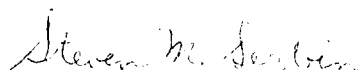


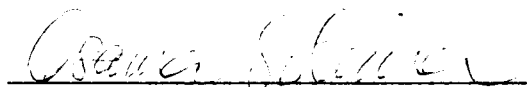
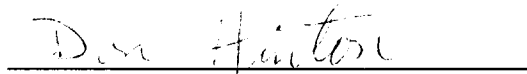
To the Graduate Council:

I am submitting herewith a dissertation written by Elizabeth B. Cohen entitled "Analysis of a Class of Two-Step Implicit Runge-Kutta Schemes for Second-Order Systems of Ordinary Differential Equations." I have examined the final copy of this dissertation for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Doctor of Philosophy, with a major in Mathematics.



Steven M. Serbin, Major Professor

We have read this dissertation
and recommend its acceptance:



Accepted for the Council:



Vice Provost
and Dean of The Graduate School

ANALYSIS OF A CLASS OF TWO-STEP IMPLICIT RUNGE-KUTTA
SCHEMES FOR SECOND-ORDER SYSTEMS OF
ORDINARY DIFFERENTIAL EQUATIONS

A Dissertation

Presented for the

Doctor of Philosophy

Degree

The University of Tennessee, Knoxville

Elizabeth Bruce Cohen

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ABSTRACT

In this dissertation a class of methods that numerically solve initial-value problems with second order ordinary differential equations of the form $y'' = f(x, y(x))$ is investigated. Methods in this class are two step implicit Runge-Kutta methods with s internal stages that do not require an update of y' . There are many examples in the literature of methods which conform to our format.

Using a type of Nyström tree and a corresponding special type of Nyström series the order conditions for this method are developed. With this technique of putting order conditions in terms of trees, we obtain a set of simplifying conditions that serve as a framework for generating and analyzing higher order methods.

Our analysis affords the development of a two-parameter family of eighth-order methods. The issue of maximum obtainable order for unconditionally stable s stage methods is investigated for $s = 1, 2$.

When implemented, these methods, in general, require at each step the solution of an algebraic equation of the form $\vec{Y} = (M \otimes I_m)F(\vec{Y})$, $\vec{Y} \in \mathbb{R}^n$ where M is an $(s+1) \times (s+1)$ matrix. To facilitate solving this equation we develop a method where M is lower triangular.

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CHAPTER 1

TWO-STEP IMPLICIT RUNGE-KUTTA METHODS

§ 1.0 Introduction.

In this dissertation we consider a class of methods that are numerical solutions to the initial value problem

$$y'' = f(x, y(x)), \quad y(x_0) = y^0, \quad y'(x_0) = y^{0'} \quad (1.1)$$

where $y \in \mathbb{R}^m$ and $f : \mathbb{R} \times \mathbb{R}^m \rightarrow \mathbb{R}^m$. Due to the absence of the term y' , this is known as a special second order system.

Special cases of these methods include:

Hairer's fourth order method [17]

$$\begin{aligned} y^{n+1} - 2y^n + y^{n-1} &= \frac{h^2}{12} [f^{n+1} + (10 - R)f^n + f^{n-1} + R\bar{f}^n] \\ \bar{y}^n &= y^n - \frac{h^2}{12R} (f^{n+1} - 2f^n + f^{n-1}) \end{aligned}$$

R is free parameter

Cash's fourth order method [5]

$$\begin{aligned} y^{n+1} - 2y^n + y^{n-1} &= h^2 \left[\frac{-11}{360} (f^{n+1} + f^{n-1}) + \frac{3}{20} f^n + \frac{41}{90} (f^{n+\frac{1}{2}} + f^{n-\frac{1}{2}}) \right] \\ \bar{y}^{n+\frac{1}{2}} &= \frac{1}{4} y^{n+1} + y^n - \frac{1}{4} y^{n-1} + h^2 \left(\frac{-3}{48} f^{n+1} + \frac{9}{48} f^n \right) \\ \bar{y}^{n-\frac{1}{2}} &= \frac{1}{2} y^n + \frac{1}{2} y^{n-1} + h^2 \left(\frac{9}{192} f^{n+1} - \frac{15}{96} f^n - \frac{1}{64} f^{n-1} \right) \end{aligned}$$

and Chawla's fourth order method [7]

$$\begin{aligned} y^{n+1} - 2y^n + y^{n-1} &= h^2 \left[\frac{-1}{18} (f^{n+1} + f^{n-1}) + \frac{5}{9} (f^{n+\frac{1}{2}} + f^{n-\frac{1}{2}}) \right] \\ \bar{y}^{n+\frac{1}{2}} &= \frac{3}{4}y^{n+1} + \frac{1}{4}y^{n-1} + h^2 \left[Bf^{n+1} - \left(\frac{3}{8} - B \right) f^{n-1} \right] \\ \bar{y}^{n-\frac{1}{2}} &= \frac{1}{4}y^{n+1} + \frac{3}{4}y^{n-1} + h^2 \left[-\left(\frac{3}{8} + B \right) f^{n+1} + Bf^{n-1} \right] \end{aligned}$$

B a free parameter.

These three methods as well as methods mentioned in [6],[8],[12],[18],[19] can be written as special cases of the general method

$$\begin{aligned} y^{n,i} &= \alpha_i y^{n-1} + \gamma_i y^n + \theta_i y^{n+1} + h^2 \sigma_i f^{n-1} + h^2 \delta_i f^n + h^2 \beta_i f^{n+1} \\ &\quad + h^2 \sum_{j=1}^s a_{ij} f(x^n + c_j h, y^{n,j}) \\ y^{n+1} &= -y^{n-1} + 2y^n + h^2 \sum_{i=1}^s b_i f(x^n + c_i h, y^{n,i}) \\ &\quad + h^2 \tilde{\sigma} f^{n-1} + h^2 \tilde{\delta} f^n + h^2 \tilde{\beta} f^{n+1} . \end{aligned} \tag{1.2}$$

A main point of this dissertation will be to investigate the order and stability of methods of the general form (1.2).

One of the more successful classes of methods for this problem is known as the Nyström methods. Nyström's method applied to problem (1.1) is

$$\begin{aligned} k_i &= f(x_0 + \alpha_i h, y^0 + \alpha_i h y^{0'} + h^2 \sum_{j=1}^2 a_{ij} k_j) \\ y^1 &= y^0 + h y^{0'} + h^2 \sum_{i=1}^s b_i k_i \\ y^{1'} &= y^{0'} + h \sum_{i=1}^s \bar{b}_i k_i . \end{aligned}$$

This is equivalent to

$$\begin{aligned}
y^{n,i} &= y^n + \alpha_i h y^{n'} + h^2 \sum_{j=1}^s a_{ij} y^{n,j} \\
y^{n+1} &= y^n + h y^{n'} + h^2 \sum_{i=1}^s b_i f(y^{n,i}) \\
y^{n+1'} &= y^{n'} + h \sum_{i=1}^s \bar{b}_i f(y^{n,i}) .
\end{aligned} \tag{1.3}$$

Note that unlike method (1.2) Nyström's method requires an update of the derivative as each step. Also note that there are choices [17] of the α_i 's, a_{ij} 's, $\bar{a}_{ij}$'s, b_i 's and $\bar{b}_i$'s that give an unconditionally stable method of order $2s$.

To find high order methods by means of matching up the Taylor series expansion of y^{n+1} and $y(x_0 + h)$ directly is a very tedious task, especially when considering the case $y(x) \in \mathbf{IR}^m$ $m \geq 2$. J. C. Butcher looked at this problem in [1], [2], [3] with respect to finding high order Runge-Kutta methods for the ODE

$$y'(x) = f(x, y(x)) , \quad y(x_0) = y^0 . \tag{1.4}$$

Then in [15], E. Hairer and G. Wanner used trees and Butcher series to find the order conditions of various methods that solve (1.4). In [16] Hairer and Wanner used a device they termed Nyström trees. Similarly, in Chapter 2 of this dissertation, a framework for discussing the accuracy, via order conditions, of the class of methods (1.2) is developed in the following manner. We show that the elementary differentials, of which the terms in the Taylor series are composed, can be represented by a certain set of trees which we call A trees. These are in fact a subset of the Nyström trees. Then, we show that these A trees can be decomposed into trees of lesser order, enabling us to write the trees in a simple form that leads to

recursive formula for coefficients (maps from the A trees to $\mathbf{IR}$) in the “A series” representations of both the true and approximate solution. Comparing these A series allows the specification of order conditions in terms of trees.

From these order conditions, certain simplifying conditions are established. Theorems relating these conditions are developed; these will be used in the remaining chapters to find high order methods with additional properties.

In Chapter 3 we investigate the limitations on order that are imposed by the requirement of unconditional stability. We analyze conditions that admit an eighth order family of methods.

In Chapter 4 we develop a fourth order unconditionally stable method for $s = 2$. The method requires solving a nonlinear algebraic system of the form $\overline{y}^n = (M \otimes I_m) f(\overline{y}^n)$ at each step. We show that the parameters in (1.4) can be chosen so that the matrix is lower triangular with distinct diagonal entries. We will establish that this form of M is useful in implementing the method.

§ 1.1 Motivation: Collocation.

In addition to noting that a wide class of known methods for solving (1.1) can be put in the form (1.2) at this point, we provide another motivation for this class of methods. This motivation parallels work done in [21], in which implicit Runge-Kutta methods for first-order systems are shown to be equivalent to a collocation approach. Our work then discovers a similar relationship when dealing with special second-order systems.

For any sufficiently smooth function u ,

$$\begin{aligned} \int_x^{x+k} (k - \tau + x) u''(\tau) d\tau &= (k - \tau + x) u'(\tau) \Big|_x^{x+k} + \int_x^{x+k} u'(\tau) d\tau \\ &= -ku'(x) + u(x+k) - u(x) . \end{aligned}$$

Hence $u(x+k) - u(x) = ku'(x) + \int_x^{x+k} (k - \tau + x) u''(\tau) d\tau$. Put $x = t_0$, $k = c_i h$, so that

$$u(t_0 + c_i h) = u(t_0) + c_i h u'(t_0) + \int_{t_0}^{t_0 + c_i h} (t_0 + c_i h - \tau) u''(\tau) d\tau . \quad (1.5)$$

Put $x = t_0$, $k = -h$ to obtain

$$u(t_0 - h) = u(t_0) - h u'(t_0) + \int_{t_0}^{t_0 - h} (t_0 - h - \tau) u''(\tau) d\tau . \quad (1.6)$$

Put $x = t_0$, $k = h$ to find

$$u(t_0 + h) = u(t_0) + h u'(t_0) + \int_{t_0}^{t_0 + h} (t_0 + h - \tau) u''(\tau) d\tau . \quad (1.7)$$

Now (1.6) $\Rightarrow$

$$\begin{aligned} -(\theta_i - c_i)u(t_0 - h) &= -(\theta_i - c_i)u(t_0) + (\theta_i - c_i)h u'(t_0) \\ &\quad - (\theta_i - c_i) \int_{t_0}^{t_0 + c_i h} (t_0 - h - \tau) u''(\tau) d\tau \end{aligned} \quad (1.8)$$

and (1.7) $\Rightarrow -\theta_i u(t_0 + h) = -\theta_i u(t_0) - \theta_i h u'(t_0)$

$$- \theta_i \int_{t_0}^{t_0 + h} (t_0 + h - \tau) u''(\tau) d\tau . \quad (1.9)$$

So, adding (1.5), (1.8), (1.9) we get

$$\begin{aligned} &u(t_0 + c_i h) - (\theta_i - c_i)u(t_0 - h) - \theta_i u(t_0 + h) \\ &= u(t_0) + c_i h u'(t_0) + \int_{t_0}^{t_0 + c_i h} (t_0 + c_i h - \tau) u''(\tau) d\tau \\ &\quad - (\theta_i - c_i)u(t_0) + (\theta_i - c_i)h u'(t_0) - (\theta_i - c_i) \int_{t_0}^{t_0 + h} (t_0 - h - \tau) u''(\tau) d\tau \\ &\quad - \theta_i u(t_0) - \theta_i h u'(t_0) - \theta_i \int_{t_0}^{t_0 + h} (t_0 + h - \tau) u''(\tau) d\tau . \end{aligned} \quad (1.10)$$

Make the change of variable $\nu = \frac{1}{h}(\tau - t_0)$ so that $t_0 + \nu h = \tau$. Then

$$\int_{t_0}^{t_0+c_i h} (t_0 + c_i h - \tau) u''(\tau) d\tau = h \int_0^{c_i} (c_i - \nu) u''(t_0 + \nu h) d\nu. \quad (1.11)$$

So, in particular, for $c_i = -1$

$$\int_{t_0}^{t_0-h} (t_0 - h - \tau) u''(\tau) d\tau = h \int_0^{-1} (-1 - \nu) u''(t_0 + \nu h) d\nu. \quad (1.12)$$

and for $c_i = 1$

$$\int_{t_0}^{t_0+h} (t_0 + h - \tau) u''(\tau) d\tau = h \int_0^1 (1 - \nu) u''(t_0 + \nu h) d\nu. \quad (1.13)$$

Using (1.11), (1.12) and (1.13) in (1.10) we obtain

$$\begin{aligned} & u(t_0 + c_i h) - (\theta_i - c_i)u(t_0 - h) - \theta_i u(t_0 + h) = \\ & (1 - 2\theta_i + c_i)u(t_0) + h^2 \left[\int_0^{c_i} (c_i - \nu) u''(t_0 + \nu h) d\nu \right] \\ & - \theta_i h^2 \left[\int_0^1 (1 - \nu) u''(t_0 + \nu h) d\nu \right] \\ & - (\theta_i - c_i) h^2 \left[\int_0^{-1} (-1 - \nu) u''(t_0 + \nu h) d\nu \right]. \end{aligned} \quad (1.14)$$

Now, define the collocation polynomial $u(t)$ of degree $(s + 4)$ by

$$u''(t_0 + c_i h) = f(t_0 + c_i h, u(t_0 + c_i h)) \equiv k_i \quad i = 1, \dots, s + 3$$

where we specify $c_{s+1} = -1$, $c_{s+2} = 0$, and $c_{s+3} = 1$ along with the condition that $u(t_0) = y^0$ and $u(t_0 - h) = y^{-1}$, which are given.

Note that this nonstandard notation of $c_{s+1} = -1$, $c_{s+2} = 0$, and $c_{s+3} = 1$ is due to the fact that our method requires us to evaluate $f(t_0, y^0)$, $f(t_0 - h, y^{-1})$,

$f(t_0 + h, y^1)$. Since $u''(t)$ has degree $s + 2$, it is reproduced by its interpolate at the $(s + 3)$ points $c_i = 1, \dots, s + 3$. It follows that

$$u''(t_0 + \nu h) = \sum_{j=1}^{s+3} u''(t_0 + c_j h) l_j(\nu) \quad (1.15)$$

where $l_j(c_i) = \delta_{ij}$ ($l_j(\nu)$ is the fundamental Lagrangian interpolating polynomial).

Then, by (1.14)

$$\begin{aligned} & u(t_0 + c_i h) - (\theta_i - c_i)u(t_0 - h) - \theta_i u(t_0 + h) = \\ & (1 - 2\theta_i + c_i)u(t_0) + h^2 \left[\int_0^{c_i} (c_i - \nu) \sum_{j=1}^{s+3} k_j l_j(\nu) d\nu \right. \\ & \left. - \theta_i \int_0^1 (1 - \delta) \sum_{j=1}^{s+3} k_j l_j(\nu) d\nu - (\theta_i - c_i) \int_0^{-1} (-\nu - 1) \sum_{j=1}^{s+3} k_j l_j(s) ds \right] \\ & = (1 - 2\theta_i + c_i)u(t_0) + h^2 \sum_{j=1}^{s+3} \left\{ \int_0^{c_i} (c_i - s) l_j(\nu) d\nu \right. \\ & \left. - \theta_i \int_0^1 (1 - \nu) l_j(\nu) d\nu - (\theta_i - c_i) \int_0^{-1} (-\nu - 1) l_j(\nu) d\nu \right\}. \end{aligned} \quad (1.16)$$

We adopt the following notation:

$$\begin{aligned} & \int_0^{c_i} (c_i - \nu) l_j(\nu) d\nu - \theta_i \int_0^1 (1 - \nu) l_j(\nu) d\nu - (\theta_i - c_i) \int_0^{-1} (-\nu - 1) l_j(\nu) d\nu \\ & = \begin{cases} a_{ij} & \text{if } 1 \leq i, j \leq s \\ \sigma_i & \text{if } j = s + 1, 1 \leq i \leq s \\ \delta_i & \text{if } j = s + 2, 1 \leq i \leq s \\ \beta_i & \text{if } j = s + 3, 1 \leq i \leq s \end{cases}. \end{aligned}$$

Then, the collocation polynomial, by (1.16) satisfies

$$\begin{aligned} & u(t_0 + c_i h) - (\theta_i - c_i)u(t_0 - h) - \theta_i u(t_0 + h) \\ & = (1 - 2\theta_i + c_i)u(t_0) + h^2 \sum_{j=1}^s a_{ij} k_j + h^2 \sigma_i k_{s+1} + h^2 \delta_i k_{s+2} + h^2 \beta_i k_{s+3} \end{aligned} \quad (1.17)$$

for $i = 1, \dots, s$ and $i = s + 3$. We note that

$$k_{s+1} = f(t_0 - h, u(t_0 - h)) = f(t_0 - h, y^{-1})$$

and

$$k_{s+2} = f(t_0, u(t_0)) = f(t_0, y^0)$$

are known quantities.

