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MULTISTEP SPLITTING METHODS OF HIGH ORDER FOR INITIAL VALUE PROBLEMS

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Multistep splitting methods of high order for initial value problems

by

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ABSTRACT

Multistep splitting formulas of third and fourth order are constructed for systems of first order differential equations. Unconditional stability is proved when the Jacobian matrix of the right hand side can be splitted into a sum of matrices with a common set of eigenvectors and negative eigenvalue spectra. The efficiency of the formulas is proportional to the computational work involved to solve the linear systems defined by these matrices.

KEY WORDS & PHRASES: *Numerical Analysis, Initial Value Problems, Ordinary Differential Equations, Partial Differential Equations, Multistep Methods, Splitting Methods.*

CONTENTS

0. INTRODUCTION

When an initial-boundary-value-problem is discretized with respect to its space variables, a system of ordinary differential equations results of which the Jacobian matrix has an eigenvalue spectrum extending far away from the origin (e.g. *parabolic* equations along the *negative* axis and *hyperbolic* equations along the *imaginary* axis). In order to integrate such systems, one may choose *backward differentiation formulas* which are known to have excellent stability properties, at least for parabolic equations; in case of hyperbolic equation, one should add dissipative terms to the differential equations when third or higher order backward differentiation formulas are chosen (cf. [4]). However, since the backward differentiation formulas are implicit, a large system of equations has to be solved in each integration step. Moreover, the iteration process to be used should be such that the stability properties of the backward differentiation formulas are not destroyed by the iteration process; on the other hand, it should be efficient enough to limit the computation time to realistic values. Hence, *Jacobi iteration* which is very cheap per iteration, cannot be used because of loosing stability, while *Newton iteration* which leaves the stability unaffected, is not a very attractive method in the case of two or higher dimensional problems unless the special structure of the Jacobian matrix is exploited. Since it is our aim to construct a *robust* integration formula, we have looked for other iteration methods.

In this paper, we investigate iteration methods in which the Jacobian matrix is splitted into a sum of "simply structured" matrices (e.g. tridiagonal matrices) and in which the "implicitness" is distributed over several iterations. The resulting integration method may be considered as a multistep analogue of *single-step splitting methods* of which the hopscotch and alternating direction methods are familiar examples.

The reason to develop *multistep splitting methods* is the desire to construct integration formulas with the following properties:

(1) *It is more accurate than single-step splitting methods which usually are only of first or second order.*

(2) *It is more stable than explicit Runge-Kutta methods which are accurate enough but require relatively small integration steps to maintain stability.*

(3) *It is as efficient as single-step splitting methods and as robust as explicit Runge-Kutta methods.*

We shall derive *third* and *fourth order* formulas which apply to general systems of the form

$$(0.1) \qquad \frac{d\vec{y}}{dx} = \vec{f}(\vec{y}).$$

The *efficiency* of the formulas is proportional to the computational work involved to solve the linear systems defined by the matrices occurring in the splitting of $\partial\vec{f}/\partial\vec{y}$. As to the stability of the formulas, where Newton's method does not influence the stability of the integration method, splitting iteration methods noticeably decrease the stability properties. It will be shown, however, that when $\partial\vec{f}/\partial\vec{y}$ can be splitted into matrices with *negative eigenvalue spectra* (parabolic equations), the stability of the backward differentiation formula is strong enough to compensate for the instabilities introduced by the iteration process so that *unconditional stability* results. The stability analysis for *hyperbolic equations* is still subject of investigation.

In the near future, we intend to report numerical experiments with the formulas analysed in this paper.

2. SINGLE-STEP SPLITTING METHODS

Suppose that we are given m functions $\vec{F}_j(\vec{u},\vec{v})$ such that the right hand side $\vec{f}$ of equation (0.1) can be splitted according to

$$(1.1) \qquad \vec{f}(\vec{y}) = \sum_{j=1}^{m} \vec{F}_j(\vec{y},\vec{y}).$$

Furthermore, suppose that all Jacobians $\partial\vec{F}_j(\vec{u},\vec{v})/\partial\vec{u}$ are band matrices with a relatively small band width. We then may define the integration formula

$$
\begin{aligned}
&\vec{y}_{n+1}^{(0)} = \vec{y}_n, \\
(1.2)\qquad &\vec{y}_{n+1}^{(j)} = \vec{y}_{n+1}^{(j-1)} + h_n \sum_{i,\ell=0}^{j} \lambda_{ji\ell}\, \vec{F}_j(\vec{y}_{n+1}^{(i)}, \vec{y}_{n+1}^{(\ell)}), \\
&\vec{y}_{n+1} = \vec{y}_{n+1}^{(m)},
\end{aligned}
$$

where the parameters λ_{jij}, $i = 0,1,\ldots,j$ vanish for $j = 1,2,\ldots,m$.

Formulas belonging to this very general class of single-step splitting schemes are studied in [2] and [3]. As is shown in these references, a large number of methods based on the various alternating direction type splittings, locally one-dimensional splittings, hopscotch type splittings, etc, can be fitted into the class (1.2) by an appropriate choice of the splitting functions $\vec{F}_j$.

As far as we know all single-step splitting methods given in the literature are first or second order accurate. Although it is possible to derive conditions for third order accuracy (cf.[2]), we did not succeed to construct third order formulas in which the implicitness is distributed over the successive stages in such a way that stability might be expected. Therefore, we have recoursed to *multistep splitting methods*.

2. MULTISTEP SPLITTING METHODS

Suppose that the right hand side of the differential equation

$$(2.1)\qquad \frac{d\vec{y}}{dx} = \vec{f}(\vec{y})$$

has a Jacobian matrix J which can be splitted into a sum of matrices with a "simple" structure (e.g. tridiagonal matrices). To be more precise, let

$$(2.2)\qquad J = \sum_{j=1}^{m} J_j,$$

where the matrices J_j are easily decomposable into a lower and upper triangular matrix. We now define the class of methods

$$
(2.3)\qquad
\begin{aligned}
\vec{y}^{(0)}_{n+1} &= \vec{y}^{(pred)}_{n+1}, \\
\vec{y}^{(1)}_{n+1} &= \sum_{\ell=1}^{k} a_\ell\, \vec{y}_{n+1-\ell} + h\, \vec{G}_1((\vec{y}^{(1)}_{n+1}, \vec{y}^{(0)}_{n+1}), \\
\vec{y}^{(j)}_{n+1} &= \sum_{\ell=1}^{k} a_\ell\, \vec{y}_{n+1-\ell} + h\, \vec{G}_j(\vec{y}^{(j)}_{n+1},\ldots,\vec{y}^{(0)}_{n+1}), \\
\vec{y}_{n+1} &= \vec{y}^{(m)}_{n+1},
\end{aligned}
$$

where $\vec{y}^{(pred)}_{n+1}$ presents a single-step predictor formula. It will be assumed that the functions $\vec{G}_j$ satisfy the conditions

$$
(2.4)\qquad \frac{\partial \vec{G}_j}{\partial \vec{y}^{(j)}_{n+1}}(\vec{y},\ldots,\vec{y}) = \mu_j J_j(\vec{y}), \qquad j = 1,2,\ldots,m,\ \mu_j \text{ scalar}
$$

This implies that (2.3) is a *computationally efficient* scheme. Of course, further conditions should be imposed on the functions $\vec{G}_j$ in order to make scheme (2.3) also an *accurate* and *stable* method for the integration of equation (2.1). These aspects will be studied in the following subsections.

2.1. The order equations for backward differentiation type formulas

When we choose

$$
(2.5)\qquad \vec{G}_j(\vec{y},\vec{y}^{(j-1)}_{n+1},\ldots,\vec{y}^{(0)}_{n+1}) \equiv b_0 \vec{f}(\vec{y}), \qquad j = 1,2,\ldots,m,
$$

scheme (2.3) reduces to a multistep method of the backward differentiation (or Curtiss-Hirschfelder) type:

$$
(2.6)\qquad \vec{y}_{n+1} = \sum_{\ell=1}^{k} a_\ell\, \vec{y}_{n+1-\ell} + b_0\, h\, \vec{f}(\vec{y}_{n+1}).
$$

These formulas are of order k when the coefficients are defined according to table 2.1 (cf.[1]).

