534(-2) \\ -0.534(-2) \\ 0.391(-1) \end{gathered}$ |
| $(0,4) ;(4,0)$ | $\begin{aligned} & \mathrm{e}_{1} \\ & \mathrm{e}_{2} \\ & \mathrm{e}_{3} \end{aligned}$ | $\begin{array}{r} -0.960(-4) \\ 0.960(-4) \\ 0.623(-4) \end{array}$ | $\begin{gathered} -0.883(-3) \\ 0.883(-3) \\ 0.245(-3) \end{gathered}$ | $\begin{gathered} -0.180(-1) \\ 0.180(-1) \\ 0.116(-1) \end{gathered}$ |
| $(0,4) ;(1,4)$ | $\mathrm{e}_{1}$ $\mathrm{e}_{2}$ $\mathrm{e}_{3}$ | $\begin{array}{r} -0.695(-5) \\ 0.694(-5) \\ -0.174(-4) \end{array}$ | $\begin{array}{r} -0.753(-4) \\ 0.753(-4) \\ -0.133(-3) \end{array}$ | $\begin{array}{r} -0.491(-2) \\ 0.491(-2) \\ -0.146(-2) \end{array}$ |

Theoretical solution is $y(0.09) \simeq(0.339,0.436,0.012)^{\mathrm{T}}$

Table 3 : Errors in y $1 \mathrm{y}_{2}$. for Problem 2 after ten steps of $\mathrm{h}=(0.001,0.0001,0,00001,0.000001$ using the $\left(0, \mathrm{k}^{*}\right) ;(1,4)$ predictor-corrector combinations $\left(\mathrm{k}^{*}=1,2,3,4\right)$

| h | Theoretical <br> solution ( $\mathrm{y}_{1}, \mathrm{y}_{2}$ ) | Errors in $\quad \mathrm{y}_{1}, \mathrm{y}_{2}$ |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $(0,1) ;(1,4)$ | $(0,2) ;(1,4)$ | $(0,3) ;(1,4)$ | $(0,4) ;(1,4)$ | Cash EBD |
| 0.001 | -0.1006914044(-1) | $\begin{aligned} & 0.241(-5) \\ & 0.135(-7) \end{aligned}$ | 0.246(-6) | $0.101(-6)$ | 0.149(-7) | 0.815(-6) |
|  | $0.8978912350(-4)$ |  | $0.728(-9)$ | 0.823 (-9) | $0.572(-9)$ | 0.628(-8) |
| 0.0001 | -0.6306050198(-2) | $\begin{aligned} & 0.394(-5) \\ & 0.392(-8) \end{aligned}$ | $0.135(-6)$ | 0.455(-8) | 0.650(-10) | 0.835(-6) |
|  | $0.3670275606(-5)$ |  | 0.132(-9) | $0.353(-11)$ | 0.662(-13) | 0.819(-9) |
| 0.00001 | $\begin{gathered} -0.9511426272(-3) \\ 0.4835591013(-7) \end{gathered}$ | $\begin{gathered} 0.929(-8) \\ 0.920(-11) \end{gathered}$ | $0.318(-10)$ | 0.104(-13) | 0.141(-13) | 0.231(-9) |
|  |  |  | 0.326(-13) | 0. 800 (-16) | $0.379(-17)$ | 0.222(-12) |
| 0.000001 | -0.9949622896(-4) | $\begin{aligned} & 0.101(-10) \\ & 0.100(-13) \end{aligned}$ | 0.348(-14) | 0.120(-18) | 0.105(-17) | 0.300(-13) |
|  | $0.4983176581(-9)$ |  | 0.345 (-17) | 0.638(-24) | 0.921(-21) | $0.246(-16)$ |



Figure 1: $\quad(0,1) ;(1,4)$ combination
........... $(0,1) ;(1,0)$ combination
---------- $(0,1) ;(1,1)$ combination (Euler-modified Euler)


Figu


Figure 4:
(0,4);(1,4) combination
$(0,4) ;(4,0)$ combination
combina--------- fourth order Adams- Bashforth-Moulton