Since $c_{s+3} = 1$ and we choose $\theta_{s+3} = 0$, for $i = s + 3$ equation (1.16) becomes

$$\begin{aligned} u(t_0 + h) + u(t_0 - h) = & 2u(t_0) + h^2 \left[\sum_{j=1}^s b_j f(t_0 + c_j h, u(t_0 + c_j h)) \right. \\ & \left. + \tilde{\sigma} f(t_0 - h, u(t_0 - h)) + \tilde{\delta} f(t_0, u(t_0)) + \tilde{\beta} f(t_0 + h, u(t_0 + h)) \right] \end{aligned}$$

where

$$\begin{aligned} a_{s+3} = b_j \quad \text{for} \quad i = 1, \dots, s \\ a_{s+3,s+1} = \tilde{\sigma}, \quad a_{s+3,s+2} = \tilde{\delta}, \quad \text{and} \quad a_{s+3,s+3} = \tilde{\beta}. \end{aligned} \quad (1.18)$$

By definition $y^1 = u(t_0 + h)$, and we have $y^0 = u(t_0)$, and $y^{-1} = u(t_0 - h)$, and let $y^{1,i} = u(t_0 + c_i h)$.

Using this in (1.16) and (1.17) suggests the method

$$\begin{aligned} y^{1,i} = & (\theta_i - c_i) y^{-1} + \theta_i y^1 + (1 - 2\theta_i + c_i) y^0 \\ & + h^2 \sum_{j=1}^s a_{ij} f(t_0 + c_j h, y^{1,j}) \\ & + h^2 \sigma_i f(t_0 - h, y^{-1}) + h^2 \delta_i f(t_0, y^0) + h^2 \beta_i f(t_0 + h, y^1) \end{aligned}$$

and

$$y^1 = 2y^0 - y^{-1} + h^2 \left[\sum_{i=1}^s b_i f(t_0 + c_i h, y^{1,i}) \right. \\ \left. + \tilde{\sigma} f(t_0 - h, y^{-1}) + \tilde{\delta} f(t_0, y^0) + \tilde{\beta} f(t_0 + h, y^1) \right]$$

where $\theta_i - c_i = \alpha_i$ and $1 - 2\theta_i + c_i = \gamma_i$. This is, with obvious correspondence of notation, the method (1.2), and hence we have established that it may be viewed either as a collocation scheme or an implicit Runge-Kutta method.

CHAPTER 2

TREE-BASED DEVELOPMENT OF ORDER CONDITIONS

§ 2.0 Introduction

In *A Theory for Nyström Methods* [16] E. Hairer and G. Wanner use Nyström trees and Nyström series to find the order conditions of Nyström methods. Nyström methods can be applied to the more general ODE

$$y'' = f(y, y'), \quad y(x_0) = y^0, \quad y'(x_0) = y^{0'} . \quad (2.1)$$

Hairer and Wanner show that there exists a one to one correspondence between the elementary differentials of (2.1) and Nyström trees, which are a type of tree whose nodes are also labeled “fat” and “meager”.

They then use this correspondence to describe the Taylor series expansion of $y(x_0 + h)$ as a Nyström series, which is a series summed over Nyström trees. Similarly the numerical estimate y^1 obtained from Nyström method is described as a Nyström series. Then the order conditions are found by matching up the coefficients of these two Nyström series.

Sections one and two of this chapter will parallel this work. Since the O.D.E. (1.1) that method (1.2) solves is independent of y' , the elementary differentials of the solution to (1.1) will be a proper subset of the elementary differentials of the solution to (2.1). Because of this, we introduce a class of trees we call A trees, which are the proper subset of the Nyström trees that correspond to the elementary differentials of the solution to (1.1), and a corresponding series, deemed an A series.

Then, as in [16], we use this 1-1 correspondence to express $y(x_1 + h)$ and y^2 as A series. The order conditions are found by matching up the coefficients of these two A series.

We note that S. Gupta in an unpublished work [14], has investigated a class of two-step methods (in his case, applied to boundary value problems) which appear to be a subclass of the methods we consider here, in that certain of the parameters in our method do not appear in his scheme, and that our interest is to investigate, in general, methods which are implicit, while his are explicit. He too uses a tree-based analysis, but does not provide detailed proofs, and correspondences between his conditions and ours are not apparent.

In [1] J. C. Butcher, who originated the whole concept of alternative ways to generate order conditions, shows that instead of looking at the order conditions directly by matching up Taylor Series, that the order can be found more easily by means of "simplifying conditions" A, B, C, D , and E . (These type of conditions have become standard in the Runge-Kutta industry). The conditions A, B, C , and E in section 2.3 are defined in the spirit of the corresponding conditions in [1]. The D condition is of necessity a little different from the D condition in [1].

The rest of § 2.3 is devoted to proving a series of theorems that show the interconnections between conditions A, B, C, D , and E and the order conditions. These theorems will greatly simplify the search for higher order methods.

§ 2.1 Trees

First we give the definition of the most basic type of tree.

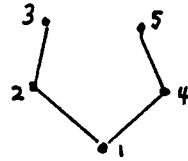
DEFINITION 1 [16] (Monotonically labelled trees (LT)). Let $n \in \mathbb{Z}$, $n \geq 0$. A monotonically labelled tree of order n is a map $t : \{2, \dots, n\} \rightarrow \{1, \dots, n\}$ such that

$t(i) < i$ for $i = 2, \dots, n$.

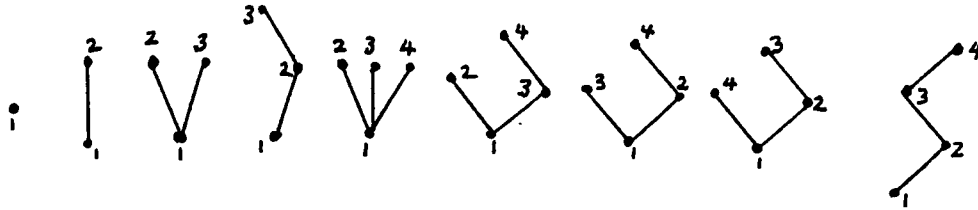
Let $\rho(t)$ denote the order of a labelled tree t .

A labelled tree t of order n can be graphically represented by n labelled points called nodes and $n - 1$ arcs connecting node i to node $t(i)$. It is traditional to locate the node labelled 1 called the root at the bottom of the graph.

EXAMPLE 2.1: Consider the fifth order tree t where t maps $2 \rightarrow 1$, $3 \rightarrow 2$, $4 \rightarrow 1$, $5 \rightarrow 4$. The graph of this labelled tree is



EXAMPLE 2.2: Here are the graphs of LT of order 4 and less:



DEFINITION 2 [16] (Trees (T)): A tree is an equivalence class of LT's which represent the same graph but differ in numeration. This equivalence relation can be defined by

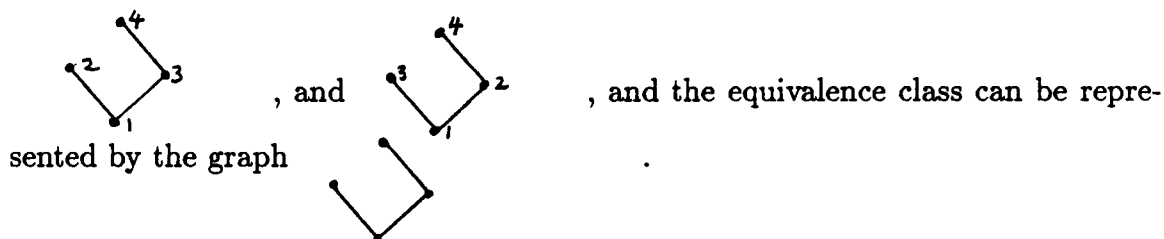
$$t \approx u \iff 1) \rho(t) = \rho(u).$$

2) There exists a permutation σ of

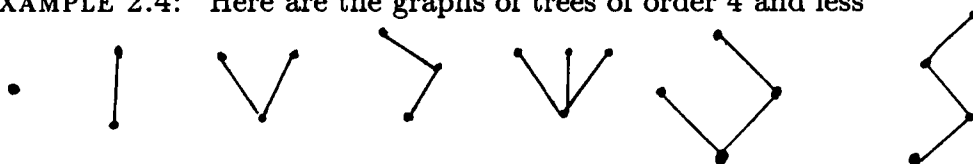
$\{1, \dots, \rho(t)\}$ such that $\sigma(1) = 1$ and

$$t(i) = \sigma u \sigma^{-1}(i) \quad (i = 2, \dots, \rho(t)).$$

EXAMPLE 2.3: The following two trees are equivalent



EXAMPLE 2.4: Here are the graphs of trees of order 4 and less



DEFINITION 3 [16] (Monotonically labelled Nyström-trees (LNT)). A m.l.N. tree of order n is a map $t \in \text{LT}$ together with a specification of its nodes into fat ones and meager ones, i.e. a second map

$$q: \{1, \dots, n\} \rightarrow \{0, 1\}$$

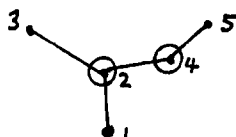
such that

- a) the root is meager, i.e. $q(1) = 0$
- b) a meager node has no ramifications and each adjacent node must be fat, i.e.:
 $q(i) = 0 \Rightarrow \text{card } \{t^{-1}(i)\} \leq 1 \text{ and } q(\{t^{-1}(i)\}) = 1 \text{ if } t^{-1}(i) \neq \emptyset.$

A labelled Nyström tree can be graphically represented in the same manner as a labelled tree but with the extra notation of a circle around the fat nodes.

EXAMPLE 2.5: Consider the 5th order LNT(t, q) where t maps: $2 \rightarrow 1, 3 \rightarrow 2, 4 \rightarrow 2, 5 \rightarrow 4$ and where q maps: $1 \rightarrow 0, 2 \rightarrow 1, 3 \rightarrow 0, 4 \rightarrow 1, 5 \rightarrow 0$.

The graph of this LNT is



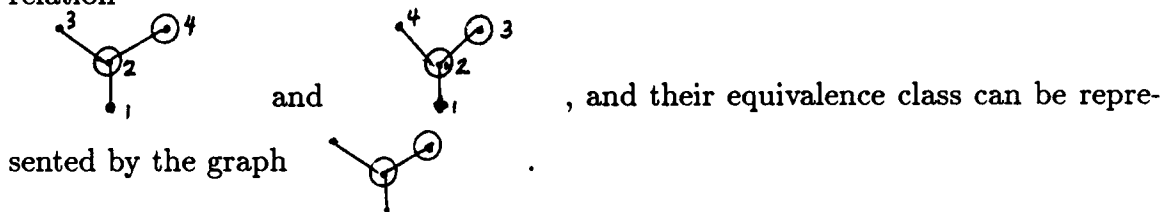
DEFINITION 4 [16] (Nyström-trees (NT)): A N -tree is an equivalence class of LNT's

with respect to the equivalence relation

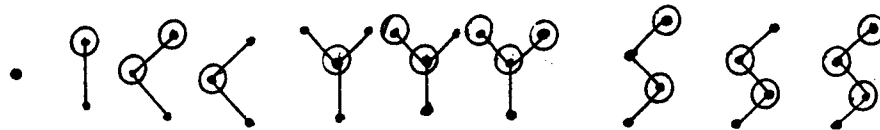
$$\left. \begin{array}{l} (t, q) \sim (u, r) \iff 1) \\ 2) \end{array} \right\} \text{ same as in definition 2}$$

$$3) \quad q(i) = r \sigma(i)$$

EXAMPLE 2.6: The following two trees are equivalent by the above equivalence relation



EXAMPLE 2.7: Here are the graphs of the Nyström-trees of order 4 and less:



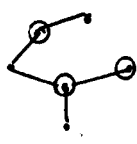
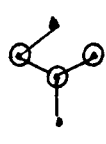
It was shown in [16] that any Nyström tree of order 3 or greater can be generated from Nyström trees of lesser order using the construction described in the following definition.

DEFINITION 5 [16] : Let $t_1, \dots, t_m \in \text{NT}$ and $k \in \mathbb{Z}$ with $0 \leq k \leq m$. Then we denote by $t = [t_1, \dots, t_k; t_{k+1}, \dots, t_m]$ a new NT of order $\sum_{i=1}^m \rho(t_i) - m + k + 2$ which is obtained by:

- 1) The roots of $t_{k+1}, \dots, t_k$ are identified to a new fat node "Charlie" say
- 2) The roots of $t_1, \dots, t_k$ are connected by a new branch to Charlie;
- 3) Finally a new root is affixed underneath of Charlie .

This has sense only if the order is ≥ 1 for $t_1, \dots, t_k$ and ≥ 2 for $t_{k+1}, \dots, t_m$.

EXAMPLE 2.8: Given $t_1 =$ and $t_2 =$ then the tree $[t_1, t_2;]$

is , the tree $[t_1; t_2]$ is , and the tree $[; t_1, t_2]$ is .

Finally we define A trees in the following manner.

DEFINITION 6 (Monotonically labelled A trees (LAT)): Let $n \in \mathbb{Z}$, $n \geq 0$. A monotonically labelled A tree of order n is a mapping $t \in \text{LT}$ together with the map q such that

$$\{2, \dots, n\} \xrightarrow{t} \{1, \dots, n\} \xrightarrow{q} \{0, 1\}$$

such that

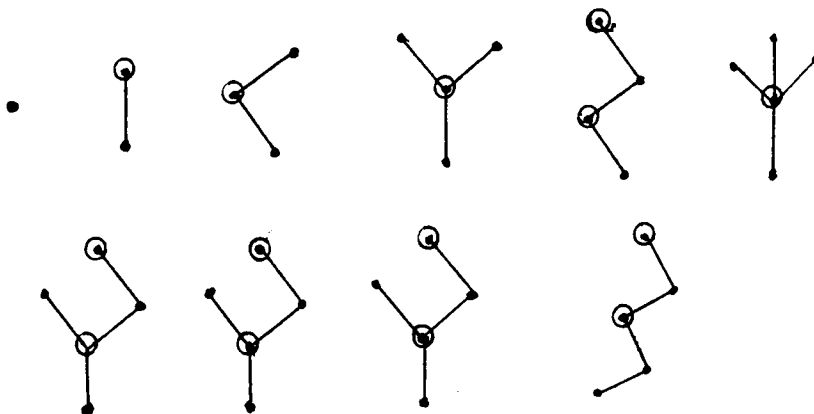
- 1) $t(2) = 1$ and $t(i) < i$
- 2) $q(1) = 0$
- 3) if $q(i) = 0$ then $\text{card } \{t^{-1}(i)\} \leq 1$
and $q(\{t^{-1}(i)\}) = 1$ if $t^{-1}(i) \neq \emptyset$
- 4) if $q(i) = 1$ then $q(\{t^{-1}(i)\}) = 0$.

As in definition 3, q labels the nodes meager if $q(i) = 0$ and fat if $q(i) = 1$.

Note condition 4) in the above definition is what distinguishes the LAT from the LNT, that is $\text{LAT} \subsetneq \text{LNT}$. Observe that the following labelled Nyström trees are not labelled A trees



EXAMPLE 2.9: The following are the LAT of order 5 and less:



DEFINITION 7 (*A* trees (AT)): An *A* tree is an equivalence class of LAT's with respect to the equivalence relation

$$(t, q) \sim (u, r) \iff 1) \rho(t) = \rho(u)$$

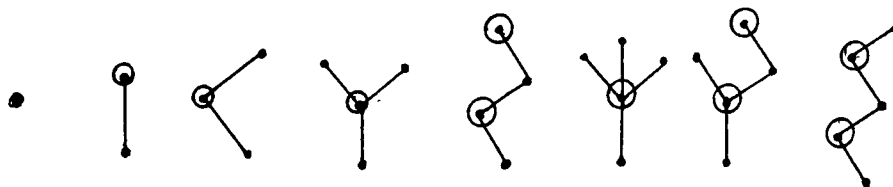
2) There exists a permutation σ such that

$$\sigma(1) = 1 \text{ and } t(i) = \sigma u \sigma^{-1}(i) \text{ } i = 2, \dots, \rho(t).$$

3) $q(i) = r\sigma(i)$

The above equivalence relation is the same as the one mentioned in definition 4 so AT is a subset of NT.

EXAMPLE 2.10: Here are the AT of order 5 and less:

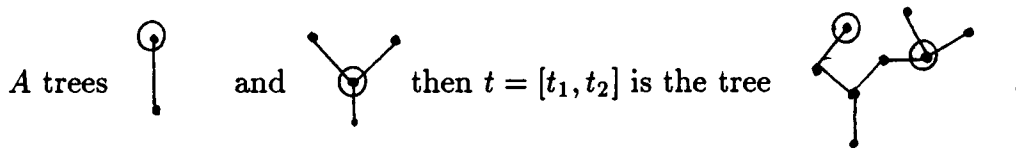


The following definition gives us a method of generating *A* trees from *A* trees of lesser order.