Table 3.1 Coefficients of the backward differentiation or Curtiss-Hirschfelder formulas

k	b_0	a_1	a_2	a_3	a_4
1	1	1			
2	2/3	4/3	-1/3		
3	6/11	18/11	-9/11	2/11	
4	12/25	48/25	-36/25	16/25	-3/25

Suppose that we do choose the coefficients a_ℓ in (2.3) according to this table, then scheme (2.3) may be interpreted as an iteration method for the solution of equation (2.6). The order of accuracy of this scheme follows from the following lemma:

LEMMA 2.1. *Let the functions* $\vec{G}_j$ *satisfy the conditions*

$$G_j(\vec{y},\ldots,\vec{y}) \equiv b_0\vec{f}(\vec{y}), \quad j = r,r+1,\ldots,m, \tag{2.7}$$

and let $S_{j\ell}$ *be defined by*

$$S_{r\ell} = L_{r\ell}(1-hL_{rr})^{-1}, \quad S_{j\ell} = [L_{j\ell} + h \sum_{i=r}^{j-1} L_{ji}S_{i\ell}](1-hL_{jj})^{-1}. \tag{2.8}$$

for $j > r$ *and* $\ell = 0,1,\ldots,r-1$, *where* $L_{j\ell}$, $\ell = j-1,\ldots,0$, *denote Lipschitz constants for the functions* $\vec{G}_j$ *with respect to their successive arguments. Then the local error of scheme* (3.1) *is bounded by* ($\vec{\tilde{y}}_{n+1}$ *solution of* (2.6))

$$h \sum_{\ell=0}^{r-1} S_{m\ell} \, \|\vec{y}^{(\ell)}_{n+1} - \vec{\tilde{y}}_{n+1}\| + O(h^{k+1}). \tag{2.9}$$

PROOF. Let $\vec{y}(x)$ denote the solution of equation (2.1) through the point $(x_n,\vec{y}_n)$ and $\vec{\tilde{y}}_{n+1}$ the solution of equation (2.6). By virtue of condition (2.7) we have for $j \geq r$

$$\begin{aligned}\vec{y}^{(j)}_{n+1} - \vec{\tilde{y}}_{n+1} &= h[\vec{G}_j(\vec{y}^{(j)}_{n+1},\ldots,\vec{y}^{(0)}_{n+1}) - b_0 \vec{f}(\vec{\tilde{y}}_{n+1})] \\ &= h[\vec{G}_j(\vec{y}^{(j)}_{n+1},\ldots,\vec{y}^{(0)}_{n+1}) - \vec{G}_j(\vec{\tilde{y}}_{n+1},\ldots,\vec{\tilde{y}}_{n+1})].\end{aligned}$$

Thus, as $h \to 0$

$$\|\vec{y}_{n+1}^{(j)} - \tilde{\vec{y}}_{n+1}\| \le h \sum_{\ell=0}^{j-1} \frac{L_{j\ell}}{1-hL_{jj}} \|\vec{y}_{n+1}^{(\ell)} - \tilde{\vec{y}}_{n+1}\|, \quad j \ge r.$$

Recursion of this inequality leads to inequalities of the form

$$\|\vec{y}_{n+1}^{(j)} - \tilde{\vec{y}}_{n+1}\| \le h \sum_{\ell=0}^{r-1} \tilde{S}_{j\ell} \|\vec{y}_{n+1}^{(\ell)} - \tilde{\vec{y}}_{n+1}\|, \quad j \ge r.$$

where the $\tilde{S}_{j\ell}$ are certain functions of the Lipschitz constants L_{ji}, $i = 0,1,\dots,j$. It is straighforwardly proved that these functions satisfy the recurrence relation (2.8), so that we may write

$$\|\vec{y}_{n+1} - \tilde{\vec{y}}_{n+1}\| \le h \sum_{\ell=0}^{r-1} S_{m\ell} \|\vec{y}_{n+1}^{(\ell)} - \tilde{\vec{y}}_{n+1}\|.$$

Hence, we finally arrive at the inequality

$$\begin{aligned}\|\vec{y}_{n+1} - \vec{y}(x_{n+1})\| &\le \|\vec{y}_{n+1} - \tilde{\vec{y}}_{n+1}\| + \|\tilde{\vec{y}}_{n+1} - \vec{y}(x_{n+1})\| \\ &\le h \sum_{\ell=0}^{r-1} S_{m\ell} \|\vec{y}_{n+1}^{(\ell)} - \tilde{\vec{y}}_{n+1}\| + \|\tilde{\vec{y}}_{n+1} - \vec{y}(x_{n+1})\|,\end{aligned}$$

and by using the property that $\tilde{\vec{y}}_{n+1}$ has a local error h^{k+1} as $h \to 0$, we obtain estimate (2.9).

COROLLARY 2.1. *When the functions* $\vec{G}_j$ *satisfy* (2.7) *and only depend on* $\vec{y}_{n+1}^{(j)}$, $\vec{y}_{n+1}^{(j-1)}$ *and* $\vec{y}_{n+1}^{(0)}$ *for all* $j \ge r > 1$, *then scheme* (2.3) *has the order*

(2.10) $\qquad p = \min\{k,\ m-r+1,\ q+1\}$,

q *being the order of the predictor formula.*

This result immediately follows from estimate (2.9) and the observation that all Lipschitz constants $L_{j\ell}$ with $j \ge r$ and $1 \le \ell \le j-2$ vanish. For then the parameters $S_{j\ell}$ also vanish except for

$$S_{rr-1} = L_{rr-1}(1-hL_{rr})^{-1},\quad S_{jr-1} = \frac{hL_{jj-1}}{1-hL_{jj}} S_{j-1\,r-1}$$

(2.8') $$j \geq r+1,$$

$$S_{r0} = L_{r0}(1-hL_{rr})^{-1},\quad S_{j0} = \frac{L_{j0}+hL_{jj-1}S_{j-10}}{1-hL_{jj}}$$

so that

(2.9') $$h[S_{mr-1}\|\vec{y}_{n+1}^{(r-1)} - \vec{\tilde{y}}_{n+1}\| + S_{m0}\|\vec{y}_{n+1}^{(0)} - \vec{\tilde{y}}_{n+1}\|] + O(h^{k+1}) =$$

$$= \|\vec{y}_{n+1}^{(r-1)} - \vec{\tilde{y}}_{n+1}\| \cdot O(h^{m-r+1}) + O(h^{q+2}) + O(h^{k+1})$$

from which (2.10) can be concluded. In particular, we have

<u>COROLLARY 2.2.</u> *When the functions* $\vec{G}_j$ *satisfy* (2.7) *with* $r = 1$ *and only depend on* $\vec{y}_{n+1}^{(j)}$ *and* $\vec{y}_{n+1}^{(j-1)}$, *then scheme* (2.3) *has the order*