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Appendix : (one- step multiderivative methods based on the first twentyfour entries of the pade Table for the exponential function.
$(0,1): y_{n+1}=y_{n}+h y_{n}^{\prime}+0\left(h^{2}\right) . \quad$ (Euler's predictor.
$(1,1): \mathrm{y}_{\mathrm{n}+1}=\mathrm{y}_{\mathrm{n}}+\frac{1}{2} \mathrm{~h}\left(\mathrm{y}_{\mathrm{n}}^{\prime}+\mathrm{y}_{\mathrm{n}+1}^{\prime}\right)+0\left(\mathrm{~h}^{3}\right)$. (Euler' s corrector ; the trapezoida 1 rule) .
$(1,0): y_{n+1}=y_{n}+h y_{n+1}^{\prime}+0\left(h^{2}\right)$.
$(0,2): y_{n+1}=y_{n}+h\left(y_{n}^{\prime}+\frac{1}{2} h^{2} y_{n}^{\prime \prime}+0\left(h^{3}\right)\right.$.
$(1,2): y_{n+1}=y_{n}+\frac{2}{3} h\left(y_{n}^{\prime}+\frac{1}{3} h y_{n+1}^{\prime}+\frac{1}{6} h^{2} y_{n}^{\prime \prime}+0\left(h^{4}\right)\right.$.
$\left.(2,2): y_{n+1}=y_{n}+\frac{1}{2} h\left(y_{n}^{\prime}+y_{n+1}^{\prime}\right)+\frac{1}{12} h^{2} y_{n}^{\prime \prime}-y_{n+1}^{\prime \prime}\right)+0\left(h^{5}\right)$.
$(2,1): y_{n+1}=y_{n}+\frac{1}{3} h\left(y_{n}^{\prime}+\frac{2}{3} h y_{n+1}^{\prime}-\frac{1}{6} h^{2} y_{n+1}^{\prime \prime}+0\left(h^{4}\right)\right.$.
$(2,0): y_{n+1}=y_{n}+h y_{n+1}^{\prime}-\frac{1}{2} h^{2} y_{n+1}^{\prime \prime}+0\left(h^{3}\right)$.
$(0,3): y_{n+1}=y_{n}+h y_{n}^{\prime}+\frac{1}{2} h^{2} y_{n}^{\prime \prime}+\frac{1}{6} h^{3} y_{n}^{(i i i)}+0\left(h^{4}\right)$.
$(1,3): y_{n+1}=y_{n}+\frac{1}{4} h\left(3 y_{n}^{\prime}+y_{n+1}^{\prime}\right)+\frac{1}{4} h^{2} y_{n}^{\prime \prime}+\frac{1}{24} h^{3} y_{n}^{(i i i)}+0\left(h^{5}\right)$
$\left.(2,3): y_{n+1}=y_{n}+\frac{1}{5} h\left(3 y_{n}^{\prime}+2 y_{n+1}^{\prime}\right)+\frac{1}{20} h^{2} 3 y_{n}^{\prime \prime}-y_{n+1}^{\prime \prime}\right)+\frac{1}{60} \mathrm{~h}^{3} \mathrm{y}_{\mathrm{n}}^{(\mathrm{iii})}+0\left(\mathrm{~h}^{6}\right)$.
$(3,3): y_{n+1}=y_{n}+\frac{1}{2} h\left(y_{n}^{\prime}+y_{n+1}^{\prime}\right)+\frac{1}{10} h^{2}\left(y_{n}^{\prime \prime}-y_{n+1}^{\prime \prime}\right)$

$$
\begin{array}{r}
+\frac{1}{120} \mathrm{~h}^{3}\left(\mathrm{y}_{\mathrm{n}}^{(\mathrm{iii})}+\mathrm{y}_{\mathrm{n}+1}^{(\mathrm{iii})}\right)+0\left(\mathrm{~h}^{7}\right) .(\text { (Milne' s starting } \\
\text { procedure }) .
\end{array}
$$

$(3,2): y_{n+1}=y_{n}+\frac{1}{5} h\left(2 y_{n}^{\prime}+3 y_{n+1}^{\prime}\right)+\frac{1}{20} h^{2}\left(y_{n}^{\prime \prime}-3 y_{n+1}^{\prime \prime}\right)+\frac{1}{60} h^{3} y_{n+1}^{(i i i)}+0\left(h^{6}\right)$.
$(3,1): y_{n+1}=y_{n}+\frac{1}{4} h\left(y_{n}^{\prime}+3 y_{n+1}^{\prime}\right)-\frac{1}{4} h^{2} y_{n+1}^{\prime \prime}+\frac{1}{24} h^{3} y_{n+1}^{(i i i)}+0\left(h^{5}\right)$.
$(3,0): y_{n+1}=y_{n}+h y_{n+1}^{\prime}-\frac{1}{2} h^{2} y_{n+1}^{\prime \prime}+\frac{1}{6} h^{3} y_{n+1}^{(i i i)}+0\left(h^{4}\right)$.
$(0,4): y_{n+1}=y_{n}+h y_{n}^{\prime}+\frac{1}{2} h^{2} y_{n}^{\prime \prime}+\frac{1}{6} h^{3} y_{n}^{(i i i)}+\frac{1}{24} h^{4} y_{n}^{(i v)}+0\left(h^{5}\right)$.
$(1,4): y_{n+1}=y_{n}+\frac{1}{5} h\left(4 y_{n}^{\prime}+y_{n+1}^{\prime}\right)+\frac{3}{10} h^{2} y_{n}^{\prime \prime}+\frac{1}{15} h^{3} y_{n}^{(i i i)}+\frac{1}{120} h^{4} y_{n}^{(i v)}+0\left(h^{6}\right)$.
$(2,4): y_{n+1}=y_{n}+\frac{1}{3} h\left(2 y_{n}^{\prime}+y_{n+1}^{\prime}\right)+\frac{1}{5} h^{2}\left(y_{n}^{\prime \prime} \frac{1}{6} y_{n+1}^{\prime \prime}\right)+\frac{1}{30} h^{3} y_{n}^{(i i i)}$