DEFINITION 8: Let $t_1, \dots, t_m \in \text{AT}$; then we denote by $t = [t_1, \dots, t_m]$ a new A tree which is obtained by connecting each root of t_i , $i = 1, \dots, m$ to a new branch. Those new branches are connected to a new fat node with one meager node underneath it.

The construction $[t_1, \dots, t_m]$ described in definition 8 produces the same tree as $[t_1, \dots, t_m;]$ defined in definition 5.

Example 2.11: Here is an example of the construction defined in definition 8. Given



The following two propositions are concerned with a tree as a composite of smaller trees.

PROPOSITION 2.1: $\rho([t_1, \dots, t_k]) = \sum_{i=1}^k \rho(t_i) + 2$

PROOF: The proof follows directly from the definition. For example just count the nodes in the above example.

PROPOSITION 2.2: Every $t \in \text{AT}$ with $\rho(t) \geq 3$ can be represented in the form $t = [t_1, \dots, t_k]$ with $t_i \in \text{AT}$, $\rho(t_i) \leq \rho(t)$. Except for permutation among $t_1, \dots, t_k$, this representation is unique.

PROOF: (The proof of this proposition is just an adaptation of the proof of Proposition 8 in [16].) Take away the lowest two nodes and the adjacent branches. What is left is a collection of A trees $t_1, \dots, t_k$ and so $t = [t_1, \dots, t_k]$.

§2.2 Elementary Differentials

As was shown in [16] the elementary differentials of y where $y'' = f(y, y')$ are:

$$\begin{aligned}
 y' &= y' \\
 y'' &= f(y, y') \\
 y^{(3)} &= D_1 f \cdot y' + D_2 f \cdot f \\
 y^{(4)} &= D_1 D_1 f \cdot (y', y') + D_2 D_1 f \cdot (y', f) + D_1 f \cdot f + D_1 D_2 f \cdot (f, y') \\
 &\quad + D_2 D_2 f \cdot (f, f) + D_2 f \cdot (D_1 f, y') + D_2 f \cdot (D_2 f \cdot f) \\
 &\quad \vdots
 \end{aligned}$$

In [16] E. Hairer and G. Wanner define a one to one, onto correspondence between these elementary differentials and the N trees in the following manner:

For $t \in NT$ define $F(t)$ recursively by:

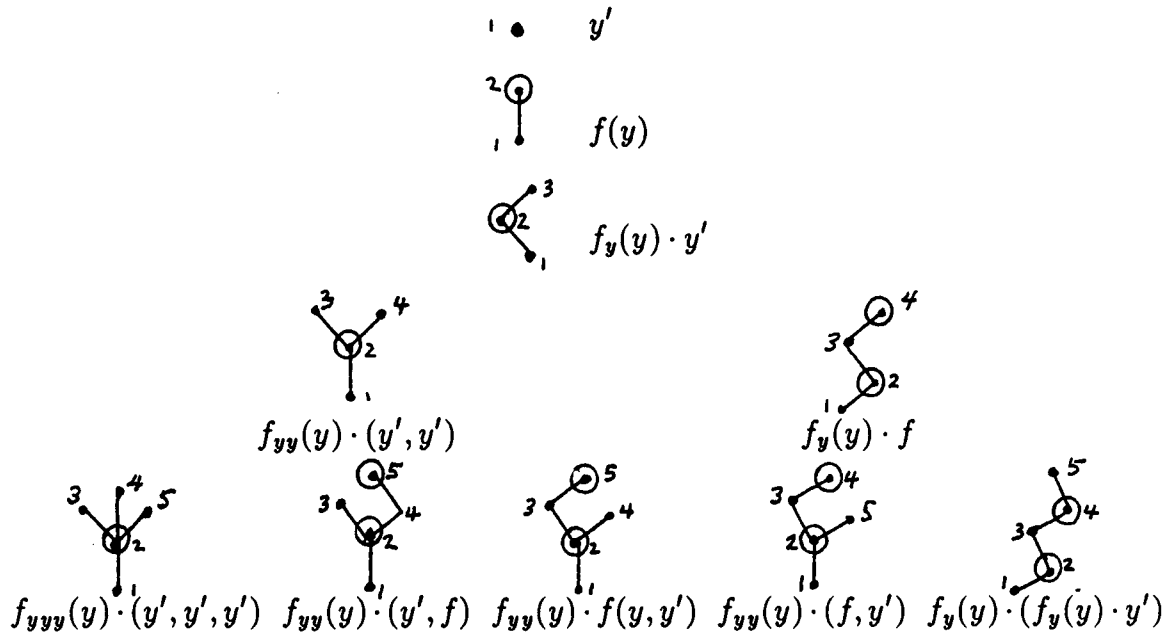
$$\begin{aligned}
 F(\phi)(y, y') &= y \\
 F(\cdot)(y, y') &= y' \\
 F(\bigcirc)(y, y') &= f(y, y') \\
 F(t)(y, y') &= D_1^k D_2^{m-k} f \cdot (F(t_1), \dots, F(t_k), F(t_{k+1}), \dots, F(t_m)) \quad (2.2)
 \end{aligned}$$

where $t = [t_1, \dots, t_k; t_{k+1}, \dots, t_m]$

In our case, the elementary differentials of y , where $y'' = f(y)$, are:

$$\begin{aligned}
 y' &= y' \\
 y'' &= f(y) \\
 y^{(3)} &= f_y(y) \cdot y' \\
 y^{(4)} &= f_{yy}(y) \cdot (y', y') + f_y(y) \cdot f \\
 y^{(5)} &= f_{yyy}(y) \cdot (y', y', y') + f_{yy}(y) \cdot (f, y') + f_{yy}(y) \cdot (y', f) + \dots
 \end{aligned}$$

These elementary differentials can be represented by monotonically labelled A trees in the following manner



Formally this correspondence is as follows.

For every $t \in \text{AT}$ we define a function $F(t) : \mathbb{R}^m \times \mathbb{R}^m \rightarrow \mathbb{R}^m$ recursively by

$$F(\phi)(y, y') = y$$

$$F(\cdot)(y, y') = y'$$

$$F(\Phi)(y, y') = f(y)$$

$$F(t)(y, y') = D_y^k f \cdot (F(t_1), \dots, F(t_k)) \text{ where } t = [t_1, \dots, t_k]. \quad (2.3)$$

Since this is the same correspondence as described in [16], restricted to $AT \subset NT$, we know it is well defined and 1 to 1. As to it's being onto, that is shown in the proof of the following theorem, which describes the actual solution at the next point as an A -series.

THEOREM (2.3). For the solution of equation (1.1) we have

$$y^p(x_0) = \sum_{\substack{t \in \text{LAT} \\ \rho(t)=p}} F(t) (y^0, y^{0'})$$

and

$$y(x_0 + h) = \sum_{t \in \text{LAT}} F(t) (y^0, y^{0'}) \frac{h^{\rho(t)}}{(\rho(t))!}$$

where F is defined by (2.3).

PROOF: We can restate the problem

$$y''(x) = f(y(x)), \quad y(x_0) = y^0, \quad y'(x_0) = y^{0'}$$

as $y''(x) = \tilde{f}(y(x), y'(x))$, $y(x_0) = y^0$, $y'(x_0) = y^{0'}$ where $\tilde{f}(y(x), y'(x)) = f(y(x))$. Since $y''(x) = \tilde{f}(y(x), y'(x))$ is the problem that [16] addresses, by Theorem 10 of [16] we have

$$y^p(x_0) = \sum_{\substack{t \in \text{LNT} \\ \rho(t)=p}} \tilde{F}(t)(y^0, y^{0'}) ,$$

where $\tilde{F}$ is defined as in (2.2) with respect to the $\tilde{f}$ defined above.

Next we show by induction that $\tilde{F}(t)(y^0, y^{0'}) = 0$ for all $t \notin \text{AT}$.

Consider the smallest tree in NT that is not in AT namely

$$\begin{array}{c} \circ \\ \diagup \quad \diagdown \\ \circ \quad \circ \end{array} ; \text{ then } \tilde{F}(\begin{array}{c} \circ \\ \diagup \quad \diagdown \\ \circ \quad \circ \end{array})(y^0, y^{0'}) = D_2 \tilde{f} \cdot \tilde{f} = 0, \quad \text{since } D_2 \tilde{f} = 0.$$

Assume the claim is true for all trees $t \in \text{NT} - \text{AT}$ of order less than p . Consider $t \in \text{NT} - \text{AT}$, $\rho(t) = p$. Since $t \notin \text{AT}$ then either $m > k$ or at least one of the t_i 's is an element of NT - AT .

If $m > k$ then

$$\tilde{F}(t)(y^0, y^{0'}) = D_1^k D_2^{m-k} \tilde{f} \cdot (\tilde{F}(t_1), \dots, \tilde{F}(t_k), \tilde{F}(t_{k+1}), \dots, \tilde{F}(t_m)),$$

but as stated before, $D_2 \tilde{f} = 0$, so if $m > k$, then $\tilde{F}(t) = 0$.

If one of the t_i 's is an element of NT-AT then by our assumption $\tilde{F}(t_i)(y^0, y^{0'}) = 0$ since $\rho(t_i) \leq p$, so $\tilde{F}(t)(y^0, y^{0'}) = 0$ for all $t \notin \text{AT}$.

Since $\tilde{F}(t)|_{\text{NT-AT}} = 0$ and $\tilde{F}(t)|_{\text{AT}} = F(t)$ we have $y^p(x_0) = \sum_{\substack{t \in \text{AT} \\ \rho(t)=p}} F(t)(y^0, y^{0'})$ and the Taylor Series of

$$y(x_0 + h) = \sum_{t \in \text{LAT}} F(t)(y^0, y^{0'}) \frac{h^{\rho(t)}}{\rho(t)!} \quad \blacksquare$$

An A series is a special case of N series which is defined as follows

DEFINITION 9 [16] (Nyström or N series): With a mapping $a: \text{NT} \rightarrow \mathbf{IR}$ we combine the series

$$N(a, y^0, y^{0'}) = \sum_{t \in \text{LNT}} a(t) F(t)(y^0, y^{0'}) \frac{h^{\rho(t)}}{\rho(t)!}$$

and call it a Nyström series. Its derivative is

$$N'(a, y^0, y^{0'}) = \sum_{\substack{t \in \text{LNT} \\ t \neq \emptyset}} a(t) F(t)(y^0, y^{0'}) \frac{h^{\rho(t)-1}}{(\rho(t)-1)!}.$$

where (2.2) defines the F .

DEFINITION 10 (A Series): Given the mapping $a: \text{AT} \rightarrow \mathbf{IR}$ then the A series $A(a, y^0, y^{0'})$ is the sum

$$A(a, y^0, y^{0'}) = \sum_{t \in \text{LAT}} a(t) F(t)(y^0, y^{0'}) \frac{h^{\rho(t)}}{\rho(t)!}.$$

Its derivative is

$$A'(a, y^0, y^{0'}) = \sum_{\substack{t \in \text{LAT} \\ t \neq \emptyset}} a(t) F(t) (y^0, y^{0'}) \frac{h^{\rho(t)-1}}{(\rho(t)-1)!},$$

where (2.3) defines the F .

So an A series is an N series where the mapping $a : \text{NT} \rightarrow \mathbf{IR}$ obeys $a(t) = 0$ for all $t \notin \text{LAT}$.

Theorem 2.3 gives us that $y(x_0 + \tau h)$ is an A -series $A(p_\tau, y^0, y^{0'})$ with $p_\tau(t) = \tau^{\rho(t)}$ where y is the exact solution to (2.1). In particular $y(x_0 + h) = y(x_1) = A(p, y^0, y^{0'})$ where $p(t) = 1$ for all t .

The following proposition allows us to say that two A series $A(a, y^0, y^{0'})$ and $A(b, y^0, y^{0'})$ are equal for all f if and only if $a(t) = b(t)$ for all t . The proof of this proposition is just a special case of the proof of Proposition 12 in 16[22].

PROPOSITION 2.4: For any tree $t \in \text{AT}$ there exists an initial value problem of the form $y'' = f(y, y'), y(x_0) = y^0, y'(x_0) = y^{0'}$ such that for the first component of $F(u)(y^0, y^{0'})$

$$F(u) (y^0, y^{0'}) \begin{cases} \neq 0 & \text{for } u = t \ u \in \text{AT} \\ = 0 & \text{for } u \neq t \ u \in \text{AT} \end{cases}$$

where the F is defined by (2.3).

PROOF: Proposition 12 in [16] states that for any tree $t \in \text{NT}$ there exists an initial value problem of the form $y'' = f(y, y'), y(x_0) = y^0, y'(x_0) = y^{0'}$ such that for the first component of $F(u)(y^0, y^{0'})$

$$F(u)(y^0, y^{0'})_1 \begin{cases} \neq 0 & \text{for } u = t \ u \in \text{NT} \\ = 0 & \text{for } u \neq t \end{cases}$$

(where F is defined by (2.2)).

This was done by considering a vector valued polynomial f of dimension $\rho(t) - 1$ where f is defined to be

$$f_i((y_2, \dots, y_{\rho(t)}), (y'_2, \dots, y'_{\rho(t)})) = \begin{cases} \prod_{k \in M(i)} y_k \prod_{k' \in M'(i)} y_{k'} & \text{if } q(i) = 1 \\ 0 & \text{if } q(i) = 0 \end{cases}$$

with the initial values $y^0 = (0, \dots, 0)$, $y^{0'} = (y'_{2,0}, \dots, y'_{\rho(t),0})$, where

$$y'_{i,0} = \begin{cases} 0 & \text{if } q(i) = 1 \\ 1 & \text{if } q(i) = 0 \end{cases}$$

The set $M'(i)$ for an index i is defined to be the set of indices of fat nodes directly above the node labelled i ; that is

$$M'(i) = \{k | i = t(k), q(k) = 1\}$$

$M(i)$ is the set of indices of fat nodes which are connected with " i " via a meager node and of the meager end nodes which are directly above " i ", that is

$$M(i) = \{k | t(k) = l, q(l) = 0, t(l) = i\} \\ \cup \{k | t(k) = i, q(k) = 0, t^{-1}(k) = \phi\}.$$

Consider $t \in AT$; then $M'(i) = \phi$ when i is a fat node, so the f_i above is

$$f_i((y_2, \dots, y_{\rho(t)}), (y'_2, \dots, y'_{\rho(t)})) = \begin{cases} \prod_{k \in M(i)} y_k & q(i) = 1 \\ 0 & \text{otherwise} . \end{cases}$$

So for $t \in AT$ the IVP formed to prove Proposition 12 in [16] is in the form of the IVP $y'' = f(y)$, $y(x_0) = y^0$, $y'(x_0) = y^{0'}$.

When applied to $y'' = f(y)$ the F defined by (2.2) and the F defined by (2.3) agree on AT , so the proposition is proved. ■

Like Theorem 13 in [16] the following theorem will be crucial in getting the recursive form of the order conditions. The proof the Theorem 2.5 just shows how to adapt Theorem 13 in [16] to the situation here.

THEOREM 2.5. Let $a : AT \rightarrow \mathbf{IR}$ be a mapping. If $a(\phi) = 1$ then

$$f(A(a, y^0, y^{0'})) = \sum_{t \in \text{LNT}} a''(t) F(t)(y^0, y^{0'}) \frac{h^{\rho(t)-2}}{(\rho(t)-2)!}$$

where $a'' : AT \rightarrow \mathbf{IR}$ is defined by $a''(\phi) = a''(\cdot) = 0$, $a''(\Phi) = 1$, and $a''(t) = a(t_1) \dots a(t_k)$ for $t = [t_1, \dots, t_k]$, and F is defined as in (2.3).

PROOF: Consider the extension $\tilde{a}$ of a to NT where $\tilde{a} \mid_{\text{NT}-AT} = 0$. Let $\tilde{a}'$ be a mapping $\tilde{a}' : \text{NT} \rightarrow \mathbf{IR}$ where $\tilde{a}'(t) = 0$ for all $t \neq \cdot$ and $\tilde{a}'(\cdot) = 1$.

Rewrite the IVP $y'' = \tilde{f}(y, y') = f(y)$, $y(x_0) = y^0$, $y'(x_0) = y^{0'}$. Then by Theorem 13 in [16]

$$\tilde{f}(N(\tilde{a}, y^0, y^{0'}), N'(\tilde{a}', y^0, y^{0'})) = \sum_{t \in \text{LNT}} \tilde{a}''(t) \tilde{F}(y^0, y^{0'}) \frac{h^{\rho(t)-2}}{(\rho(t)-2)!}$$

where $\tilde{F}$ is defined as in (2.2) and with respect to $\tilde{f}$ above. By Theorem 13 in [16] the $\tilde{a}'' : \text{NT} \rightarrow \mathbf{IR}$ is defined as follows:

$$\tilde{a}''(\phi) = \tilde{a}''(\cdot) = 0, \tilde{a}''(\Phi) = 1$$

$$\tilde{a}''(t) = \tilde{a}(t_1) \dots \tilde{a}(t_k) \tilde{a}'(t_{k+1}) \dots \tilde{a}'(t_m)$$

$$t = [t_1, \dots, t_k; t_{k+1}, \dots, t_m].$$

If $t \in \text{LNT} - \text{LAT}$ $t = [t_1, \dots, t_k; t_{k+1}, \dots, t_m]$ then either $m > k$ or $t_i \notin \text{LAT}$ for at least one i , for $i = 1, \dots, k$. If $m > k$ then by definition 5, $\rho(t_{k+1}) > 2$. Therefore $\tilde{a}'(t_{k+1}) = 0$ so $\tilde{a}''(t) = 0$. If $t_i \notin \text{LAT}$ then $\tilde{a}(t_i) = 0$; therefore $a''(t) = 0$. So if $t \in \text{LNT} - \text{LAT}$ then $\tilde{a}''(t) = 0$.