(2.11) $$p = \min\{k, m+q\}.$$

2.2. <u>Remarks on general order equations</u>

In the preceding considerations scheme (2.3) was interpreted as an iteration process for the solution of formula (2.6). We now derive the order equations for first and second order accuracy by expanding $\vec{y}_{n+1}$ in a power series of h. Denoting by $J_{j\ell}$ the Jacobian matrix $\partial\vec{G}_j/\partial\vec{y}_{n+1}^{(\ell)}$ at the point $(\vec{y}_n,\ldots,\vec{y}_n)$, it is easily seen that

$$\vec{y}_{n+1} = \sum_{\ell=1}^{k} a_\ell \vec{y}_n + h[\sum_{\ell=1}^{k} (1-\ell)a_\ell \vec{f}(\vec{y}_n) +$$

$$+ \vec{G}_m(\vec{y}_n,\ldots,\vec{y}_n)] + \tfrac{1}{2}h^2 \sum_{\ell=1}^{k} (\ell-1)^2 a_\ell J \vec{f}(\vec{y}_n)$$

$$+ h \sum_{\ell=0}^{m} J_{m\ell}[\vec{y}_{n+1}^{(\ell)} - \vec{y}_n] + O(h^3)$$

$$= \sum_{\ell=1}^{k} a_\ell \vec{y}_n + h[\sum_{\ell=1}^{k} (1-\ell)a_\ell \vec{y}_n' + \vec{G}_m(\vec{y}_n,\ldots,\vec{y}_n)] +$$

$$+ \tfrac{1}{2}h^2 \sum_{\ell=1}^{k} (1-\ell)^2 a_\ell \vec{y}_n'' +$$

$$+ h \sum_{\ell=1}^{m} J_{m\ell}[(\sum_{i=1}^{k} a_i - 1)\vec{y}_n +$$

$$+ h \sum_{i=1}^{k} (1-i)a_i \; \vec{y}\,'_n + h\vec{G}_\ell(\vec{y}_n,\ldots,\vec{y}_n)] +$$

$$+ hJ_{m0}[\vec{y}^{(pred)}_{n+1} - \vec{y}_n] + 0(h^3).$$

Hence, first order consistency is obtained when

$$\sum_{\ell=1}^{k} a_\ell = 1,$$

$$\sum_{\ell=1}^{k} (1-\ell)a_\ell + b = 1, \text{ b arbitrary} \tag{2.12}$$

$$\vec{G}_m(\vec{y},\ldots,\vec{y}) = b\vec{f}(\vec{y}).$$

The local error is then given by

$$\vec{y}_{n+1} - \vec{y}(x_{n+1}) = \tfrac{1}{2}h^2[\sum_{\ell=1}^{k} (\ell-1)^2 a_\ell - 1]\vec{y}\,''_n + \tag{2.13}$$

$$+ h^2[\sum_{\ell=1}^{m} J_{m\ell}((1-b)\vec{y}\,'_n + \vec{G}_\ell(\vec{y}_n,\ldots,\vec{y}_n))+$$

$$+ J_{m0}\;\vec{y}\,'_n] + 0(h^3).$$

It is not clear how to derive from this expression a priori conditions for second order accuracy. Higher order conditions become increasingly more complicated, so that we conclude that a consistency analysis by Taylor expansions may be useful to *check* the order of accuracy of a given method, but is less appropriate to *construct* higher order methods. Therefore, our further considerations will be confined to multistep methods of the backward differentiation type to which lemma 2.1 can be applied.

2.3. Stability

Introducing perturbations $\Delta\vec{y}_{n+1-\ell}$, $\ell = 1,2,\ldots,k$, into scheme (2.3) yields the variational equations

$$
\begin{aligned}
\Delta\vec{y}^{(0)}_{n+1} &= \Delta\vec{y}^{(\text{pred})}_{n+1}\,, \\
\Delta\vec{y}^{(j)}_{n+1} &= \sum_{\ell=1}^{k} a_\ell\, \Delta\vec{y}_{n+1-\ell} + h \sum_{\ell=0}^{j} J_{j\ell}\, \Delta\vec{y}^{(\ell)}_{n+1}\,, \qquad (2.14) \\
\Delta\vec{y}_{n+1} &= \Delta\vec{y}^{(m)}_{n+1}\,.
\end{aligned}
$$

It will turn out that (2.14) is conveniently written either, in the form

$$
(2.14') \quad
\begin{bmatrix}
\sum_{\ell=1}^{k} a_\ell \Delta\vec{y}_{n+1-\ell} \\
\Delta\vec{y}^{(1)}_{n+1} \\
\Delta\vec{y}^{(2)}_{n+1} \\
\vdots \\
\Delta\vec{y}^{(j)}_{n+1} \\
\vdots \\
\Delta\vec{y}_{n+1}
\end{bmatrix}
=
\begin{bmatrix}
I & & & & \\
B_1 & hB_1J_{10} & & & \bigcirc \\
B_2 & hB_2J_{20} & hB_2J_{21} & & \\
\vdots & \vdots & & \ddots & \\
B_j & hB_jJ_{j0} & \cdots & hB_jJ_{jj-1} & \\
\vdots & \vdots & & & \ddots \\
B_m & hB_mJ_m & \cdots & & hB_mJ_{mm-1}
\end{bmatrix}
\begin{bmatrix}
\sum_{\ell=1}^{k} a_\ell \Delta\vec{y}_{n+1-\ell} \\
\Delta\vec{y}^{(0)}_{n+1} \\
\vdots \\
\Delta\vec{y}^{(m-1)}_{n+1}
\end{bmatrix}
$$

or in the equivalent form

$$
\text{2.14")}\qquad
\begin{bmatrix}
\sum_{\ell=1}^{k} a_\ell \Delta\vec{y}_{n+1-\ell} \\
\Delta\vec{y}^{(1)}_{n+1} \\
\Delta\vec{y}^{(2)}_{n+1} \\
\vdots \\
\Delta\vec{y}^{(j)}_{n+1} \\
\vdots \\
\Delta\vec{y}_{n+1}
\end{bmatrix}
=
\begin{bmatrix}
I & & & & & \\
B_1 & B_1D_{10} & & & & \\
0 & B_2D_{20} & B_2(I+D_{21}) & & & \\
\vdots & \vdots & \ddots & \ddots & & \\
0 & B_jD_{j0} & \cdots & B_jD_{jj-2} & B_j(I+D_{jj-1}) & \\
\vdots & \vdots & & \ddots & \ddots & \\
0 & B_mD_{m0} & \cdots & & B_mD_{mm-2} & B_m(I+D_{mm-1})
\end{bmatrix}
\begin{bmatrix}
\sum_{\ell=1}^{k} a_\ell \Delta\vec{y}_{n+1-\ell} \\
\Delta\vec{y}^{(0)}_{n+1} \\
\Delta\vec{y}^{(1)}_{n+1} \\
\vdots \\
 \\
 \\
\Delta\vec{y}^{(m-1)}_{n+1}
\end{bmatrix}
$$

where

$$
(2.15)\qquad
\begin{aligned}
&B_j = [I - hJ_{jj}]^{-1}, \qquad J_{00} = 0 \\
& \hspace{18em} , \; j = 1,2,\dots,m \\
&D_{j\ell} = h[J_{j\ell} - J_{j-1\ell}], \quad \ell = 0,1,\dots,j-1
\end{aligned}
$$

It is easily seen that both (2.14') and (2.14") result in a relation of the form

$$
(2.16)\qquad \Delta\vec{y}_{n+1} = Q \sum_{\ell=1}^{k} a_\ell \, \Delta\vec{y}_{n+1-\ell} + R\Delta\vec{y}^{(0)}_{n+1},
$$

where Q and R are matrices determined by scheme (2.14).

For future reference, we consider two special cases. Firstly, let the functions $\vec{G}_j$ depend on $\vec{y}^{(j)}_{n+1}$ and $\vec{y}^{(j-1)}_{n+1}$ only. Then,

$$
(2.17)\qquad J_{j\ell} = 0, \; \ell = 0,1,\dots,j-2; \; j = 2,3,\dots,m.
$$

Substitution into (2.14') leads to the expressions

$$(2.18)\qquad R = \prod_{j=m}^{1} A_j, \quad Q = \sum_{i=1}^{m-1} \left[\prod_{j=m}^{i+1} A_j\right] B_i + B_m,$$

where

$$(2.19)\qquad A_j = hB_j J_{jj-1}.$$

Together with the error equation of the predictor formula,

$$\Delta\vec{y}_{n+1}^{(0)} = \Delta\vec{y}_{n+1}^{(pred)} = C\Delta\vec{y}_n$$

say, the equations (2.16),(2.18),(2.19) determine the stability of scheme (2.3).