$$
+\frac{1}{360} h^{4} y_{n}^{(i v)}+0\left(h^{7}\right)
$$

$(3,4): y_{n+1}=y_{n}+\frac{1}{7} h\left(4 y_{n}^{\prime}+3 y_{n+1}^{\prime}\right)+\frac{1}{14} h^{2}\left(2 y_{n}^{\prime \prime}-y_{n+1}^{\prime \prime}\right)$

$$
+\frac{1}{210} h^{3}\left(4 y_{n}^{(i i i)}+\mathrm{y}_{\mathrm{n}+1}^{(\mathrm{iii})}\right)+\frac{1}{840} \mathrm{~h}^{4} \mathrm{y}_{\mathrm{n}}^{(\mathrm{iv})}+0\left(\mathrm{~h}^{8}\right)
$$

$(4,4): y_{n+1}=y_{n}+\frac{1}{2} h\left(y_{n}^{\prime}+y_{n+1}^{\prime}\right)+\frac{3}{28} h^{2}\left(y_{n}^{\prime \prime}-y_{n+1}^{\prime \prime}\right)$

$$
+\frac{1}{84} h^{3}\left(\mathrm{y}_{\mathrm{n}}^{(\mathrm{iii})}+\mathrm{y}_{\mathrm{n}+1}^{(\mathrm{iii})}\right)+\frac{1}{1680} \mathrm{~h}^{4}\left(\mathrm{y}_{\mathrm{n}}^{(\mathrm{iv})}-\mathrm{y}_{\mathrm{n}+1}^{(\mathrm{iv})}\right)+0\left(\mathrm{~h}^{9}\right) .
$$

$(4,3): y_{n+1}=y_{n}+\frac{1}{7} h\left(y_{n}^{\prime}+4 y_{n+1}^{\prime}\right)+\frac{1}{14} h^{2}\left(y_{n}^{\prime \prime}-2 y_{n+1}^{\prime \prime}\right)+\frac{1}{120} h^{3}\left(y_{n}^{(i i i)}+4 y_{n+1}^{(\text {iii })}\right)$

$$
-\frac{1}{840} \mathrm{~h}^{4} \mathrm{y}_{\mathrm{n}}^{(\mathrm{iv})}+0\left(\mathrm{~h}^{8}\right)
$$

$(4,2): y_{n+1}=y_{n}+\frac{1}{3} h\left(y_{n}^{\prime}+2 y_{n+1}^{\prime}\right)+\frac{1}{30} h^{2}\left(y_{n}^{\prime \prime}-6 y_{n+1}^{\prime \prime}\right)+\frac{1}{30} h^{3}\left(y_{n+1}^{(i i i)}\right.$

$$
-\frac{1}{360} h^{4} y_{n+1}^{(i v)}+0\left(h^{7}\right)
$$

$(4,1): y_{n+1}=y_{n}+\frac{1}{5} h\left(y_{n}^{\prime}+4 y_{n+1}^{\prime}\right)-\frac{3}{10} h^{2} y_{n+1}^{\prime \prime}+\frac{1}{15} h^{3} y_{n+1}^{(i i i)}$

$$
-\frac{1}{120} h^{4} y_{n+1}^{(i v)}+0\left(h^{6}\right)
$$

(4,0): $\mathrm{y}_{\mathrm{n}+1}=\mathrm{hy}_{\mathrm{n}+1}^{\prime}-\frac{1}{2} \mathrm{~h}^{2} \mathrm{y}_{\mathrm{n}+1}^{\prime \prime}+\frac{1}{6} \mathrm{~h}^{3} \mathrm{y}_{\mathrm{n}+1}^{(\text {(iii })}-\frac{1}{24} \mathrm{~h}^{4} \mathrm{y}_{\mathrm{n}+1}^{(\text {(iv })}+0\left(\mathrm{~h}^{5}\right)$.