Using this result we obtain

$$\tilde{f}(N(\tilde{a}, y^0, y^{0'}), N'(\tilde{a}', y^0, y^{0'})) = \sum_{t \in \text{LAT}} \tilde{a}''(t) \tilde{F}(y^0, y^{0'})(t) \frac{h^{\rho(t)-2}}{(\rho(t)-2)!}$$

By the way $\tilde{f}$ is defined we have

$$\tilde{f}(N(\tilde{a}, y^0, y^{0'}), N'(\tilde{a}', y^0, y^{0'})) = f(N(\tilde{a}, y^0, y^{0'})) = f(A(a, y^0, y^{0'}))$$

and

$$\tilde{F}(y^0, y^{0'})|_{AT} = F(y^0, y^{0'})|_{AT}$$

For $t = [t_1, \dots, t_k] \in AT$ then $\tilde{a}''(t) = \tilde{a}(t_1) \dots \tilde{a}(t_k) = a(t_1) \dots a(t_k) = a''(t)$.

Using these last four results we obtain the desired result. ■

From now on when we use F we will be referring to the F defined by (2.3).

§2.3 Order Conditions

Before investigating the order conditions we will find certain compatibility conditions, i. e. conditions on the coefficients under which our method yields the same result whether it is applied directly to (1.1) or to the equivalent autonomous system in the following manner. Solving the problem $y'' = f(x, y(x))$ is equivalent to solving the following problem.

Let

$$\vec{Y}(x) = \begin{bmatrix} y_1(x) \\ y_2(x) \end{bmatrix} = \begin{bmatrix} y(x) \\ x \end{bmatrix} ;$$

then

$$\vec{Y}''(x) = \begin{bmatrix} f(y_1, y_2) \\ 0 \end{bmatrix} = f(\vec{Y}(x)) . \quad (2.4)$$

We want the numerical solution of applying our method to $y''(x) = f(x, y(x))$ to agree with the numerical solution of applying our method to (2.4).

Applying our method to (2.4) yields

$$\begin{aligned}
Y^{n,i} &= \begin{bmatrix} p_i^n \\ q_i^n \end{bmatrix} = \alpha_i \begin{bmatrix} y_1^{n-1} \\ y_2^{n-1} \end{bmatrix} + \gamma_i \begin{bmatrix} y_1^n \\ y_2^n \end{bmatrix} + \theta_i \begin{bmatrix} y_1^{n+1} \\ y_2^{n+1} \end{bmatrix} + h^2 \sigma_i \begin{bmatrix} f(y_2^{n-1}, y_1^{n-1}) \\ 0 \end{bmatrix} \\
&+ h^2 \delta_i \begin{bmatrix} f(y_2^n, y_1^n) \\ 0 \end{bmatrix} + h^2 \beta_i \begin{bmatrix} f(y_2^{n+1}, y_1^{n+1}) \\ 0 \end{bmatrix} + h^2 \sum_{j=1}^s a_{ij} \begin{bmatrix} f(q_j^n, p_j^n) \\ 0 \end{bmatrix} \\
&= \begin{bmatrix} \alpha_i y_1^{n-1} + \gamma_i y_1^n + \theta_i y_1^{n+1} + h^2 \sigma_i f(y_2^{n-1}, y_1^{n-1}) + h^2 \delta_i f(y_2^n, y_1^n) \\ \alpha_i y_2^{n-1} + \gamma_i y_2^n + \theta_i y_2^{n+1} \\ + h^2 \beta_i f(y_2^{n+1}, y_1^{n+1}) + h^2 \sum_{j=1}^s a_{ij} f(q_j^n, p_j^n) \end{bmatrix} \\
&+ 0
\end{aligned} \tag{2.5}$$

and

$$\begin{aligned}
\bar{Y}^{n+1} &= \begin{bmatrix} y_1^{n-1} \\ y_2^{n-1} \end{bmatrix} + 2 \begin{bmatrix} y_1^n \\ y_2^n \end{bmatrix} + h^2 \tilde{\beta} \begin{bmatrix} f(y_2^{n+1}, y_1^{n+1}) \\ 0 \end{bmatrix} \\
&+ h^2 \tilde{\sigma} \begin{bmatrix} f(y_2^{n-1}, y_1^{n-1}) \\ 0 \end{bmatrix} + h^2 \tilde{\delta} \begin{bmatrix} f(y_2^n, y_1^n) \\ 0 \end{bmatrix} + h^2 \sum_{i=1}^s b_i \begin{bmatrix} f(q_i^n, p_i^n) \\ 0 \end{bmatrix}
\end{aligned} \tag{2.6}$$

By using equation (2.5) in (2.6) we obtain

$$\begin{aligned}
\bar{Y}^{n+1} &= - \begin{bmatrix} y_1^{n-1} \\ y_2^{n-1} \end{bmatrix} + 2 \begin{bmatrix} y_1^n \\ y_2^n \end{bmatrix} + h^2 \tilde{\sigma} \begin{bmatrix} f(y_2^{n-1}, y_1^{n-1}) \\ 0 \end{bmatrix} + h^2 \tilde{\delta} \begin{bmatrix} f(y_2^n, y_1^n) \\ 0 \end{bmatrix} \\
&+ h^2 \tilde{\beta} \begin{bmatrix} f(y_2^{n+1}, y_1^{n+1}) \\ 0 \end{bmatrix} + h^2 \sum_{i=1}^s b_i \times \\
&\begin{bmatrix} f(\alpha_i y_2^{n-1} + \gamma_i y_2^n + \theta_i y_2^{n+1}, \alpha_i y_1^{n-1} + \gamma_i y_1^n + \theta_i y_1^{n+1} + h^2 \sigma_i f(y_2^{n-1}, y_1^{n-1}) \\ 0 \\ + h^2 \delta_i f(y_2^n, y_1^n) + h^2 \beta_i f(y_2^{n+1}, y_1^{n+1}) + h^2 \sum_{j=1}^s a_{ij} f(q_j^n, p_j^n) \end{bmatrix} \\
&+ 0
\end{aligned}$$

Now directly applying the method to the problem $y''(x) = f(x, y(x))$ yields

$$\begin{aligned}
y^{n+1} &= -y^{n-1} + 2y^n + h^2 \sum_{i=1}^s b_i f(x_n + c_i h, y^{n,i}) + h^2 \tilde{\sigma} f_{n-1} + h^2 \tilde{\delta} f_n + h^2 \tilde{\beta} f_{n+1} \\
&= -y^{n-1} + 2y^n + h^2 \sum_{i=1}^s b_i f(x_n + c_i h, \alpha_i y^{n-1} + \gamma_i y^n + \theta_i y^{n+1} + h^2 \sigma_i f^{n-1} \\
&\quad + h^2 \delta_i f^n + h^2 \beta_i f^{n+1} + h^2 \sum_{j=1}^s a_{ij} f(x_n + c_i h, y^{n,j})) \\
&\quad + h^2 \tilde{\sigma} f^{n-1} + h^2 \tilde{\delta} f^n + h^2 \tilde{\beta} f^{n+1} .
\end{aligned}$$

We want the two approaches to produce the same result, that is $y^{n+1} = y_1^{n+1}$.

For this to happen we must have

$$\begin{aligned}
x_n + c_i h &= \alpha_i y_2^{n-1} + \gamma_i y_2^n + \theta_i y_2^{n+1} \\
&= \alpha_i (x_n - h) + \gamma_i (x_n) + \theta_i (x_n + h) \\
&= (\alpha_i + \gamma_i + \theta_i) x_n + (-\alpha_i + \theta_i) h .
\end{aligned}$$

This happens if and only if

$$\alpha_i + \gamma_i + \theta_i = 1 \quad \text{and} \quad \theta_i - \alpha_i = c_i, \quad i = 1, \dots, s . \quad (2.7)$$

The above equations are the compatibility conditions. From now on we will assume these compatibility conditions. With these compatibility conditions we are able to look at the simpler problem $y'' = f(y)$ and the method (1.2) applied to it becomes

$$\begin{aligned}
y^{n,i} &= \alpha_i y^{n-1} + \gamma_i y^n + \theta_i y^{n+1} + h^2 \sigma_i f^{n-1} + h^2 \delta_i f^n + h^2 \beta_i f^{n+1} \\
&\quad + h^2 \sum_{j=1}^s a_{ij} f(y^{n,j})
\end{aligned} \quad (2.8)$$

$$y^{n+1} = -y^{n-1} + 2y^n + h^2 \sum_{i=1}^s b_i f(y^{n,i}) + h^2 \tilde{\sigma} f^{n-1} + h^2 \tilde{\delta} f^n + h^2 \tilde{\beta} f^{n+1} .$$

When we say a method has local truncation error of order p we mean

$$\|y^{n+1} - y(t_n + h)\| = \mathcal{O}(h^p)$$

where y^{n+1} is the numerical solution obtained from method (2.8) assuming y^n, y^{n-1} are exact. This happens when the coefficients of the Taylor series of the exact solution, $y(x_n + h)$, and the approximate solution, y^{n+1} , match up for all the elementary differentials corresponding to trees of order $p - 1$ or less.

Using this idea we will derive the order conditions for our method by finding the A series representations for the estimate y^2 and equating it with the A series of the true solution $y(x_1 + h)$ up to a certain order. (In doing so, we are following the usual practice in the literature of going from time steps 0, 1 to 2, rather than $n - 1, n$ to $n + 1$.) To do this first we find the A series representation of $y^{1,i}$.

Let $y^{1,i}$ (the i th intermediate stage), and y^2 (the approximate solution at the next step), be expanded in A -series about x_1 (instead of x_0), corresponding to the maps $a_i, \Psi : \mathbf{AT} \rightarrow \mathbf{IR}$ respectively. That is, $y^{1,i} = A(a_i, y^1, y^{1'})$ and $y^2 = A(\Psi, y^1, y^{1'})$.

Then

$$\begin{aligned} y^{1,i} &= A(a_i, y^1, y^{1'}) = \alpha_i A(p_{-1}, y^1, y^{1'}) + \gamma_i A(p_0, y^1, y^{1'}) \\ &\quad + \theta_i A(\Psi, y^1, y^{1'}) + h^2 \sigma_i f(A(p_{-1}, y^1, y^{1'})) + h^2 \delta_i f(A(p_0, y^1, y^{1'})) \\ &\quad + h^2 \beta_i f(A(\Psi, y^1, y^{1'})) + h^2 \sum_{j=1}^s a_{ij} f(A(a_j, y^1, y^{1'})) \end{aligned} \quad (2.9)$$

and

$$\begin{aligned} y^2 &= A(\Psi, y^1, y^{1'}) = -A(p_{-1}, y^1, y^{1'}) + 2A(p_0, y^1, y^{1'}) \\ &\quad + h^2 \tilde{\sigma} f(A(p_{-1}, y^1, y^{1'})) + h^2 \tilde{\beta} f(A(\Psi, y^1, y^{1'})) \\ &\quad + h^2 \sum_{i=1}^s b_i f(A(a_i, y^1, y^{1'})) . \end{aligned}$$

In these formulae , p_{-1} and p_0 are defined as follows

$$p_0(t) = \begin{cases} 1 & \text{if } t = \emptyset \\ 0 & \text{otherwise} \end{cases}$$

and $p_{-1}(t) = (-1)^{\rho(t)}$.

If we require $a_i(\emptyset) = 1$ then by Theorem 2.5

$$\begin{aligned} h^2 f(A(a_i, y^1, y^{1'})) &= \sum_{t \in \text{LAT}} a_i''(t) F(t)(y^1, y^{1'}) \frac{h^{\rho(t)}}{(\rho(t) - 2)!} \\ &= \sum_{t \in \text{LAT}} (\rho(t))(\rho(t) - 1) a_i''(t) F(t)(y^1, y^{1'}) \frac{h^{\rho(t)}}{(\rho(t))!} = A(\tilde{a}_i, y^1, y^{1'}) \end{aligned} \quad (2.10)$$

where $\tilde{a}_i(t) = \rho(t)(\rho(t) - 1) a_i''(t)$.

Therefore $\tilde{a}_i(\emptyset) = \tilde{a}_i(\cdot) = 0$, $\tilde{a}_i(\overset{Q}{\underset{1}{\uparrow}}) = 2$ and $\tilde{a}_i(t) = \rho(t)(\rho(t) - 1) a_i(t_1) \dots a_i(t_m)$ where $t = [t_1, \dots, t_m]$.

Now, $p_{-1}(\emptyset) = p_0(\emptyset) = 1$, so by applying Theorem 2.5 again and doing the same calucations as before we get the following results

$$h^2 f(A(p_0, y^1, y^{1'})) = A(\tilde{p}_0, y^1, y^{1'}) \quad (2.11)$$

where

$$\begin{aligned} \tilde{p}_0(\emptyset) &= \tilde{p}_0(\cdot) = 0, \tilde{p}_0(\overset{Q}{\underset{1}{\uparrow}}) = 2, \tilde{p}_0(t) = 0 \quad \text{and} \\ h^2 f(A(p_{-1}, y^1, y^{1'})) &= A(\tilde{p}_{-1}, y^1, y^{1'}) \end{aligned} \quad (2.12)$$

where $\tilde{p}_{-1}(t) = \rho(t)(\rho(t) - 1) p_{-1}(t) \dots p_{-1}(t_m) = \rho(t)(\rho(t) - 1) (-1)^{\rho(t)-2}$ where $t = [t_1, \dots, t_m]$.

If we require $\Psi(\emptyset) = 1$ then by the same reasoning

$$h^2 f(A(\Psi, y^1, y^{1'})) = A(\tilde{\Psi}, y^1, y^{1'}) \quad (2.13)$$

where $\tilde{\Psi}(\emptyset) = \tilde{\Psi}(\cdot) = 0$, $\tilde{\Psi}(\mathcal{Q}) = 2$ and $\tilde{\Psi}(t) = \rho(t)(\rho(t) - 1)\Psi(t_1) \dots \Psi(t_m)$ where $t = [t_1, \dots, t_m]$.

Applying these results to (2.9) we get

$$\begin{aligned} y^{1,i} &= A(a_i, y^1, y^{1'}) = \alpha_i A(p_{-1}, y^1, y^{1'}) + \gamma_i A(p_0, y^1, y^{1'}) \\ &+ \theta_i A(\Psi, y^1, y^{1'}) + \sigma_i A(\tilde{p}_{-1}, y^1, y^{1'}) + \delta_i A(\tilde{p}_0, y^1, y^{1'}) \\ &+ \beta_i A(\tilde{\Psi}, y^1, y^{1'}) + \sum_{j=1}^s a_{ij} A(\tilde{a}_j, y^1, y^{1'}) . \end{aligned}$$

Therefore

$$\begin{aligned} a_i(t) &= \alpha_i p_{-1}(t) + \gamma_i p_0(t) + \theta_i \Psi(t) + \sigma_i \tilde{p}_{-1}(t) + \delta_i \tilde{p}_0(t) \\ &+ \beta_i \tilde{\Psi}(t) + \sum_{j=1}^s a_{ij} \tilde{a}_j(t) . \end{aligned}$$

It follows that

$$a_i(\emptyset) = \alpha_i + \gamma_i + \theta_i = 1 .$$

Note this agrees with the compatibility conditions. If $\Psi(\cdot) = 1$ then $a_i(\cdot) = -\alpha_i + \theta_i$ and by one of the compatibility conditions, $a_i(\cdot) = -\alpha_i + \theta_i = c_i$.

We have

$$a_i(\mathcal{Q}) = \alpha_i + \theta_i \Psi(\mathcal{Q}) + 2\sigma_i + 2\delta_i + 2\beta_i + 2 \sum_{j=1}^s a_{ij}$$

and for $\rho(t) > 2$ we get

$$\begin{aligned} a_i(t) &= \alpha_i (-1)^{\rho(t)} + \theta_i \Psi(t) + \sigma_i (-1)^{\rho(t)-2} (\rho(t)) (\rho(t) - 1) \\ &+ \beta_i \Psi(t_1) \dots \Psi(t_m) \rho(t) (\rho(t) - 1) + (\rho(t)) (\rho(t) - 1) \sum_{j=1}^s a_{ij} a_j(t_1) \dots a_j(t_m) \end{aligned}$$

where $t = [t_1, \dots, t_m]$.

DEFINITION 11: A method has the property $A(p)$ if its local truncation error is of order $\geq p + 1$, that is $\Psi(t) = 1$ for all $t \in AT$, $\rho(t) \leq p$.

If a method has property $A(p)$, and $t \in AT$, $\rho(t) \leq p$, then

$$a_i(t) = \alpha_i(-1)^{\rho(t)} + \theta_i + \sigma_i \rho(t)(\rho(t) - 1)(-1)^{\rho(t)-2} \\ + \beta_i \rho(t)(\rho(t) - 1) + \rho(t)(\rho(t) - 1) \sum_{j=1}^s a_{ij} a_j(t_1) \dots a_j(t_m)$$

where $t = [t_1, \dots, t_m]$.