In order to continue the stability analysis it will from now on be assumed that the matrices A_j, B_j and C have the same set of eigenvectors. This assumption is rather severe, but an important class of differential equations, viz. classes of semi-discretized partial differential equations, do allow splitting functions $\vec{G}_j$ satisfying the above requirement. Let α_j, β_j and γ denote the eigenvalues of A_j, B_j and C, then (2.16) leads to the characteristic equation

$$(2.20)\qquad \zeta^k - [a_1(\beta_m + \sum_{i=1}^{m-1} \prod_{j=m}^{i+1} \alpha_j \cdot \beta_i) + \gamma \prod_{j=m}^{1} \alpha_j]\zeta^{k-1} + \\ - (\beta_m + \sum_{i=1}^{m-1} \prod_{j=m}^{i+1} \alpha_j \cdot \beta_i) \sum_{\ell=2}^{k} a_\ell \zeta^{k-\ell} = 0.$$

In the second case, representation (2.14") is taken as the starting point. Let us now choose

$$(2.17')\qquad D_{j\ell} = 0, \quad \ell = 1,2,\ldots,j-1, \quad j = 2,3,\ldots,m.$$

Substitution into (2.14") leads to the expressions

$$(2.18')\qquad R = \sum_{i=1}^{m-1} \left[\prod_{j=m}^{i+1} B_j\right] E_m + E_m, \quad Q = \prod_{j=m}^{1} B_j,$$

where

$$(2.19') \qquad E_j = B_j D_{j0}.$$

Just as above we assume that the matrices B_j, C and E_j have a common set of eigenvectors with eigenvalues β_j, γ and ε_j. The characteristic equation of (2.16) then becomes

$$(2.20') \qquad \zeta^k - [a_1 \prod_{j=1}^{m} \beta_j + \gamma(\varepsilon_m + \sum_{i=1}^{m-1} \prod_{j=m}^{i+1} \beta_j . \varepsilon_i)]\zeta^{k-1} + - \prod_{j=1}^{m} \beta_j . \sum_{\ell=2}^{k} a_\ell \zeta^{k-\ell} = 0.$$

3. TWO-ARGUMENT SPLITTING FUNCTIONS

In many cases, the right hand side $\vec{f}(\vec{y})$ can be written as a function $\vec{F}(\vec{y},\vec{y})$ in which the Jacobian matrices

$$(3.1) \qquad J_1 = \frac{\partial\vec{F}(\vec{u},\vec{v})}{\partial\vec{u}}, \quad J_2 = \frac{\partial\vec{F}(\vec{u},\vec{v})}{\partial\vec{v}}$$

have a simple structure (e.g. tridiagonal matrices). In such cases we may define splitting functions $\vec{G}_j$ with only two arguments:

$$(3.2) \qquad \vec{G}_j(\vec{y}^{(j)},\vec{y}^{(j-1)},\ldots,\vec{y}^{(0)}) = \begin{cases} b_0\vec{F}(\vec{y}^{(j)},\vec{y}^{(j-1)}) & j \text{ odd} \\ b_0\vec{F}(\vec{y}^{(j-1)},\vec{y}^{(j)}) & j \text{ even} \end{cases}.$$

Evidently, these functions satisfy condition (2.2) and (2.4) (cf.(2.7)).

Let a_ℓ and b_0 be defined by table 2.1, and consider the class of formulas

$$\vec{y}^{(0)}_{n+1} = \vec{y}^{(pred)}_{n+1},$$

$$(3.3) \qquad \vec{y}^{(j)}_{n+1} = \sum_{\ell=1}^{k} a_\ell \vec{y}_{n+1-\ell} + b_0 h \vec{F}(\vec{y}^{(j)}_{n+1}, \vec{y}^{(j-1)}_{n+1}), \ j \text{ odd},$$

$$(3.3)\qquad \vec{y}^{(j)}_{n+1} = \sum_{\ell=1}^{k} a_\ell \vec{y}_{n+1-\ell} + b_0 h \vec{F}(\vec{y}^{(j-1)}_{n+1}, \vec{y}^{(j)}_{n+1}),\ j \text{ even},$$

$$\vec{y}_{n+1} = \vec{y}^{(m)}_{n+1}.$$

According to corollary 2.2, this scheme is of order $p = \min(k, m+q)$. We shall call scheme (3.3) a *method of successive corrections* since the order of accuracy of $\vec{y}^{(j)}_{n+1}$ increases with j until the maximum order k is reached.

It is easily verified that condition (2.17) is satisfied, hence it follows from (2.15) and (2.19) that

$$(3.4)\qquad A_j = \begin{cases} b_0 h[I - b_0 h J_1]^{-1} J_2 & \\ & \text{for } j = \\ b_0 h[I - b_0 h J_2]^{-1} J_1 & \end{cases}\begin{matrix}\text{odd}\\ \\ \text{even}\end{matrix},$$

$$B_j = \begin{cases} [I - b_0 h J_1]^{-1} & \\ & \text{for } j = \\ [I - b_0 h J_2]^{-1} & \end{cases}\begin{matrix}\text{odd}\\ \\ \text{even}\end{matrix}.$$

Let us denote the eigenvalues of $b_0 h J_1$ and $b_0 h J_2$ by z_1 and z_2, respectively. Then, by (2.18)

$$(3.5)\qquad \begin{aligned} \alpha_j &= \frac{z_2}{1-z_1}, \quad \beta_j = \frac{1}{1-z_1}, \quad j \text{ odd} \\ \alpha_j &= \frac{z_1}{1-z_2}, \quad \beta_j = \frac{1}{1-z_2}, \quad j \text{ even} \end{aligned}.$$

Substitution of these expressions into (2.20) yields the characteristic equation of scheme (3.3'). It should be remarked that, unless the eigenvalues γ of the predictor formula behave like $(1-z_1)/z_2$ as $|z_1|$ or $|z_2| \to \infty$, the value of m has to be even, otherwise the coefficient of ζ^{k-1} in (3.20) may become infinite as $|z_2| \to \infty$. Restricting our considerations to even m-values, we conclude from Corollary 2.2 that the optimal choices for k, and m are given by the values listed in the following table

Table 3.1 Optimal (k,q,m) values

p = k	q	m
2	0	2
3	1	2
4	2	2
4	0	4
5	1	4
6	2	4

1 where it is assumed that at most second order accurate predictors are used. In the following subsections we analyse the stability of the first four formulas. Since splitting methods are primarily designed for partial differential equations, the fifth and sixth order formula generally are unnecessarily accurate and are therefore are not analysed in this paper.

3.1. A second order formula

Choosing $\vec{y}^{(pred)}_{n+1} = \vec{y}_n$, i.e. $q = 0$, and $k = m = 2$ we obtain the second order formula

$$\text{(3.6)}\qquad \begin{aligned} \vec{y}^{(1)}_{n+1} &= \frac{4}{3}\vec{y}_n - \frac{1}{3}\vec{y}_{n-1} + \frac{2}{3} h \vec{F}(\vec{y}^{(1)}_{n+1}, \vec{y}_n) \\ \vec{y}_{n+1} &= \frac{4}{3}\vec{y}_n - \frac{1}{3}\vec{y}_{n-1} + \frac{2}{3} h \vec{F}(\vec{y}^{(1)}_{n+1}, \vec{y}_{n+1}) \end{aligned}$$

with the characteristic equation

$$\text{(3.7)}\qquad \zeta^2 - \frac{4+3z_1z_2}{3(1-z_1)(1-z_2)}\zeta + \frac{1}{3(1-z_1)(1-z_2)} = 0.$$

It is easily verified that the roots of this equation are within the unit circle for all negative z_1 and z_2 values. Thus, *scheme (3.6) is stable for all splitting functions with negative eigenvalue spectra.*