Now, we proceed to find a formula for $\Psi(t)$. Using the results (2.10), (2.11), (2.12), and (2.13) we obtain

$$\Psi(t) = -(-1)^{\rho(t)} + 2p_0(t) + \tilde{\sigma}\tilde{p}_{-1}(t) + \tilde{\delta}\tilde{p}_0(t) + \tilde{\beta}\Psi(t) \\ + \sum_{i=1}^s b_i \tilde{a}_i(t) .$$

So we have

$$\Psi(\emptyset) = -1 + 2 = 1$$

$$\Psi(\cdot) = 1$$

$$\Psi(\bigcirc) = -1 + 2\tilde{\sigma} + 2\tilde{\delta} + 2\tilde{\beta} + 2 \sum_{i=1}^s b_i$$

and $\Psi([t_1, \dots, t_m]) = -(-1)^{\rho(t)} + \tilde{\sigma}(-1)^{\rho(t)-2} \rho(t)(\rho(t) - 1) + \tilde{\beta} \rho(t)(\rho(t) - 1) \times \Psi(t_1) \dots \Psi(t_m) + \sum_{i=1}^s b_i \rho(t)(\rho(t) - 1) a_i(t_1) \dots a_i(t_m)$. If $\Psi(t_i) = 1$ for $i = 1, \dots, m$ then $\Psi([t_1, \dots, t_m]) = -(-1)^{\rho(t)} + \tilde{\sigma}(-1)^{\rho(t)-2} \rho(t)(\rho(t) - 1) + \tilde{\beta} \rho(t)(\rho(t) - 1) + \rho(t)(\rho(t) - 1) \sum_{i=1}^s b_i a_i(t_1) \dots a_i(t_m)$.

In summary, here are the order conditions up to order 5 if the method obeys the compatibility conditions

$$\alpha_i + \gamma_i + \theta_i = 1, \quad \theta_i = \alpha_i - c_i .$$

By the above, $\Psi(\emptyset) = 1$ and $\Psi(\cdot) = 1$

$$\Psi(\overset{\circ}{\uparrow}) = 1 \iff -1 + 2\tilde{\sigma} + 2\tilde{\delta} + 2\tilde{\beta} + 2 \sum_{i=1}^s b_i = 1$$

$$\Psi([\cdot]) = 1 \iff -(-1) - 6\tilde{\sigma} + 6\tilde{\beta} + 6 \sum_{i=1}^s b_i c_i = 1$$

$$\Psi([\cdot, \cdot]) = 1 \iff -1 + 12\tilde{\sigma} + 12\tilde{\beta} + 12 \sum_{i=1}^s b_i c_i^2 = 1$$

$$\begin{aligned} \Psi([\overset{\circ}{\uparrow}]) = 1 \iff & -1 + 12\tilde{\sigma} + 12\tilde{\beta} + 12 \sum_{i=1}^s b_i(\alpha_i + \theta_i + 2\sigma_i + 2\delta_i \\ & + 2\beta_i + 2 \sum_{j=1}^s a_{ij}) = 1 \end{aligned}$$

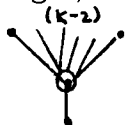
$$\Psi([\cdot, \cdot, \cdot]) = 1 \iff 1 - 20\tilde{\sigma} + 20\tilde{\beta} + 20 \sum_{i=1}^s b_i c_i^3 = 1$$

$$\begin{aligned} \Psi([\cdot, \overset{\circ}{\uparrow}]) = 1 \iff & 1 - 20\tilde{\sigma} + 20\tilde{\beta} + 20 \sum_{i=1}^s b_i c_i(\alpha_i + \theta_i \\ & + 2\sigma_i + 2\delta_i + 2\beta_i + 2 \sum_{j=1}^s a_{ij}) = 1 \end{aligned}$$

and

$$\begin{aligned} \Psi([[\cdot]]]) = 1 \iff & 1 - 20\tilde{\sigma} + 20\tilde{\beta} + 20 \sum_{i=1}^s b_i(c_i \\ & - 6\sigma_i + 6\beta_i + 6 \sum_{j=1}^s a_{ij} c_j) = 1 . \end{aligned}$$

It is customary to relate these conditions to quadrature and other properties. So, to begin, consider the following tree $t = [\underbrace{\cdot, \dots, \cdot}_{k-2}]$, which is represented by the graph



where $k \geq 2$.

Then

$$\begin{aligned}\Psi(t) = & -(-1)^k + \tilde{\sigma}\rho(t)(\rho(t) - 1)(-1)^{k-2} + \tilde{\delta}p(t)(\rho(t) - 1)(0)^{k-2} \\ & + \tilde{\beta}\rho(t)(\rho(t) - 1)(1)^{k-2} + \sum_{i=1}^s b_i \rho(t)(\rho(t) - 1)c_i^{k-2}.\end{aligned}$$

So $\Psi(t) = 1 \Leftrightarrow \tilde{\sigma}(-1)^{k-2} + \tilde{\delta}(0)^{k-2} + \tilde{\beta}(1)^{k-2} + \sum_{i=1}^s b_i c_i^{k-2} = \frac{1 + (-1)^k}{k(k-1)}$, since $\rho(t) = k$.

DEFINITION 12: A method of the form (2.8) has property $B(p)$ if

$$\tilde{\sigma}(-1)^{k-2} + \tilde{\delta}(0)^{k-2} + \tilde{\beta}(1)^{k-2} + \sum_{i=1}^s b_i c_i^{k-2} = \frac{1 + (-1)^k}{k(k-1)}$$

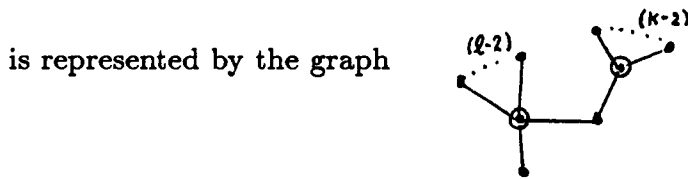
for all k such that $2 \leq k \leq p$.

We begin the presentation of simplifying conditions with the following theorem, which is an implication about quadrature.

THEOREM 2.6. For any method of the form (2.8), $A(p) \Rightarrow B(p)$.

PROOF: $A(p) \Rightarrow \Psi(t) = 1$ where $t = [\underbrace{\cdot, \dots, \cdot}_{k-2}]$ for $2 \leq k \leq p$ so the theorem is proved by the above work. ■

Next, consider the following tree $t = [\underbrace{\cdot, \dots, \cdot}_{l-2}, [\underbrace{\cdot, \dots, \cdot}_{k-2}]]$ where $l, k \geq 2$. This tree



Then

$$\begin{aligned}\Psi(t) = & -(-1)^{l+k} + \tilde{\sigma}(-1)^{l+k}(l+k)(l+k-1) + \tilde{\beta}(l+k)(l+k-1) \\ & + \Psi([\underbrace{\cdot, \dots, \cdot}_{k-2}]) \cdot (\Psi(\cdot))^{l-2} + \sum_{i=1}^s b_i (l+k)(l+k-1) a_i([\underbrace{\cdot, \dots, \cdot}_{k-2}]) (a_i(\cdot))^{l-2}\end{aligned}$$

First we calculate $a_i(\underbrace{[\cdot, \dots, \cdot]}_{k-2})$:

$$\begin{aligned} a_i(\underbrace{[\cdot, \dots, \cdot]}_{k-2}) &= \alpha_i(-1)^k + \theta_i + \sigma_i(-1)^{k-2}(k)(k-1) + (k)(k-1)\delta_i(0)^{k-2} \\ &\quad + (k)(k-1)\beta_i(1)^{k-2} + (k)(k-1) \sum_{j=1}^s a_{ij}c_j^{k-2}. \end{aligned}$$

As stated before, it is obvious that $\Psi(\cdot) = 1$. So if we assume $\Psi([\cdot, \dots, \cdot]) = 1$ then

$$\begin{aligned} \Psi(t) &= -(-1)^{l+k} + \tilde{\sigma}(-1)^{l+k}(l+k)(l+k-1) + (l+k)(l+k-1)\tilde{\beta}(1)^{l+k} \\ &\quad + (l+k)(l+k-1) \sum_{i=1}^s b_i c_i^{l-2} (\alpha_i(-1)^k + \theta_i + (k)(k-1)\sigma_i(-1)^{k-2} \\ &\quad + (k)(k-1)\delta_i(0)^{k-2} + (k)(k-1)\beta_i + (k)(k-1) \sum_{j=1}^s a_{ij}c_j^{k-2}). \end{aligned}$$

So $\Psi(t) = 1$ if and only if

$$\begin{aligned} &\tilde{\sigma}(-1)^{l+k} + \tilde{\beta}(1)^{l+k} + \sum_{i=1}^s b_i c_i^{l-2} (\alpha_i(-1)^k + \theta_i + \sigma_i(-1)^{k-2}(k)(k-1) \\ &\quad + (k)(k-1)\delta_i(0)^{k-2} + (k)(k-1)\beta_i + (k)(k-1) \sum_{j=1}^s a_{ij}c_j^{k-2}) \\ &= \frac{1 + (-1)^{l+k}}{(l+k)(l+k-1)}. \end{aligned}$$

DEFINITION 13: A method of the form (2.8) obeys property $E(\xi, \eta)$ if

$$\begin{aligned} &\tilde{\sigma}(-1)^{l+k} + \tilde{\beta}(1)^{l+k} + \sum_{i=1}^s b_i c_i^{l-2} (\alpha_i(-1)^k + \theta_i + (k)(k-1)\sigma_i(-1)^{k-2} \\ &\quad + (k)(k-1)\delta_i(0)^{k-2} + (k)(k-1)\beta_i + (k)(k-1) \sum_{j=1}^s a_{ij}c_j^{k-2}) \\ &= \frac{1 + (-1)^{l+k}}{(l+k)(l+k-1)} \end{aligned}$$

for all k, l such that $2 \leq l \leq \xi$ and $2 \leq k \leq \eta$.

Hence, by the above argument we have shown:

THEOREM 2.7. $A(p) \rightarrow E(\xi, \eta)$ where $\xi + \eta \leq p$.

Next we develop a condition like the C condition in [4].

Consider the following initial value problem:

$$y''(t) = 0 \quad \text{where} \quad y'(t) = c, \quad y(t) = ct.$$

If y^0, y^1, y^2 are exact, that is, $y^0 = 0, y^1 = ch, y^2 = 2ch$ then $y^{1,i}$ exact implies

$$y^{1,i} = \gamma_i hc + \theta_i 2hc_i = (h + hc_i)c.$$

This happens if and only if $\gamma_i + 2\theta_i = 1 + c_i$.

Since we have assumed $\gamma_i + \theta_i + \alpha_i = 1$ and $\theta_i - \alpha_i = c_i$ we get $\gamma_i + \theta_i + \theta_i = 1 - \theta_i - \alpha_i + c_i + \alpha_i = 1 + c_i$. So the compatibility conditions imply $y^{1,i}$ is exact when determined for the problem $y'' = 0$.

Now consider the following problem

$$y''(t) = t^k, \quad y'(t) = \frac{t^{k+1}}{(k+1)}, \quad y(t) = \frac{t^{k+2}}{(k+1)(k+2)}.$$

If y^0, y^1, y^2 are exact, then $y^{1,i}$ is exact if and only if

$$\begin{aligned} y^{1,i} &= \frac{(h + hc_i)^{k+2}}{(k+2)(k+1)} = \alpha_i \cdot 0 + \frac{\gamma_i h^{k+2}}{(k+2)(k+1)} + \frac{\theta_i (2h)^{k+2}}{(k+1)(k+2)} \\ &\quad + \sigma_i \cdot 0 + h^2 \delta_i (h)^k + h^2 \beta_i (2h)^k + h^2 \sum_{j=1}^s a_{ij} (h + c_j h)^k. \end{aligned} \quad (2.14)$$

So factoring out the h from both sides of (2.14) we get $y^{1,i}$ is exact if and only if

$$\begin{aligned} \frac{(1 + c_i)^{k+2}}{(k+2)(k+1)} &= \frac{\gamma_i}{(k+2)(k+1)} + \frac{\theta_i 2^{k+2}}{(k+2)(k+1)} \\ &\quad + \delta_i + \beta_i (2)^k + \sum_{j=1}^s a_{ij} (1 + c_j)^k. \end{aligned}$$

This leads us to the following definition, which is a statement of exactness of internal quadrature.

DEFINITION 14: A method has property $C(p)$ if

$$\begin{aligned} & \sigma_i(1-1)^{k-2} + \delta_i(1-0)^{k-2} + \beta_i(1+1)^{k-2} + \sum_{j=1}^s a_{ij}(1+c_j)^{k-2} \\ &= \frac{(1+c_i)^k}{(k)(k-1)} - \frac{\gamma_i}{(k)(k-1)} - \frac{\theta_i 2^k}{(k)(k-1)} \quad \text{for } 2 \leq k \leq p. \end{aligned}$$

Next the property $C(p)$ will be put in a more useable form.

PROPOSITION 2.8: Property $C(p)$ implies

$$(0)^{k-2}\delta_i + \beta_i + (-1)^{k-2}\sigma_i + \sum_{j=1}^s a_{ij} c_j^{k-2} = \frac{c_i^k + (-1)^k c_i - \theta_i(1 + (-1)^k)}{(k)(k-1)} \quad (2.15)$$

for $2 \leq k \leq p$

PROOF: Proof by induction. For $p = 2$, $C(2)$ gives us

$$\sigma_i + \delta_i + \beta_i + \sum_{j=1}^s a_{ij} = \frac{(1+c_i)^2}{2} - \frac{\gamma_i}{2} - \theta_i \cdot 2. \quad (2.16)$$

Using the compatibility conditions the right hand side of (2.16) is

$$\begin{aligned} &= \frac{1 + 2c_i + c_i^2 - (\gamma_i + \theta_i) - 3\theta_i}{2} = \frac{1 + 2c_i + c_i^2 - (1 - \theta_i + c_i) - 3\theta_i}{2} \\ &= \frac{c_i^2 + c_i - 2\theta_i}{2}. \end{aligned}$$

Therefore $\delta_i + \beta_i + \sigma_i + \sum_{j=1}^s a_{ij} = (c_i^2 + c_i - 2\theta_i)/2$ so the claim is true for $p = 2$.

Assuming that it's true for $p < n$, we then prove it's true for $p = n$. $C(n) \Rightarrow C(n-1)$ which implies (2.15) is true for $2 \leq k \leq n-1$, so all that is left to show is that (2.15) is true for $k = n$, which asks that

$$\delta_i + \beta_i(2)^{n-2} + \sum_{j=1}^s a_{ij}(1+c_j)^{n-2} = \frac{(1+c_i)^n}{n(n-1)} - \frac{\gamma_i}{n(n-1)} - \frac{\theta_i 2^n}{n(n-1)}.$$

That is,

$$\begin{aligned} & \delta_i + \beta_i(2)^{n-2} + \sum_{j=1}^s a_{ij} \left[\sum_{l=0}^{n-2} \binom{n-2}{l} c_j^l \right] \\ &= \frac{1}{n(n-1)} \left\{ \left[\sum_{l=0}^n \binom{n}{l} c_i^l \right] - \gamma_i - \theta_i 2 \right\}. \end{aligned}$$

Therefore by expanding this, (2.15) with $k = n$ can be stated as

$$\begin{aligned} & \delta_i + \beta_i(2)^{n-2} + \sum_{l=1}^{n-3} \sum_{j=1}^s a_{ij} \binom{n-2}{l} c_j^l + \sum_{j=1}^s \binom{n-2}{n-2} a_{ij} c_j^{n-2} \\ &+ \sum_{j=1}^s a_{ij} \binom{n-2}{0} c_j^0 = \frac{1}{n(n-1)} \left\{ \left[\sum_{l=0}^n \binom{n}{l} c_i^l \right] - \gamma_i - \theta_i 2 \right\}. \end{aligned} \quad (2.17)$$

By using the assumption that the claim is true for $k < n$, the result $\gamma_i = 1 - 2\theta_i + c_i$, and simple algebra we obtain

$$\begin{aligned} & \beta_i + (-1)^n \sigma_i + \sum_{j=1}^s a_{ij} c_j^{n-2} = \beta_i \left(1 - 2^{n-2} + \sum_{l=1}^{n-3} \binom{n-2}{l} + \binom{n-2}{0} \right) \\ &+ \sigma_i \left((-1)^n + \sum_{l=1}^{n-3} \binom{n-2}{l} (-1)^l + 1 \right) + \delta_i (-1 + 1) \\ &+ \frac{1}{n(n-1)} \left\{ \sum_{l=0}^n \binom{n}{l} c_i^l - (1 - 2\theta_i + c_i) - \theta_i 2^n \right\} \\ &- \sum_{l=1}^{n-3} \binom{n-2}{l} \left\{ \frac{c_i^{l+2} + (-1)^{l+2} c_i - \theta_i (1 + (-1)^{l+2})}{(l+2)(l+1)} \right\} \\ &- \binom{n-2}{0} \left\{ \frac{c_i^2 + (-1)^2 c_i - \theta_i (1 + (-1)^2)}{2} \right\}. \end{aligned}$$

The Binomial Theorem gives us

$$1 - 2^{n-2} + \sum_{l=1}^{n-3} \binom{n-2}{l} + \binom{n-2}{0} = 0$$

and

$$(-1)^n + \sum_{l=1}^{n-3} \binom{n-2}{l} (-1)^l + 1 = 0.$$

Note that $\frac{\binom{n-2}{l}}{(l+2)(l+1)} = \frac{(n-2)!}{l!(n-2-l)!} \cdot \frac{1}{(l+2)(l+1)} = \frac{(n-2)!}{(l+2)!(n-(l+2))!}$
 $= \frac{1}{n(n-1)} \cdot \frac{n!}{(l+2)!(n-(l+2))!} = \frac{1}{n(n-1)} \binom{n}{l+2}.$ Using this we obtain the following equality

$$\sum_{l=1}^{n-3} \binom{n-2}{l} \frac{c_i^{l+2}}{(l+2)(l+1)} = \frac{1}{n(n-1)} \sum_{l=3}^{n-1} \binom{n}{l} c_i^l$$

and

$$\sum_{l=1}^{n-3} \binom{n-2}{l} \frac{(-1)^{l+2}}{(l+2)(l+1)} = \frac{1}{(n-1)(n)} \sum_{l=3}^{n-1} \binom{n}{l} (-1)^l.$$

By using these results and the Binomial Theorem we obtain

$$\begin{aligned} & \beta_i(1)^n + (-1)^n \sigma_i + \sum_{j=1}^s a_{ij} c_j^{n-2} \\ &= \frac{1}{n(n-1)} \left\{ c_i^n + 1 + nc_i + \frac{n(n-1)}{2} c_i^2 - 1 - 2\theta_i - c_i - \theta_i 2^n \right\} \\ & - \frac{1}{n(n-1)} \left\{ c_i \sum_{l=3}^{n-1} \binom{n}{l} (-1)^l - \theta_i \left[\sum_{l=3}^{n-1} \binom{n}{l} (-1)^l + \sum_{l=3}^{n-1} \binom{n}{l} (1)^l \right] \right\} \\ & - \left\{ \frac{c_i^2 + (-1)^2 c_i - \theta_i(1 + (-1)^2)}{2} \right\} \\ &= \frac{1}{n(n-1)} \{ c_i^n + (-1)^n c_i - \theta_i(1 + (-1)^n) \}. \end{aligned}$$

So by induction the proposition is true. ■

We now present a major result, which connects simplifying conditions with A -series of the intermediate stages and the true solution. This will be useful in generating order conditions.

THEOREM 2.9. *If a method of the form (2.8) obeys properties $C(p)$ and $B(p)$ then $a_i(t) = c_i^{\rho(t)}$ and $\Psi(t) = 1$ for all trees $t \in AT$ such that $\rho(t) \leq p$.*

PROOF (by induction on p): First, consider the case $p = 2$. Then if $\rho(t) \leq 2$ then $t = \phi$, or $\cdot$, or $\begin{smallmatrix} \circ \\ | \\ \circ \end{smallmatrix}$. By the compatibility conditions the result holds for $t = \phi$, or $\cdot$. If $t = \begin{smallmatrix} \circ \\ | \\ \circ \end{smallmatrix}$ then

$$\Psi\left(\begin{smallmatrix} \circ \\ | \\ \circ \end{smallmatrix}\right) = -1 + 2\tilde{\sigma} + 2\tilde{\delta} + 2\tilde{\beta} + 2 \sum_{i=1}^s b_i,$$

$B(2)$ gives us $\Psi\left(\begin{smallmatrix} \circ \\ | \\ \circ \end{smallmatrix}\right) = 1$. This gives us

$$a_i\left(\begin{smallmatrix} \circ \\ | \\ \circ \end{smallmatrix}\right) = \alpha_i + \theta_i + 2\sigma_i + 2\delta_i + \beta_i + 2 \sum_{j=1}^s a_{ij}.$$

By using $C(2)$ and the compatibility condition we get

$$a_i\left(\begin{smallmatrix} \circ \\ | \\ \circ \end{smallmatrix}\right) = \theta_i - c_i + \theta_i + 2 \left(\frac{c_i^2 + c_i - \theta_i \cdot 2}{2} \right) = c_i^2.$$

So the theorem is true for $p \leq 2$.

Now, we assume the theorem is true for $p \leq k$ and prove it is true for $p = k + 1$. $C(k + 1)$, $B(k + 1) \Rightarrow C(k)$, $B(k)$, so by our assumption $a_i(t) = c_i^{\rho(t)}$ and $\Psi(t) = 1$ for all $t, \rho(t) \leq k$.

So the only case we have to consider is $\rho(t) = k + 1$. Let $t = [t_1, \dots, t_m]$ where $\rho(t_i) \leq k - 1$. By our assumption $\Psi(t_j) = 1$ and $a_i(t_j) = c_i^{\rho(t_j)}$ for $j = 1, \dots, m$. Recall that

$$\begin{aligned} \Psi(t) &= -(-1)^{k+1} + \tilde{\sigma}(k+1)(k)(-1)^{k-1} + (k+1)(k)\tilde{\beta} \\ &\quad + (k+1)(k) \sum_{i=1}^s b_i c_i^{\rho(t_1)} \dots c_i^{\rho(t_m)} \\ &= -(-1)^{k+1} + (k+1)(k)\tilde{\sigma}(-1)^{k-1} + (k+1)(k)\tilde{\beta} + (k+1)(k) \sum_{i=1}^s b_i c_i^{k-1}. \end{aligned}$$

By $B(k+1)$, this is equal to 1. Using this, the following holds

$$\begin{aligned}
a_i(t) &= \alpha_i(-1)^{k+1} + \theta_i + (k+1)(k)\sigma_i(-1)^{k-1} + (k+1)(k)\beta_i \\
&\quad + (k+1)(k) \sum_{j=1}^s a_{ij} c_j^{\rho(t_1)} \dots c_j^{\rho(t_m)} \\
&= \alpha_i(-1)^{k+1} + \theta_i + (k+1)(k)\sigma_i(-1)^{k-1} + (k+1)(k)\beta_i + (k)(k+1) \sum_{j=1}^s a_{ij} c_j^{k-1} .
\end{aligned}$$

By $C(k+1)$ and the compatibility conditions we have

$$\begin{aligned}
a_i(t) &= (\theta_i - c_i)(-1)^{k+1} + \theta_i + (k+1)(k) \left(\frac{c_i^{k+1} + (-1)^{k+1}c_i - \theta_i(1 + (-1)^{k+1})}{(k+1)(k)} \right) \\
&= c_i^{k+1}
\end{aligned}$$

So by induction the theorem is true. ■

The next theorem shows that in the quest of high order, a broad class of trees are easily handled, and, at the same time singles out those which require individual attention.

THEOREM 2.10. *If a method of the form (2.8) obeys properties $C(p-2)$ and $B(k)$ where $k \geq p$, then $\Psi(t) = 1$ for all trees $t \in AT$ such that $t = [t_1, \dots, t_m]$, $\rho(t_i) \leq p-2$ and $\rho(t) \leq k$.*

PROOF: Consider $t \in AT$ where $\rho(t) \leq k$, $t = [t_1, \dots, t_m]$ and $\rho(t_i) \leq p-2$. Then by Theorem 2.9, $a_i(t_j) = c_i^{\rho(t_j)}$ and $\Psi(t_j) = 1$ for $j = 1, \dots, m$. So

$$\begin{aligned}
\Psi(t) &= -(-1)^{\rho(t)} + \tilde{\sigma}(-1)^{\rho(t)-2} \rho(t)(\rho(t)-1) + \tilde{\beta} \rho(t)(\rho(t)-1) \\
&\quad + \rho(t)(\rho(t)-1) \sum_{i=1}^s b_i c_i^{\rho(t)-2} .
\end{aligned}$$

The property $B(k)$ gives us that the above is equal to 1, that is $\Psi(t) = 1$. ■

The next two results give an indication of what is to be required of the C -condition with respect to certain order.

THEOREM 2.11. *Given a method of the form (2.8) where $b_i \neq 0$ for $i = 1, \dots, s$ and the c_i 's are distinct, then $B(\xi + s + 1) + E(s + 1, \xi) \Rightarrow C(\xi)$, for $s \geq 1$ and $\xi \geq 2$.*

PROOF: Fix k , for $2 \leq k \leq \xi$. Then for $2 \leq l \leq s + 1$ the property $B(\xi + s + 1)$ implies

$$\begin{aligned} \tilde{\sigma}(-1)^{l+k-2} + \tilde{\delta}(0)^{l+k-2} + \tilde{\beta}(1)^{l+k-2} + \sum_{i=1}^s b_i c_i^{l+k-2} \\ = \frac{1 + (-1)^{l+k-2}}{(l+k)(l+k-1)}. \end{aligned} \quad (2.18)$$

Also, the property $E(s + 1, \xi)$ implies

$$\begin{aligned} \tilde{\sigma}(-1)^{l+k} + \tilde{\beta} + \sum_{i=1}^s b_i c_i^{l-2} (\alpha_i(-1)^k + \theta_i + \sigma_i(-1)^{k-2}(k)(k-1) \\ + (k)(k-1)\delta_i(0)^{k-2} + (k)(k-1)\beta_i + (k)(k-1) \sum_{j=1}^s a_{ij} c_j^{k-2}) \\ = \frac{1 + (-1)^{l+k}}{(l+k)(l+k-1)}. \end{aligned} \quad (2.19)$$

By subtracting equations (2.18) from (2.19) we obtain

$$\begin{aligned} \sum_{i=1}^s b_i c_i^{l-2} (\alpha_i(-1)^k + \theta_i + (k)(k-1)\sigma_i(-1)^{k-2} + (k)(k-1)\delta_i(0)^{k-2} \\ + (k)(k-1)\beta_i + (k)(k-1) \sum_{j=1}^s a_{ij} c_j^{k-2}) - \sum_{i=1}^s b_i c_i^{l+k-2} = 0 \end{aligned} \quad (2.20)$$

for $2 \leq l \leq s + 1$.

Equation (2.20) implies

$$\begin{aligned} \sum_{i=1}^s b_i c_i^{l-2} (\alpha_i(-1)^k + \theta_i + \sigma_i(-1)^{k-2}(k)(k-1) + (k)(k-1)\delta_i(0)^{k-2} \\ + (k)(k-1)\beta_i + (k)(k-1) \sum_{j=1}^s a_{ij} c_i^{k-2} - c_i^k) = 0 \end{aligned} \quad (2.21)$$

for $2 \leq l \leq s+1$.

For c_i distinct, the matrix $V = \begin{bmatrix} 1 & \dots & 1 \\ c_1 & \dots & c_s \\ \vdots & & \vdots \\ c_1^{s-1} & \dots & c_s^{s-1} \end{bmatrix}$ is a Vandermonde matrix,

therefore nonsingular. Also the matrix $B = \begin{bmatrix} b_1 & & & \\ & b_2 & & \\ & & \ddots & \\ & & & b_s \end{bmatrix}$ is nonsingular since

we assumed $b_i \neq 0$ for $i = 1, \dots, s$. Let

$$x_i = \alpha_i(-1)^k + \theta_i + (k)(k-1)\sigma_i(-1)^{k-2} + (k)(k-1)\delta_i(0)^{k-2} \\ + (k)(k-1)\beta_i + (k)(k-1) \sum_{j=1}^s a_{ij} c_j^{k-2} - c_i^k.$$

Using the above notation (2.21) can be restated as the vector equation

$$VB\vec{x} = \vec{0} \quad \text{where} \quad \vec{0} = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}.$$

Since VB is nonsingular we must have $\vec{x} = \vec{0}$. This gives us

$$\sigma_i(-1)^{k-2} + \delta_i(0)^{k-2} + \beta_i + \sum_{j=1}^s a_{ij} c_j^{k-2} = \frac{c_i^k - \alpha_i(-1)^k - \theta_i}{(k)(k-1)} \quad (2.22)$$

for $i = 1, \dots, s$.

Using the compatibility condition $\alpha_i = \theta_i - c_i$ in (2.22) gives us

$$\sigma_i(-1)^{k-2} + \delta_i(0)^{k-2} + \beta_i + \sum_{j=1}^s a_{ij} c_j^{k-2} = \frac{c_i^k + (-1)^k c_i - \theta_i(1 + (-1)^k)}{(k)(k-1)} \quad (2.23)$$

for $i = 1, \dots, s$. Since (2.23) is true for any k where $2 \leq k \leq \xi$, the property $C(\xi)$ holds. ■

The following theorem shows the naturalness of the C condition. Because of the form of the C condition this theorem will prove very valuable in finding methods of a certain order condition.

THEOREM 2.12. For a method of the form (2.8) where the c_i 's are distinct and $b_i \neq 0$, the property $A(s+1+\xi) \Rightarrow C(\xi)$.

PROOF: $A(s+1+\xi) \Rightarrow B(\xi+s+1)$ and $E(s+1, \xi)$, which implies, by Theorem (2.11), $C(\xi)$.

Before developing the D condition we will introduce the following notation that will aid forthcoming calculations.

Let

$$\begin{aligned}\tilde{a}_{i,s+1} &= \sigma_i, \quad \tilde{a}_{i,s+2} = \beta_i, \quad \tilde{a}_{i,s+3} = \delta_i \quad \text{for } i = 1, \dots, s \\ \tilde{a}_{ij} &= a_{ij} \quad \text{for } i, j = 1, \dots, s\end{aligned}$$

and

$$\tilde{a}_{s+1,j} = \tilde{a}_{s+2,j} = \tilde{a}_{s+3,j} = 0 \quad \text{for } j = 1, \dots, s+3.$$

That is

$$\tilde{A} = [\tilde{a}_{ij}] = \left[\begin{array}{cc|ccc} & & & \sigma_1 & \beta_1 & \delta_1 \\ & & & \vdots & & \\ & A & & \sigma_s & \beta_s & \delta_s \\ \hline 0 \dots & \dots & & \dots & 0 & \\ 0 \dots & \dots & & \dots & 0 & \\ 0 \dots & \dots & & \dots & 0 & \end{array} \right].$$

Let

$$\begin{aligned}\tilde{c}_{s+1} &= -1 & \tilde{c}_{s+2} &= 1 & \tilde{c}_{s+3} &= 0 & \text{and } \tilde{c}_i &= c_i & \text{for } 1 \leq i \leq s \\ \tilde{b}_{s+1} &= \tilde{\sigma} & \tilde{b}_{s+2} &= \tilde{\beta} & \tilde{b}_{s+3} &= \tilde{\delta} & \text{and } \tilde{b}_i &= b_i & \text{for } 1 \leq i \leq s \\ \tilde{\theta}_{s+1} &= 0 & \tilde{\theta}_{s+2} &= 1 & \tilde{\theta}_{s+3} &= 0 & \text{and } \tilde{\theta}_i &= \theta_i & \text{for } 1 \leq i \leq s.\end{aligned}$$

The following calculations will be helpful later

$$(1 + (-1)^k) \tilde{\theta}_{s+1} - (-1)^k \tilde{c}_{s+1} = ((1 + (-1)^k)0 - (-1)^k(-1)) = -(-1)^k \quad (2.24)$$

$$(1 + (-1)^k) \tilde{\theta}_{s+2} - (-1)^k \tilde{c}_{s+2} = ((1 + (-1)^k) \cdot 1 - (-1)^k \cdot 1) = 1 \quad (2.25)$$

$$(1 + (-1)^k) \tilde{\theta}_{s+3} - (-1)^k \tilde{c}_{s+3} = (1 + (-1)^k) \cdot 0 - (-1)^k \cdot 0 = 0 \quad (2.26)$$

Now, we state the B and E conditions in this new notation. Condition $B(\xi)$ holds if and only if

$$\sum_{i=1}^{s+3} \tilde{b}_i \tilde{c}_i^{k-2} = \frac{1 + (-1)^k}{(k)(k-1)} \quad \text{for} \quad 2 \leq k \leq \xi.$$

Recall the compatibility conditions give us $\alpha_i = \theta_i - c_i$, so

$$\alpha_i(-1)^k + \theta_i = (\theta_i - c_i)(-1)^k + \theta_i = (1 + (-1)^k)\theta_i - (-1)^k c_i. \quad (2.27)$$

By using (2.27) we get the condition $E(\xi, \eta)$ holds $\iff$

$$\begin{aligned} & \tilde{\sigma}(-1)^{l+k} + \tilde{\delta}(0)^{l+k} + \tilde{\beta}(1)^{l+k} + \sum_{i=1}^s b_i c_i^{l-2} ((1 + (-1)^k)\theta_i - (-1)^k c_i) \\ & + (k)(k-1)(\sigma_i(-1)^{k-2} + \delta_i(0)^{k-2} + \beta_i + \sum_{j=1}^s a_{ij} c_j^{k-2}) \\ & = \frac{1 + (-1)^{l+k}}{(l+k)(l+k-1)} \end{aligned} \quad (2.28)$$

for $2 \leq l \leq \xi$, $2 \leq k \leq \eta$.

With the new notation we get

$$\sigma_i(-1)^{k-2} + \delta_i(0)^{k-2} + \beta_i + \sum_{j=1}^s a_{ij} c_j^{k-2} = \sum_{j=1}^{s+3} \tilde{a}_{ij} \tilde{c}_j^{k-2} \quad (2.29)$$

for $i = 1, \dots, s$.