3.2. Third order formulas

Suppose that we are given a *first order* predictor formula with real eigenvalues γ. We then may use the *third order* scheme

$$\vec{y}_{n+1}^{(0)} = \vec{y}_{n+1}^{(pred)},$$

$$(3.8) \qquad \vec{y}_{n+1}^{(1)} = \frac{1}{11}[18\vec{y}_n - 9\vec{y}_{n+1} + 2\vec{y}_{n-2}] + \frac{6}{11} h\, \vec{F}(\vec{y}_{n+1}^{(1)}, \vec{y}_{n+1}^{(0)}),$$

$$\vec{y}_{n+1} = \frac{1}{11}[18\vec{y}_n - 9\vec{y}_{n-1} + 2\vec{y}_{n-2}] + \frac{6}{11} h\, \vec{F}(\vec{y}_{n+1}^{(1)}, \vec{y}_{n+1}),$$

with characteristic equation

$$(3.9) \qquad \zeta^3 - \frac{18+11z_1z_2\gamma}{11(1-z_1)(1-z_2)}\zeta^2 + \frac{1}{11(1-z_1)(1-z_2)}[9\zeta - 2] = 0.$$

Applying Hurwitz's criterion we find for $z_1 < 0$ and $z_2 < 0$ the conditions

$$(1-\gamma)\, z_1z_2 - (z_1+z_2) > 0,$$

$$(1+\gamma)\, z_1z_2 - (z_1+z_2) + \frac{40}{11} > 0,$$

$$(3+\gamma)\, z_1z_2 - 3(z_1+z_2) + \frac{36}{11} > 0,$$

$$(1+2\gamma)\, z_1z_2 - (z_1+z_2) + \frac{34}{11} > 0,$$

guaranteeing that the roots of (3.9) are within the unit circle. These conditions are satisfied when

$$(3.10) \qquad -1 < \gamma < 1.$$

Thus, *scheme (3.8) is stable for all stable predictors and all splitting functions with negative eigenvalue spectra.*

3.3. Fourth order formulas

Let now $\vec{y}_{n+1}^{(pred)}$ be second order correct, again with real eigenvalues γ. Consider the fourth order scheme

$$\vec{y}_{n+1}^{(0)} = \vec{y}_{n+1}^{(pred)},$$

$$(3.11) \quad \vec{y}_{n+1}^{(1)} = \frac{1}{25}[48\vec{y}_n - 36\vec{y}_{n-1} + 16\vec{y}_{n-2} - 3\vec{y}_{n-3}] + \\ + \frac{12}{25} h\, F(\vec{y}_{n+1}^{(1)}, \vec{y}_{n+1}^{(0)})],$$

$$\vec{y}_{n+1} = \vec{y}_{n+1}^{(1)} + \frac{12}{25} h[\vec{F}(\vec{y}_{n+1}^{(1)}, \vec{y}_{n+1}) - \vec{F}(\vec{y}_{n+1}^{(1)}, \vec{y}_{n+1}^{(0)})].$$

Its characteristic equation is given by

$$(3.12) \quad \zeta^4 - \frac{48+25z_1z_2\gamma}{25(1-z_1)(1-z_2)}\zeta^3 + \frac{1}{25(1-z_1)(1-z_2)}[36\zeta^2 - 16\zeta + 3] = 0.$$

Hurwitz' criterion yields in the region $z_1 < 0$, $z_2 < 0$ the conditions

$$\gamma_0 = 1 + \alpha + 55\beta > 0,$$
$$\gamma_1 = 4 + 2\alpha - 44\beta > 0,$$
$$\gamma_2 = 6 - 54\beta > 0,$$
$$\gamma_3 = 4 - 2\alpha + 20\beta > 0,$$
$$\gamma_4 = 1 - \alpha + 23\beta > 0,$$
$$\gamma_5 = \gamma_1\gamma_2\gamma_3 - \gamma_1^2\gamma_4 - \gamma_0\gamma_3^2 > 0,$$

where

$$\alpha = \frac{48+25z_1z_2\gamma}{25(1-z_1)(1-z_2)}, \quad \beta = \frac{1}{25(1-z_1)(1-z_2)}.$$

It is easily verified that the expressions γ_j, $j = 1,\ldots,4$ are all positive provided that

$$(3.13) \quad -1 < \gamma < 1.$$

The last condition was numerically verified. By observing that

$$(3.14)\qquad -1 < \alpha \le \frac{48}{25}, \quad 0 < \beta < \frac{1}{25},$$

in the negative (z_1,z_2)-plane, we first considered α and β as independent variables and checked the value of γ_5 on a grid with mesh sizes $(\Delta\alpha,\Delta\beta) = (.01,.0004)$ in the rectangle defined by (3.14). We found stability for

$$(3.15)\qquad 0 < \beta < .0164$$

irrespective the value of α. This implies that we have stability in the region (see figure 3.2)

$$(3.15')\qquad |\gamma| < 1,\ z_1 < 0,\ z_2 < 0,\ (1-z_1)(1-z_2) > 2.47.$$

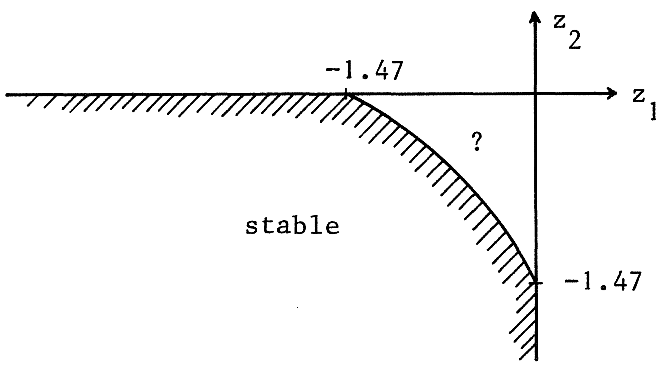

Fig. 3.1 Region of verified stable (z_1,z_2)-points

The region

$$(3.16)\qquad |\gamma| < 1,\ z_1 < 0,\ z_2 < 0,\ (1-z_1)(1-z_2) \le 2.47$$

was checked by computing γ_5 in grid points with meshes $(\Delta\gamma,\Delta z_1,\Delta z_2) = (.01,.01,.01)$. No points of instability were found so that it is reasonable to assume that scheme (3.21) is stable for all stable predictors and all splitting functions with negative eigenvalue spectra.

Another possibility to construct fourth order formulas is iterating formula (3.21) four times with the predictor $y_{n+1}^{(pred)} = y_n$, i.e. the scheme

$$\vec{y}_{n+1}^{(0)} = \vec{y}_n$$

(3.17)
$$\vec{y}_{n+1}^{(j)} = \frac{1}{25}[48\vec{y}_n - 36\vec{y}_{n-1} + 16\vec{y}_{n-2} - 3\vec{y}_{n-3}] + \frac{12}{25} h\, \vec{F}(\vec{y}_{n+1}^{(\ell)}, \vec{y}_{n+1}^{(2j-1-\ell)}), \quad j = 1,2,3,4,$$

$$\vec{y}_{n+1} = \vec{y}_{n+1}^{(4)},$$

where $\ell = j$ if j odd and $\ell = j-1$ if j even. The characteristic equation is given by

(3.18)
$$\zeta^4 - \tilde{\alpha}(z_1,z_2)\, \zeta^3 + \tilde{\beta}(z_1,z_2)[36\zeta^2 - 16\zeta + 3] = 0$$

where

$$\tilde{\alpha}(z_1,z_2) = \frac{48(1-z_1-z_2+2z_1z_2)+25z_1^2z_2^2}{25(1-z_1)^2(1-z_2)^2}$$

$$\tilde{\beta}(z_1,z_2) = \frac{1-z_1-z_2+2z_1z_2}{25(1-z_1)^2(1-z_2)^2}$$

In a similar way as done for equation (3.12), we verified that (3.18) has its roots within the unit circle for all negative z_1 and z_2 values.

4. MULTI-ARGUMENT SPLITTING FUNCTIONS

In this section the case will be considered where $\vec{f}(\vec{y})$ has to be written as an m-argument function $\vec{F}(\vec{y},\vec{y},\ldots,\vec{y})$ with $m > 2$ in order to satisfy the requirement that the Jacobian matrices of F have a simple band structure. We first try to generalize the method of successive corrections discussed in the preceding section. It will be shown that this method is no longer unconditionally stable. We then consider multi-argument splitting functions which again generate unconditionally stable schemes.