Using (2.29) and the fact that $\tilde{a}_{s+1,j} = \tilde{a}_{s+2,j} = \tilde{a}_{s+3,j} = 0$ for $j = 1, \dots, s+3$ we get

$$\begin{aligned} & \sum_{i=1}^s b_i c_i^{l-2} \left(\sigma_i(-1)^k + \delta_i(0)^{k-2} + \beta_i + \sum_{j=1}^s a_{ij} c_j^{k-2} \right) \\ &= \sum_{i=1}^{s+3} \tilde{b}_i \tilde{c}_i^{l-2} \left(\sum_{j=1}^{s+3} \tilde{a}_{ij} \tilde{c}_j^{k-2} \right). \end{aligned} \quad (2.30)$$

Using (2.24), (2.25), (2.26), we get

$$\begin{aligned} & \tilde{\sigma}(-1)^{l+k} + \tilde{\delta}(0)^{l+k} + \tilde{\beta}(1)^{l+k} + \sum_{i=1}^s b_i c_i^{l-2} ((1 + (-1)^k) \theta_i - (-1)^k c_i) \\ &= \tilde{b}_{s+1} \tilde{c}_{s+1}^{l-2} ((1 + (-1)^k) \tilde{\theta}_{s+1} - (-1)^k \tilde{c}_{s+1}) \\ &+ \tilde{b}_{s+2} \tilde{c}_{s+2}^{l-2} ((1 + (-1)^k) \tilde{\theta}_{s+2} - (-1)^k \tilde{c}_{s+2}) \\ &+ \tilde{b}_{s+3} \tilde{c}_{s+3}^{l-2} ((1 + (-1)^k) \tilde{\theta}_{s+3} - (-1)^k \tilde{c}_{s+3}) \\ &+ \sum_{i=1}^s \tilde{b}_i \tilde{c}_i^{l-2} ((1 + (-1)^k) \tilde{\theta}_i - (-1)^k \tilde{c}_i) \\ &= \sum_{i=1}^{s+3} \tilde{b}_i \tilde{c}_i^{l-2} ((1 + (-1)^k) \tilde{\theta}_i - (-1)^k \tilde{c}_i). \end{aligned} \quad (2.31)$$

So using (2.30), and (2.31), the $E(\xi, \eta)$ condition in the new notation is

$$\begin{aligned} & \sum_{i=1}^{s+3} \tilde{b}_i \tilde{c}_i^{l-2} ((1 + (-1)^k) \tilde{\theta}_i - (-1)^k \tilde{c}_i) + (k)(k-1) \sum_{i=1}^{s+3} \tilde{b}_i \tilde{c}_i^{l-2} \left(\sum_{j=1}^{s+3} \tilde{a}_{ij} \tilde{c}_j^{k-2} \right) \\ &= \frac{1 + (-1)^{l+k}}{(l+k)(l+k-1)} \quad \text{for} \quad 2 \leq k \leq \eta \quad \text{and} \quad 2 \leq l \leq \xi. \end{aligned}$$

If we have the $B(\xi+1)$ condition, then $E(\xi, \eta)$ can be rewritten as

$$\begin{aligned} & \sum_{i=1}^{s+3} \tilde{b}_i \tilde{c}_i^{l-2} ((1 + (-1)^k) \tilde{\theta}_i) + \sum_{i,j=1}^{s+3} \tilde{b}_i \tilde{c}_i^{l-2} \tilde{a}_{ij} \tilde{c}_j^{k-2} \\ &= \frac{1 + (-1)^{l+k}}{(k)(k-1)(l+k)(l+k-1)} + \frac{(-1)^k(1 + (-1)^{l+1})}{(l+1)(l)k(k-1)}, \quad 2 \leq k \leq \eta, \quad 2 \leq l \leq \xi. \end{aligned}$$

Now consider the following tree

$$t = \left[\underbrace{\cdot, \dots, \cdot}_{l-2}, \left[\underbrace{\cdot, \dots, \cdot}_{k-4} \right] \right] \quad \text{where } l \geq 2 \quad \text{and } k \geq 4.$$

To calculate $\Psi(t)$, we first note if $\Psi(\left[\underbrace{\cdot, \dots, \cdot}_{k-4} \right]) = 1$ then

$$\begin{aligned} a_i(\left[\underbrace{\cdot, \dots, \cdot}_{k-4} \right]) &= (1 + (-1)^k) \tilde{\theta}_i - \tilde{c}_i (-1)^k \\ &+ (k)(k-1) \sum_{j=1}^{s+3} \tilde{a}_{ij} ((1 + (-1)^k) \tilde{\theta}_j - \tilde{c}_j (-1)^k) \\ &+ (k)(k-1)(k-2)(k-3) \sum_{j,n=1}^{s+3} \tilde{a}_{ij} \tilde{a}_{jn} \tilde{c}_n^{k-4}. \end{aligned} \quad (2.32)$$

By using (2.32) and assuming $\Psi(\left[\underbrace{\cdot, \dots, \cdot}_{k-4} \right]) = 1$ we obtain

$$\begin{aligned} \Psi\left(\left[\underbrace{\cdot, \dots, \cdot}_{l-2}, \left[\underbrace{\cdot, \dots, \cdot}_{k-4} \right] \right]\right) &= -(-1)^{l+k} \\ &+ (l+k)(l+k-1) \sum_{i=1}^{s+3} \tilde{b}_i \tilde{c}_i^{l-2} \{(1 + (-1)^k) \tilde{\theta}_i - \tilde{c}_i (-1)^k\} \\ &+ (k)(k-1)(l+k)(l+k-1) \sum_{i,j=1}^{s+3} \tilde{b}_i \tilde{c}_i^{l-2} \tilde{a}_{ij} ((1 + (-1)^k) \tilde{\theta}_j - \tilde{c}_j (-1)^k) \\ &+ (k)(k-1)(k-2)(k-3)(l+k)(l+k-1) \sum_{i,j,n=1}^{s+3} \tilde{b}_i \tilde{c}_i^{l-2} \tilde{a}_{ij} \tilde{a}_{jn} \tilde{c}_n^{k-4}. \end{aligned}$$

Therefore $\Psi\left(\left[\underbrace{\cdot, \dots, \cdot}_{l-2}, \left[\underbrace{\cdot, \dots, \cdot}_{k-4} \right] \right]\right) = 1$ and $\Psi(\left[\underbrace{\cdot, \dots, \cdot}_{k-4} \right]) = 1$ if and only if

$$\begin{aligned} &\sum_{i=1}^{s+3} \frac{\tilde{b}_i \tilde{c}_i^{l-2} \{(1 + (-1)^k) \tilde{\theta}_i\}}{(k)(k-1)(k-2)(k-3)} - (-1)^k \sum_{i=1}^{s+3} \frac{\tilde{b}_i \tilde{c}_i^{l-1}}{(k)(k-1)(k-2)(k-3)} \\ &+ \sum_{i,j=1}^{s+3} \frac{\tilde{b}_i \tilde{c}_i^{l-2} \tilde{a}_{ij} (1 + (-1)^k) \tilde{\theta}_j}{(k-2)(k-3)} - (-1)^k \sum_{i,j=1}^{s+3} \frac{\tilde{b}_i \tilde{c}_i^{l-2} \tilde{a}_{ij} \tilde{c}_j}{(k-2)(k-3)} \\ &+ \sum_{i,j,n=1}^{s+3} \tilde{b}_i \tilde{c}_i^{l-2} \tilde{a}_{ij} \tilde{a}_{jn} \tilde{c}_n^{k-4} = \frac{1 + (-1)^{l+k}}{(l+k)(l+k-1)(k)(k-1)(k-2)(k-3)}. \end{aligned}$$

DEFINITION 15: A method in the form of (2.8) obeys condition $F(\xi, \eta)$ if $\Psi(\underbrace{[\cdot, \dots, \cdot]}_{l-2} [\underbrace{[\cdot, \dots, \cdot]}_{k-4}]) = 1$ and $\Psi([\underbrace{[\cdot, \dots, \cdot]}_{k-4}]) = 1$ for all l, k such that $2 \leq l \leq \xi$ and $4 \leq k \leq \eta$.

If we have condition $B(\xi+1)$ and $E(\xi, 3)$ holding then condition $F(\xi, \eta)$ becomes

$$\begin{aligned} & \sum_{i=1}^{s+3} \frac{\tilde{b}_i \tilde{c}_i^{l-2} \{(1+(-1)^k) \tilde{\theta}_i\}}{(k)(k-1)(k-2)(k-3)} + \sum_{i,j=1}^{s+3} \frac{\tilde{b}_i \tilde{c}_i^{l-2} \tilde{a}_{ij} (1+(-1)^k) \tilde{\theta}_j}{(k-2)(k-3)} \\ & + \sum_{i,j,n=1}^{s+3} \frac{\tilde{b}_i \tilde{c}_i^{l-2} \tilde{a}_{ij} \tilde{a}_{jn} \tilde{c}_n^{k-4}}{(l+k)(l+k-1)(k)(k-1)(k-2)(k-3)} = \frac{1+(-1)^{l+k}}{(l+k)(l+k-1)(k)(k-1)(k-2)(k-3)} \\ & + \frac{(-1)^k (1+(-1)^{l+1})}{(k)(k-1)(k-2)(k-3)(l+1)(l)} + \frac{(-1)^k}{(k-2)(k-3)} \times \\ & \left\{ \frac{1+(-1)^{l+3}}{6(l+3)(l+2)} + \frac{(-1)^3 (1+(-1)^{l+1})}{6(l+1)(l)} \right\} \end{aligned} \quad (2.33)$$

for $2 \leq l \leq \xi$ and $4 \leq k \leq \eta$.

DEFINITION 16: A method of the form (2.8) obeys property $D(\eta)$ if the following holds:

$$\begin{aligned} & \sum_{i,j=1}^{s+3} \tilde{b}_i \tilde{c}_i^{l-2} \tilde{a}_{ij} \tilde{a}_{jn} = - \sum_{i,j=1}^{s+3} (\tilde{b}_i \tilde{c}_i^{l-2} \tilde{\theta}_i \tilde{b}_j \tilde{\theta}_j \tilde{b}_n + \tilde{b}_i \tilde{c}_i^{l-2} \tilde{\theta}_i \tilde{b}_j \tilde{a}_{jn} \\ & + \tilde{b}_i \tilde{c}_i^{l-2} \tilde{a}_{ij} \tilde{\theta}_j \tilde{b}_n) \\ & + \sum_{j=1}^{s+3} \left(\frac{1}{6} (\tilde{b}_j \tilde{c}_j^l \tilde{\theta}_j \tilde{b}_n + \tilde{b}_j \tilde{c}_j^l \tilde{a}_{jn}) - \frac{1}{3} (\tilde{b}_j \tilde{c}_j^{l-1} \tilde{\theta}_j \tilde{b}_n \tilde{c}_n + \tilde{b}_j \tilde{c}_j^{l-1} \tilde{a}_{jn} \tilde{c}_n) \right. \\ & + \frac{1}{6} (\tilde{b}_j \tilde{c}_j^{l-2} \tilde{\theta}_j \tilde{b}_n \tilde{c}_n^2 + \tilde{b}_j \tilde{c}_j^{l-2} \tilde{a}_{ij} \tilde{c}_n^2) \left. + \left(\frac{1+(-1)^{l+2}}{(l+2)(l+1)} + \frac{1+(-1)^{l+1}}{(l+1)(l)} \right) \right. \\ & \times \left. \left\{ \frac{-1}{12} \tilde{b}_n + \frac{1}{6} \tilde{b}_n \tilde{c}_n - \frac{1}{12} \tilde{b}_n \tilde{c}_n^2 + \frac{1}{12} \sum_{j=1}^{s+3} (\tilde{b}_j \tilde{\theta}_j \tilde{b}_n + \tilde{b}_j \tilde{a}_{jn}) \right\} \right) \end{aligned}$$

for $n = 1, \dots, s+3$ and $2 \leq l \leq \eta$.

To conclude this chapter we establish the necessity of a certain D condition if a certain order is to be attained.

THEOREM 2.13. *If a method of the form (2.8) obeys properties $F(\eta, s+6)$, $E(\eta, 3)$, $B(s+6)$, $E(\eta+2, s+4)$ and $E(\eta+1, s+5)$ and has $\tilde{c}_i$'s that are distinct, then the method obeys property $D(\eta)$.*

PROOF: Basic algebra will prove the following

$$\begin{aligned}
& \frac{1 + (-1)^{l+k}}{(l+k)(l+k-1)(k)(k-1)(k-2)(k-3)} + \frac{(-1)^k(1 + (-1)^{l+1})}{(k)(k-1)(k-2)(k-3)(l+1)(l)} \\
& + \frac{(-1)^k}{(k-2)(k-3)} \left\{ \frac{1 + (-1)^{l+3}}{(l+3)(l+2)6} + \frac{(-1)^3(1 + (-1)^{l+1})}{6(l+1)(l)} \right\} \\
& - \frac{1}{6} \left\{ \frac{1 + (-1)^{l+k}}{(l+k)(l+k-1)(k-2)(k-3)} + \frac{(-1)^k(1 + (-1)^{l+1})}{(k-2)(k-3)(l+3)(l+2)} \right\} \\
& + \frac{1}{3} \left\{ \frac{1 + (-1)^{l+k}}{(l+k)(l+k-1)(k-1)(k-2)} + \frac{(-1)^k(1 + (-1)^{l+2})}{(k-1)(k-2)(l+2)(l+1)} \right\} \\
& - \frac{1}{6} \left\{ \frac{1 + (-1)^{l+k}}{(l+k)(l+k-1)(k)(k-1)} + \frac{(-1)^k(1 + (-1)^{l+1})}{(k)(k-1)(l+1)(l)} \right\} \\
& + \left(\frac{1 + (-1)^l}{(l+2)(l+1)} + \frac{1 + (-1)^{l+1}}{(l+1)(l)} \right) \left\{ \frac{1}{12} \left(\frac{1 + (-1)^k}{(k-2)(k-3)} \right) - \frac{1}{6} \left(\frac{1 + (-1)^{k-1}}{(k-1)(k-2)} \right) \right. \\
& \left. + \frac{1}{12} \left(\frac{1 + (-1)^k}{(k-1)(k)} \right) - \frac{1}{2} \left(\frac{1 + (-1)^k}{(k)(k-1)(k-2)(k-3)} \right) \right\} = 0. \tag{2.34}
\end{aligned}$$

Since properties $F(l, k)$, $E(l+2, k-2)$, $E(l+1, k-1)$, $E(l, k)$, $B(k)$, $B(l+3)$, $E(l, 3)$ and $E(2, k-2)$ and equation (2.34) hold, we get

$$\begin{aligned}
& \sum_{i=1}^{s+3} \frac{\tilde{b}_i \tilde{c}_i^{l-2}(1 + (-1)^k)\tilde{\theta}_i}{(k)(k-1)(k-2)(k-3)} + \sum_{i,j=1}^{s+3} \frac{\tilde{b}_i \tilde{c}_i^{l-2} \tilde{a}_{ij}(1 + (-1)^k)\tilde{\theta}_j}{(k-2)(k-3)} \\
& + \sum_{i,j,n=1}^{s+3} \tilde{b}_i \tilde{c}_i^{l-2} \tilde{a}_{ij} \tilde{a}_{jn} \tilde{c}_n^{k-4} - \frac{1}{6} \left\{ \sum_{j=1}^{s+3} \frac{\tilde{b}_j \tilde{c}_j^l(1 + (-1)^{k-2})\tilde{\theta}_j}{(k-2)(k-3)} + \sum_{j,n=1}^{s+3} \tilde{b}_j \tilde{c}_j^l \tilde{a}_{ij} \tilde{c}_n^{k-4} \right\} \\
& + \frac{1}{3} \left\{ \sum_{j=1}^{s+3} \frac{\tilde{b}_j \tilde{c}_j^{l-1}(1 + (-1)^{k-1})\tilde{\theta}_j}{(k-1)(k-2)} + \sum_{j,n=1}^{s+3} \tilde{b}_j \tilde{c}_j^{l-1} \tilde{a}_{jn} \tilde{c}_n^{k-3} \right\}
\end{aligned}$$

$$\begin{aligned}
& -\frac{1}{6} \left\{ \sum_{j=1}^{s+3} \frac{\tilde{b}_j \tilde{c}_j^{l-2} (1 + (-1)^k) \tilde{\theta}_j}{(k)(k-1)} + \sum_{j,n=1}^{s+3} \tilde{b}_j \tilde{c}_j^{l-2} \tilde{a}_{jn} \tilde{c}_n^{k-2} \right\} \\
& + \left(\frac{1 + (-1)^{l+1}}{(l+2)(l+1)} + \frac{1 + (-1)^{l+1}}{(l+1)(l)} \right) \left\{ \frac{1}{12} \sum_{n=1}^{s+3} \tilde{b}_n \tilde{c}_n^{k-4} - \frac{1}{6} \sum_{n=1}^{s+3} \tilde{b}_n \tilde{c}_n^{k-3} \right. \\
& + \frac{1}{12} \sum_{n=1}^{s+3} \tilde{b}_n \tilde{c}_n^{k-2} - \frac{1}{2} \sum_{j=1}^{s+3} \frac{\tilde{b}_j (1 + (-1)^{k-2}) \tilde{\theta}_j}{(k-2)(k-3)} \\
& \left. - \frac{1}{2} \sum_{j,n=1}^{s+3} \tilde{b}_j \tilde{a}_{jn} \tilde{c}_n^{k-4} \right\} = 0 \tag{2.35}
\end{aligned}$$