4.1. The method of successive corrections

In section 3 we considered splitting functions $\vec{G}_j$ which only depend on the first two arguments $\vec{y}^{(j)}$ and $\vec{y}^{(j-1)}$. This suggests to define for the case where we have

$$\vec{f}(\vec{y}) = \vec{F}(\vec{y},\vec{y},\ldots,\vec{y}) \tag{4.1}$$

the splitting functions

$$\vec{G}_j(\vec{y}^{(j)},\vec{y}^{(j-1)},\ldots,\vec{y}^{(0)}) = b_0\vec{F}(\vec{y}^{(j-1)},\ldots,\vec{y}^{(j-1)},\vec{y}^{(j)},\vec{y}^{(j-1)},\ldots,\vec{y}^{(j-1)}), \tag{4.2}$$

where $\vec{y}^{(j)}$ occurs at the j-th place in the row of arguments of the function $\vec{F}$. Note that (4.2) again defines a class of two-argument splitting functions.

The splitting functions 4.2 generate the scheme

$$\begin{aligned}
\vec{y}^{(0)}_{n+1} &= \vec{y}^{(pred)}_{n+1}, \\
\vec{y}^{(1)}_{n+1} &= \sum_{\ell=1}^{k} a_\ell\, \vec{y}_{n+1-\ell} + b_0 h\vec{F}(\vec{y}^{(1)}_{n+1},\vec{y}^{(0)}_{n+1},\ldots,\vec{y}^{(0)}_{n+1}), \\
\vec{y}^{(2)}_{n+1} &= \sum_{\ell=1}^{k} a_\ell\, \vec{y}_{n+1-\ell} + b_0 h\vec{F}(\vec{y}^{(1)}_{n+1},\vec{y}^{(2)}_{n+1},\vec{y}^{(1)}_{n+1},\ldots,\vec{y}^{(1)}_{n+1}), \\
&\ldots \\
\vec{y}^{(m)}_{n+1} &= \sum_{\ell=1}^{k} a_\ell\, \vec{y}_{n+1-\ell} + b_0 h\vec{F}(\vec{y}^{(m-1)}_{n+1},\ldots,\vec{y}^{(m-1)}_{n+1},\vec{y}^{(m)}_{n+1}), \\
\vec{y}_{n+1} &= \vec{y}^{(m)}_{n+1}.
\end{aligned} \tag{4.3}$$

As for scheme (3.3), we have an order of accuracy $p = \min(k,m+q)$ when the coefficients a_ℓ and b_0 are identified with those in table 2.1. Furthermore, it is a computationally efficient scheme provided that all Jacobian matrices of $\vec{F}(\vec{y},\vec{y},\ldots.)$ have the appropriate band structure. Denoting these matrices by J_j, $j = 1,2,\ldots,m$, the matrices A_j and B_j as defined by (2.15), (2.19) assume the form (note that (2.17) is satisfied)

$$A_j = b_0 h[I - b_0 hJ_j]^{-1} [J_1+J_2+\ldots+J_{j-1}+J_{j+1}+\ldots+J_m]$$
$$B_j = [I - b_0 hJ_j]^{-1} ,$$

so that the eigenvalues α_j and β_j are given by

$$\alpha_j = \frac{z_1+z_2+\ldots+z_{j-1}+z_{j+1}+\ldots+z_m}{1-z_j}$$
$$\beta_j = \frac{1}{1-z_j} , \quad j = 1,2,\ldots,m,$$

where z_j represent the eigenvalues of the matrix $b_0 hJ_j$. Unfortunately, the product $\prod_1^m \alpha_j$ is not bounded in the planes $z_j = 0$, $j = 1,\ldots,m$, so that no unconditional stability can be expected. For instance, for $m = 3$, $k = 3$ and $\vec{y}_{n+1}^{(0)} = \vec{y}_n$ (i.e. $q = 0$) we find the characteristic equation

(4.4)
$$\zeta^3 - \frac{1}{11}\frac{18(1+z_1z_2+z_1z_3+z_2z_3)+11(z_1+z_2)(z_1+z_3)(z_2+z_3)}{(1-z_1)(1-z_2)(1-z_3)}\zeta^2 + \frac{1}{11}\frac{1+z_1z_2+z_1z_3+z_2z_3}{(1-z_1)(1-z_2)(1-z_3)}[9\zeta - 2] = 0.$$

In the (z_1,z_2)-plane this equation has the stability region defined by the inequalities

$$-11(z_1+z_2) + z_1z_2[40+11(z_1+z_2)] + 40 > 0,$$

(4.5)
$$[-260(z_1+z_2) + 288z_1z_2 - 227\, z_1z_2(z_1+z_2) + 63] + [(121 - 11z_1z_2)(z_1+z_2)^2 + (171+33(z_1+z_2))z_1^2z_2^2] > 0.$$

This region is approximately given by figure 4.1.

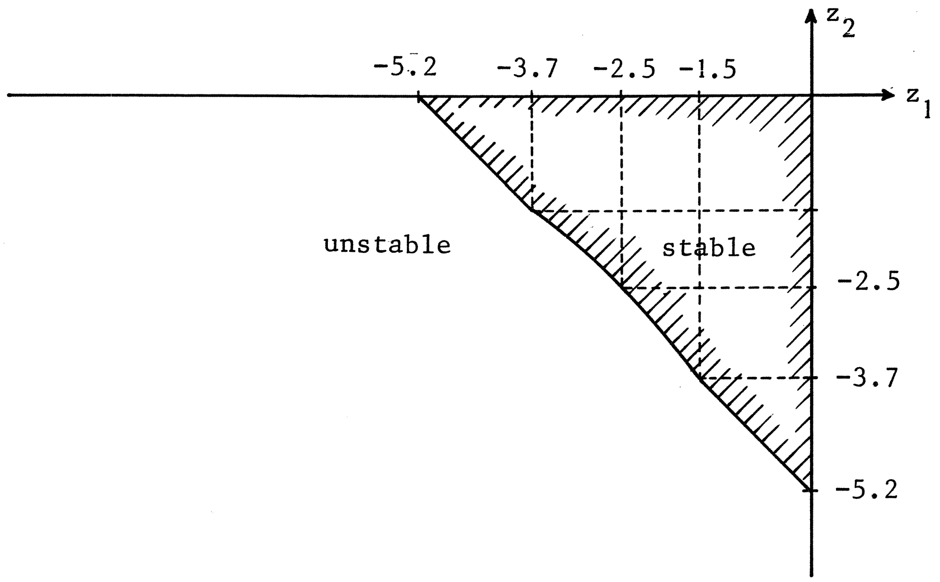

Fig. 4.1 Stability in the (z_1,z_2) plane of formula (4.1) with m = 3

4.2. The method of stabilizing corrections

In [3] a generalization of Douglas' *method of stabilizing corrections* is given which is unconditionally stable provided that the eigenvalues of all component Jacobians are negative. This method reads as follows:

$$\vec{y}^{(1)}_{n+1} = \vec{y}_n + \tfrac{1}{2}h[\vec{F}(\vec{y}^{(1)}_{n+1},\vec{y}_n,\ldots,\vec{y}_n) + \vec{F}(\vec{y}_n,\ldots,\vec{y}_n)],$$

$$\vec{y}^{(j)}_{n+1} = \vec{y}^{(j-1)}_{n+1} + \tfrac{1}{2}h[\vec{F}(\vec{y}_n,\ldots,\vec{y}_n,\vec{y}^{(j)}_{n+1},\vec{y}_n,\ldots,\vec{y}_n) - \vec{F}(\vec{y}_n,\ldots,\vec{y}_n)], \tag{4.6}$$

$$\vec{y}_{n+1} = \vec{y}^{(m)}_{n+1},$$

where $\vec{F}(\vec{y},\ldots,\vec{y})$ equals $\vec{f}(\vec{y})$. It can be proved that (4.6) is of second order.

This scheme suggests to define the multi-argument splitting functions:

$$\vec{G}_1(\vec{y}^{(1)},\vec{y}^{(0)}) = \mu_1[\vec{F}(\vec{y}^{(1)},\vec{y}^{(0)},\ldots,\vec{y}^{(0)}) + \vec{F}(\vec{y}^{(0)},\ldots,\vec{y}^{(0)})],$$

(4.7)

$$\vec{G}_2(\vec{y}^{(2)},\vec{y}^{(1)},\vec{y}^{(0)}) = \vec{G}_1(\vec{y}^{(1)},\vec{y}^{(0)}) + \\ + \mu_2[\vec{F}(\vec{y}^{(0)},\vec{y}^{(2)},\vec{y}^{(0)},\ldots,\vec{y}^{(0)}) - \vec{F}(\vec{y}^{(0)},\ldots,\vec{y}^{(0)})],$$

$$\vec{G}_j(\vec{y}^{(j)},\vec{y}^{(j-1)},\ldots,\vec{y}^{(0)}) = \vec{G}_{j-1}(\vec{y}^{(j-1)},\ldots,\vec{y}^{(0)}) + \\ + \mu_j[\vec{F}(\vec{y}^{(0)},\ldots,\vec{y}^{(0)},\vec{y}^{(j)},\vec{y}^{(0)},\ldots,\vec{y}^{(0)}) - \\ \vec{F}(\vec{y}^{(0)},\ldots,\vec{y}^{(0)})], \quad j = 3,\ldots,m,$$

to obtain a method which may be considered as a multistep formula with *stabilizing corrections*:

(4.8)

$$\vec{y}^{(0)}_{n+1} = \vec{y}^{(pred)}_{n+1},$$

$$\vec{y}^{(1)}_{n+1} = \sum_{\ell=1}^{k} a_\ell\, \vec{y}_{n+1-\ell} + \mu_1\, h[\vec{F}(\vec{y}^{(1)}_{n+1},\vec{y}^{(0)}_{n+1},\ldots,\vec{y}^{(0)}_{n+1}) + \\ + \vec{F}(\vec{y}^{(0)}_{n+1},\ldots,\vec{y}^{(0)}_{n+1})],$$

$$\vec{y}^{(j)}_{n+1} = \vec{y}^{(j-1)}_{n+1} + \mu_j\, h[\vec{F}(\vec{y}^{(0)}_{n+1},\ldots,\vec{y}^{(0)}_{n+1},\vec{y}^{(j)}_{n+1},\vec{y}^{(0)}_{n+1},\ldots,\vec{y}^{(0)}_{n+1}) \\ - \vec{F}(\vec{y}^{(0)}_{n+1},\ldots,\vec{y}^{(0)}_{n+1})],$$

$$\vec{y}_{n+1} = \vec{y}^{(m)}_{n+1}.$$

Firstly, the stability of this scheme will be analyzed. From (4.7) it is immediate that

(4.9) $$J_{10} = \mu_1[J_1 + 2(J_2+\ldots+J_m)],\ J_{11} = \mu_1 J_1$$

$$(4.9)\qquad J_{20} = J_{10} - \mu_2 J_2,\ J_{21} = J_{11},\ J_{22} = \mu_2 J_2$$

$$J_{j0} = J_{j-10} - \mu_j J_j,\ J_{j1} = J_{j-1},\dots,J_{jj-1} = J_{j-1j-1}, J_{jj} = \mu_j J_j,$$

$$j = 3,\dots,m.$$

It is easily verified that (2.17') is satisfied and that

$$(4.10)\qquad \begin{aligned} D_{10} &= \mu_1 h[J_1 + 2(J_2+\dots+J_m)], \\ D_{j0} &= -\mu_j h J_j, \quad j = 2,\dots,m. \end{aligned}$$

The matrices B_j and E_j determining the matrices Q and R in the error equation (2.16), are given by

$$(4.11)\qquad \begin{aligned} B_j &= [I - \mu_j h J_j]^{-1}, \quad j = 1,2,\dots,m, \\ E_1 &= \mu_1 h[I - \mu_1 h J_1]^{-1}[J_1 + 2(J_2+\dots+J_m)] \\ E_j &= -\mu_j h[I - \mu_j h J_j]^{-1} J_j, \quad j = 2,3,\dots,m. \end{aligned}$$

In the case $\mu_j = \mu$, $j = 1,2,\dots,m$, the eigenvalues are given by

$$(4.12)\qquad \begin{aligned} \beta_j &= \frac{1}{1-z_j}, \quad j = 1,2,\dots,m \\ \varepsilon_1 &= \frac{z_1+2(z_2+\dots+z_m)}{1-z_1}, \\ \varepsilon_j &= \frac{-z_j}{1-z_j}, \quad j = 2,3,\dots,m, \end{aligned}$$

where z_j denotes an eigenvalue of the matrix $\mu\ h\ J_j$.

The characteristic equations are given by (cf.(2.20'))

$$(4.13)\qquad \zeta^k - \frac{a_1+\gamma \sum_{i=1}^{m} z_i(2-\Pi_{i-1})}{\Pi_m} \zeta^{k-1} - \frac{1}{\Pi_m} \sum_{\ell=2}^{k} a_\ell\, \zeta^{k-\ell} = 0,$$

where

$$(4.14) \qquad \Pi_0 = 1, \quad \Pi_i = \prod_{j=1}^{i} (1 - z_j), \qquad i = 1,2,\ldots,m.$$

Before deriving stability regions from these characteristic equations we have to consider the accuracy of scheme (4.8). Evidently, the corollaries 2.1 and 2.2 do not apply so that a renewed investigation of the order of consistency is required. The following theorem can be stated:

<u>THEOREM 4.1</u>. *Let* a_ℓ *and* b_0 *be defined as in table* 2.1, *let* $\mu_j = b_0/2$ *and let* q *be the order of the predictor formula. Then scheme* (4.8) *is at least of order* $p = \min\{k,q+1\}$.

<u>PROOF</u>. Let $\vec{y}(x)$ be the solution of the differential equation through $(x_n,\vec{y}_n)$ and $\vec{\tilde{y}}_{n+1}$ the solution of equation (2.6). Firstly, we apply corollary 2.2 to the integration formula $\vec{y}^{(1)}_{n+1}$ in scheme (4.8). This results in the estimate

$$(4.16) \qquad \vec{y}^{(1)}_{n+1} - \vec{y}(x_{n+1}) = O(h^{\min\{k+1,q+2\}}).$$

Secondly, (4.8) yields for $\vec{y}^{(j)}_{n+1} - \vec{\tilde{y}}_{n+1}$ the relation

$$\begin{aligned}\vec{y}^{(j)}_{n+1} - \vec{\tilde{y}}_{n+1} &= \vec{y}^{(j-1)}_{n+1} - \vec{\tilde{y}}_{n+1} + \tfrac{1}{2}b_0hJ_j(\vec{y}^{(j)}_{n+1} - \vec{y}^{(0)}_{n+1}) + \ldots \\ &= \vec{y}^{(j-1)}_{n+1} - \vec{\tilde{y}}_{n+1} + \tfrac{1}{2}b_0hJ_j(\vec{y}^{(j)}_{n+1} - \vec{\tilde{y}}_{n+1}) + O(h^{q+2}) + \ldots\end{aligned}$$

Hence, as $h \to 0$

$$\vec{y}^{(j)}_{n+1} - \vec{\tilde{y}}_{n+1} = (I - \tfrac{1}{2}b_0hJ_j)^{-1}\,[\vec{y}^{(j-1)}_{n+1} - \vec{\tilde{y}}_{n+1} + O(h^{q+2}) + \ldots\,],$$

so that, by iterating this relation,

$$\begin{aligned}\vec{y}_{n+1} - \vec{y}(x_{n+1}) &= [\vec{y}_{n+1} - \vec{\tilde{y}}_{n+1}] + [\vec{\tilde{y}}_{n+1} - \vec{y}(x_{n+1})] = \\ &= [\vec{y}^{(1)}_{n+1} - \vec{\tilde{y}}_{n+1}]O(1) + [\vec{\tilde{y}}_{n+1} - \vec{y}(x_{n+1})] + O(h^{q+2}) \\ &= [\vec{y}^{(1)}_{n+1} - y(x_{n+1}) + \vec{y}(x_{n+1}) - \vec{\tilde{y}}_{n+1}]\,O(1) + O(h^{q+2})\end{aligned}$$

Finally, by (4.16)

$$\vec{y}_{n+1} - \vec{y}(x_{n+1}) = O(h^{k+1}) + O(h^{q+2})$$

which proves the theorem.

From this theorem it follows that scheme (4.2) is *third order accurate* when the second order formula (4.1) is used as predictor formula.

4.3. Third order formulas.

As shown above the class of three-step formulas

$$\vec{y}^{(0)}_{n+1} = \vec{y}^{(pred)}_{n+1},$$

$$\vec{y}^{(1)}_{n+1} = \frac{1}{11}[18\vec{y}_n - 9\vec{y}_{n-1} + 2\vec{y}_{n-2}] +$$

$$(4.17)\qquad + \frac{6}{11}h[\vec{F}(\vec{y}^{(1)}_{n+1},\vec{y}^{(0)}_{n+1},\ldots,\vec{y}^{(0)}_{n+1}) + \vec{F}(\vec{y}^{(0)}_{n+1},\ldots,\vec{y}^{(0)}_{n+1})]$$

$$\vec{y}^{(2)}_{n+2} = \vec{y}^{(1)}_{n+1} + \frac{6}{11}h[\vec{F}(\vec{y}^{(0)}_{n+1},\vec{y}^{(2)}_{n+1},\vec{y}^{(0)}_{n+1},\ldots,\vec{y}^{(0)}_{n+1}) -$$

$$\vec{F}(\vec{y}^{(0)}_{n+1},\ldots,\vec{y}^{(0)}_{n+1})],$$

$$\ldots$$

$$\vec{y}_{n+1} = \vec{y}^{(m)}_{n+1}$$

is third order accurate provided that $\vec{y}^{(pred)}_{n+1}$ is of second order. The characteristic equation of (4.17) is of the form (cf.(4.3))

$$(4.18)\qquad \zeta^3 - \frac{18+11\gamma\sum_{i=1}^{m} z_i(z-\Pi_{i-1})}{11\Pi_m}\zeta^2 + \frac{9}{11\Pi_m}\zeta - \frac{2}{11\Pi_m} = 0.$$

Assuming that $z_j < 0$ and applying Hurwitz' criterion yields the conditions

$$\Pi_m - \gamma\textstyle\sum_m - 1 > 0,$$

$$\Pi_m + \gamma\textstyle\sum_m + \frac{29}{11} > 0,$$

(4.19)

$$3\Pi_m + \gamma\textstyle\sum_m + \frac{3}{11} > 0,$$

$$11\Pi_m^2 - 9\Pi_m + 2\gamma\textstyle\sum_m + \frac{32}{11} > 0,$$

where we have written

$$\textstyle\sum_m = \sum_{i=1}^{m} z_i(2 - \Pi_{i-1}). \tag{4.20}$$

In figure 4.2 the stability region is shown in the $(\Pi_m, \gamma \sum_m)$-plane. From this figure it may be concluded that a *sufficient* condition for stability is given by (note that $z_j < 0$ implies $\Pi_m > 1$)

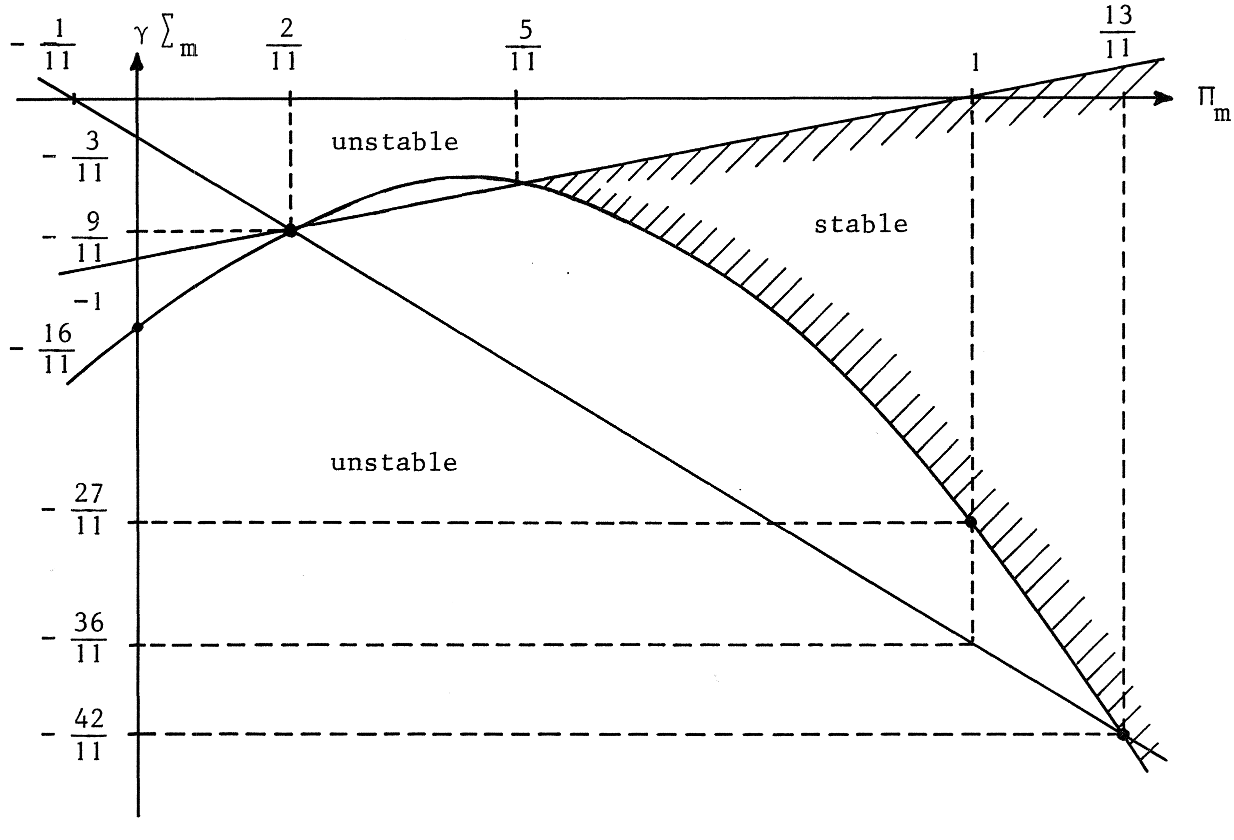

Fig. 4.2 Stability region of scheme (4.17) in the $(\Pi_m,\gamma\sum_m)$-plane

$$(4.21)\qquad \begin{cases} -1 < \gamma < 1 \\ |\Sigma_m| < \Pi_m - 1 \end{cases}.$$

We will investigate this condition for m = 3. From (4.14) and (4.20) it follows that

$$\Pi_3 = 1 - z_1 - z_2 - z_3 + z_1z_2 + z_1z_3 + z_2z_3 - z_1z_2z_3$$

$$\Sigma_3 = z_1 + z_2 + z_3 + z_1z_2 + z_1z_3 + z_2z_3 - z_1z_2z_3$$

It is now easily verified that (4.21) is satisfied since $z_j < 0$, $j = 1,2,3$. Thus, scheme (4.17) with $m = 3$ is unconditionally stable when the predictor formula is stable and when the Jacobian matrices J_j have a negative eigenvalue spectrum. (Note that this result also holds for $m = 2$ which can be proved by simply putting $z_3 = 0$.)

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