Since properties $B(s+6)$ and $E(2, s+4)$ hold the following equations hold:

$$\sum_{i=1}^{s+3} \tilde{b}_i \tilde{c}_i^{k-4} = \frac{1 + (-1)^{k-2}}{(k-2)(k-3)}, \tag{2.36}$$

$$\sum_{i=1}^{s+3} \tilde{b}_i \tilde{c}_i^{k-3} = \frac{1 + (-1)^{k-1}}{(k-1)(k-2)}, \tag{2.37}$$

$$\sum_{i=1}^{s+3} \tilde{b}_i \tilde{c}_i^{k-2} = \frac{1 + (-1)^k}{(k)(k-1)}, \tag{2.38}$$

and

$$\sum_{i=1}^{s+3} \frac{\tilde{b}_i (1 + (-1)^{k-2}) \tilde{\theta}_i}{(k-2)(k-3)} + \sum_{i,j=1}^{s+3} \tilde{b}_i \tilde{a}_{ij} \tilde{c}_j^{k-4} = \frac{1 + (-1)^k}{(k)(k-1)(k-2)(k-3)}. \tag{2.39}$$

By using (2.36) in (2.39) we get

$$\sum_{i=1}^{s+3} \tilde{b}_i \tilde{\theta}_i \left(\sum_{j=1}^{s+3} \tilde{b}_j \tilde{c}_j^{k-4} \right) + \sum_{i,j=1}^{s+3} \tilde{b}_i \tilde{a}_{ij} \tilde{c}_j^{k-4} = \frac{1 + (-1)^k}{(k)(k-1)(k-2)(k-3)}. \tag{2.40}$$

Using (2.36), (2.37), (2.38), and (2.40) in (2.35) we get

$$\sum_{i=1}^{s+3} \tilde{b}_i \tilde{c}_i^{l-2} \tilde{\theta}_i \left(\sum_{j=1}^{s+3} \tilde{b}_j \tilde{\theta}_j \sum_{n=1}^{s+3} \tilde{b}_n \tilde{c}_n^{k-4} + \sum_{j,n=1}^{s+3} \tilde{b}_j \tilde{a}_{jn} \tilde{c}_n^{k-4} \right)$$

$$\begin{aligned}
& + \sum_{i,j=1}^{s+3} \tilde{b}_i \tilde{c}_i^{l-2} \tilde{a}_{ij} \tilde{\theta}_j \sum_{n=1}^{s+3} \tilde{b}_n \tilde{c}_n^{k-4} + \sum_{i,j,n=1}^{s+3} \tilde{b}_i \tilde{c}_i^{l-2} \tilde{a}_{ij} \tilde{a}_{jn} \tilde{c}_n^{k-4} \\
& - \frac{1}{6} \left\{ \sum_{j=1}^{s+3} \tilde{b}_j \tilde{c}_j^l \tilde{\theta}_j \left(\sum_{n=1}^{s+3} \tilde{b}_n \tilde{c}_n^{k-4} \right) + \sum_{j,n=1}^{s+3} \tilde{b}_j \tilde{c}_j^l \tilde{a}_{jn} \tilde{c}_n^{k-4} \right\} \\
& + \frac{1}{3} \left\{ \sum_{j=1}^{s+3} \tilde{b}_j \tilde{c}_j^{l-1} \tilde{\theta}_j \left(\sum_{n=1}^{s+3} \tilde{b}_n \tilde{c}_n^{k-3} \right) + \sum_{j,n=1}^{s+3} \tilde{b}_j \tilde{c}_j^{l-1} \tilde{a}_{jn} \tilde{c}_n^{k-3} \right\} \\
& - \frac{1}{6} \left\{ \sum_{j=1}^{s+3} \tilde{b}_j \tilde{c}_j^{l-2} \tilde{\theta}_j \left(\sum_{n=1}^{s+3} \tilde{b}_n \tilde{c}_n^{k-2} \right) + \sum_{j,n=1}^{s+3} \tilde{b}_j \tilde{c}_j^{l-2} \tilde{a}_{jn} \tilde{c}_n^{k-2} \right\} \\
& + \left(\frac{1+(-1)^{l+2}}{(l+2)(l+1)} + \frac{1+(-1)^{l+1}}{(l+1)(l)} \right) \left\{ \frac{1}{12} \sum_{n=1}^{s+3} \tilde{b}_n \tilde{c}_n^{k-4} - \frac{1}{6} \sum_{n=1}^{s+3} \tilde{b}_n \tilde{c}_n^{k-3} \right. \\
& \left. + \frac{1}{12} \sum_{n=1}^{s+3} \tilde{b}_n \tilde{c}_n^{k-2} - \frac{1}{2} \sum_{j=1}^{s+3} \tilde{b}_j \tilde{\theta}_j \left(\sum_{n=1}^{s+3} \tilde{b}_n \tilde{c}_n^{k-4} \right) - \frac{1}{2} \sum_{j,n=1}^{s+3} \tilde{b}_j \tilde{a}_{jn} \tilde{c}_n^{k-4} \right\} = 0.
\end{aligned}$$

Therefore

$$\begin{aligned}
& \sum_{n=1}^{s+3} \tilde{c}_n^{k-4} \left\{ \sum_{i,j=1}^{s+3} (\tilde{b}_i \tilde{c}_i^{l-2} \tilde{\theta}_i \tilde{b}_j \tilde{\theta}_j \tilde{b}_n + \tilde{b}_i \tilde{c}_i^{l-2} \tilde{\theta}_i \tilde{b}_j \tilde{a}_{jn} + \tilde{b}_i \tilde{c}_i^{l-2} \tilde{a}_{ij} \tilde{\theta}_j \tilde{b}_n \right. \\
& + \tilde{b}_i \tilde{c}_i^{l-2} \tilde{a}_{ij} \tilde{a}_{jn}) + \sum_{j=1}^{s+3} \left(-\frac{1}{6} (\tilde{b}_j \tilde{c}_j^l \tilde{\theta}_j \tilde{b}_n + \tilde{b}_j \tilde{c}_j^l \tilde{a}_{jn}) \right. \\
& + \frac{1}{3} (\tilde{b}_j \tilde{c}_j^{l-1} \tilde{\theta}_j \tilde{b}_n \tilde{c}_n + \tilde{b}_j \tilde{c}_j^{l-1} \tilde{a}_{jn} \tilde{c}_n) \\
& - \frac{1}{6} (\tilde{b}_j \tilde{c}_j^{l-2} \tilde{\theta}_j \tilde{b}_n \tilde{c}_n^2 + \tilde{b}_j \tilde{c}_j^{l-2} \tilde{a}_{jn} \tilde{c}_n^2) \\
& + \left(\frac{1+(-1)^{l+2}}{(l+2)(l+1)} + \frac{1+(-1)^{l+1}}{(l+1)(l)} \right) \left\{ \frac{1}{12} \tilde{b}_n - \frac{1}{6} \tilde{b}_n \tilde{c}_n + \frac{1}{12} \tilde{b}_n \tilde{c}_n^2 \right. \\
& \left. \left. - \frac{1}{2} \sum_{j=1}^{s+3} (\tilde{b}_j \tilde{\theta}_j \tilde{b}_n + \tilde{b}_j \tilde{a}_{jn}) \right\} \right\} = 0
\end{aligned}$$

where

$$2 \leq l \leq \eta \quad \text{and} \quad 4 \leq k \leq s+6. \quad (2.41)$$

Fix l and let $\tilde{v}_n$ be defined as follows

$$\begin{aligned} \tilde{v}_n = & \sum_{i,j=1}^{s+3} (\tilde{b}_i \tilde{c}_i^{l-2} \tilde{\theta}_i \tilde{b}_j \tilde{\theta}_j \tilde{b}_n + \tilde{b}_i \tilde{c}_i^{l-2} \tilde{\theta}_i \tilde{b}_j \tilde{a}_{jn} + \tilde{b}_i \tilde{c}_i^{l-2} \tilde{\theta}_j \tilde{b}_n \\ & + \tilde{b}_i \tilde{c}_i^{l-2} \tilde{a}_{ij} \tilde{a}_{jn}) + \sum_{j=1}^{s+3} \left(-\frac{1}{6} (\tilde{b}_j \tilde{c}_j^l \tilde{\theta}_j \tilde{b}_n + \tilde{b}_j \tilde{c}_j^l \tilde{a}_{jn}) + \frac{1}{3} (\tilde{b}_j \tilde{c}_j^{l-1} \tilde{\theta}_j \tilde{b}_n \tilde{c}_n \right. \\ & + \tilde{b}_j \tilde{c}_j^{l-1} \tilde{a}_{jn} \tilde{c}_n) - \frac{1}{6} (\tilde{b}_j \tilde{c}_j^{l-2} \tilde{\theta}_j \tilde{b}_n \tilde{c}_n^2 + \tilde{b}_j \tilde{c}_j^{l-2} \tilde{a}_{jn} \tilde{c}_n^2) \Big) \\ & + \left(\frac{1 + (-1)^{l+2}}{(l+2)(l+1)} + \frac{1 + (-1)^{l+1}}{(l+1)(l)} \right) \times \\ & \left\{ \frac{1}{12} \tilde{b}_n - \frac{1}{6} \tilde{b}_n \tilde{c}_n + \frac{1}{12} \tilde{b}_n \tilde{c}_n^2 - \frac{1}{2} \sum_{j=1}^{s+3} (\tilde{b}_j \tilde{\theta}_j \tilde{b}_n + \tilde{b}_j \tilde{a}_{jn}) \right\}. \end{aligned}$$

So we can restate (2.41) as $\sum_{n=1}^{s+3} \tilde{c}_n^{k-4} \tilde{v}_n = 0$ for $4 \leq k \leq s+6$; this can be put into matrix form in the following way

$$\begin{bmatrix} 1 & \cdots & 1 \\ \tilde{c}_1 & \cdots & \tilde{c}_{s+3} \\ \vdots & & \vdots \\ \tilde{c}_1^{s+2} & \cdots & \tilde{c}_{s+3}^{s+2} \end{bmatrix} \begin{bmatrix} \tilde{v}_1 \\ \vdots \\ \tilde{v}_{s+3} \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}.$$

Since the $\tilde{c}_i$'s are distinct $\begin{bmatrix} 1 & \cdots & 1 \\ \tilde{c}_1 & & \tilde{c}_{s+3} \\ \vdots & & \vdots \\ \tilde{c}_1^{s+2} & \cdots & \tilde{c}_{s+3}^{s+2} \end{bmatrix}$ is a Vandermonde matrix and is

therefore nonsingular, so $\tilde{v}_n = 0$ for $n = 1, \dots, s+3$. $\tilde{v}_n = 0$ gives us the following

equality

$$\begin{aligned}
\sum_{i,j=1}^{s+3} \tilde{b}_i \tilde{c}_i^{l-2} \tilde{a}_{ij} \tilde{a}_{jn} &= - \sum_{i,j=1}^{s+3} (\tilde{b}_i \tilde{c}_i^{l-2} \tilde{\theta}_i \tilde{b}_j \tilde{\theta}_j \tilde{b}_n + \tilde{b}_i \tilde{c}_i^{l-2} \tilde{\theta}_i \tilde{b}_j \tilde{a}_{jn} \\
&+ \tilde{b}_i \tilde{c}_i^{l-2} \tilde{a}_{ij} \tilde{\theta}_j \tilde{b}_n) + \sum_{j=1}^{s+3} \left(\frac{1}{6} (\tilde{b}_j \tilde{c}_j^l \tilde{\theta}_j \tilde{b}_n + \tilde{b}_j \tilde{c}_j^l \tilde{a}_{jn}) \right. \\
&- \frac{1}{3} (\tilde{b}_j \tilde{c}_j^{l-1} \tilde{\theta}_j \tilde{b}_n \tilde{c}_n + \tilde{b}_j \tilde{c}_j^{l-1} \tilde{a}_{jn} \tilde{c}_n) + \frac{1}{6} (\tilde{b}_j \tilde{c}_j^{l-2} \tilde{\theta}_j \tilde{b}_n \tilde{c}_n^2 + \tilde{b}_j \tilde{c}_j^{l-2} \tilde{a}_{jn} \tilde{c}_n^2) \Big) \\
&+ \left(\frac{1 + (-1)^{l+2}}{(l+2)(l+1)} + \frac{1 + (-1)^{l+1}}{(l+1)(l)} \right) \times \\
&\quad \left\{ \frac{-1}{12} \tilde{b}_n + \frac{1}{6} \tilde{b}_n \tilde{c}_n - \frac{1}{12} \tilde{b}_n \tilde{c}_n^2 + \frac{1}{2} \sum_{j=1}^{s+3} (\tilde{b}_j \tilde{\theta}_j \tilde{b}_n + \tilde{b}_j \tilde{a}_{jn}) \right\}.
\end{aligned}$$

This holds for $2 \leq l \leq \eta$, thus proving the theorem. ■

THEOREM 2.14. *For a method of the form (2.8) $A(\eta + s + 6) \Rightarrow D(\eta)$.*

PROOF: $A(\eta + s + 6) \Rightarrow F(\eta, s + 6)$, $E(\eta, 3)$, $B(s + 6)$, $E(\eta + 2, s + 4)$, and $E(\eta + 1, s + 5) \Rightarrow D(\eta)$ by Theorem (2.13).

Having established these theorems for methods with an arbitrary number of stages, we shall now go on to demonstrate their applicability to some cases with few stages, which are of practical interest.

CHAPTER 3

ORDER AND UNCONDITIONAL STABILITY

§ 3.0 Introduction.

In this chapter the question of what the maximum obtainable order of an unconditionally stable method for $s = 1$ and $s = 2$ is addressed. Section 3.1, which deals with the case $s = 1$, shows that the maximum obtainable order is 4. For $s = 1$ there do exist fourth order methods that are unconditionally stable. In section 3.2 it is shown for $s = 2$ there exists eighth order methods; these, however, are not unconditionally stable. In fact it is shown that for $s = 2$ any method of order 6 or more can not be unconditionally stable.

The characteristic equation for our method is shown to be

$$\begin{aligned} & (1 + z^2 b^T (I + z^2 A)^{-1} (\vec{\theta} - z^2 \vec{\beta}) + \tilde{\beta} z^2) \xi^2 \\ & + (-2 + z^2 b^T (I + z^2 A)^{-1} (\vec{\gamma} - z^2 \vec{\delta}) + \tilde{\delta} z^2) \xi \\ & + (1 + z^2 b^T (I + z^2 A)^{-1} (\vec{\alpha} - z^2 \vec{\sigma}) + \tilde{\sigma} z^2) = 0 \end{aligned}$$

If $(1 + z^2 b^T (I + z^2 A)^{-1} (\vec{\theta} - z^2 \vec{\beta}) + \tilde{\beta} z^2) = (1 + z^2 b^T (I + z^2 A)^{-1} (\vec{\alpha} - z^2 \vec{\sigma}) + \tilde{\sigma} z^2)$, then the roots of the characteristic equation are the same as the roots to the following equation

$$\xi^2 - \frac{2(1 - \frac{1}{2} z^2 b^T (I + z^2 A)^{-1} (\vec{\gamma} - z^2 \vec{\delta}) - \frac{1}{2} \tilde{\delta} z^2)}{(1 + z^2 b^T (I + z^2 A)^{-1} (\vec{\theta} - z^2 \vec{\beta}) + \tilde{\beta} z^2)} \xi + 1 = 0.$$

So the method is unconditionally stable if and only if the absolute value of the rational function

$$R(z^2) = \frac{1 - \frac{1}{2} z^2 b^T (I + z^2 A)^{-1} (\vec{\gamma} - z^2 \vec{\delta}) - \frac{1}{2} \tilde{\delta} z^2}{1 + z^2 b^T (I + z^2 A)^{-1} (\vec{\theta} - z^2 \vec{\beta}) + \tilde{\beta} z^2}$$

is less than or equal to one for all real z .

In [11] John P. Coleman uses the following definition.

DEFINITION 3.1: (Order of Dispersion [11]): For any method corresponding to the characteristic equation of the form

$$\xi^2 - 2R_{nm}(r^2)\xi + 1 = 0$$

the quantity

$$\varphi(r) = r - \cos^{-1} |R_{nm}(r^2)|$$

is called the dispersion (or phase lag). If $\varphi(r) = \mathcal{O}(r^{q+1})$ as $r \rightarrow 0$ the order of dispersion is q . Effectively, the order of dispersion deals with the order that will be seen when a method of our type is applied to a *linear* problem, and hence the order of dispersion is greater than or equal to the “order” of a method.

For a method with s stages the corresponding rational function is $R_{nm}(z^2)$ as we have described it where $n, m \leq \max(s + 1, 3)$. Coleman in [11] shows that for a method that solves second order ODE's that has a characteristic equation of the form

$$\xi^2 - 2R_{nm}(r^2)\xi + 1 = 0$$

if the method is unconditionally stable then the order of dispersion can not exceed $2m$.

So for $s = 2$ [11] tells us that for an unconditionally stable method the order of dispersion is less than or equal to 6; this does not disagree with what is shown here, but, in fact our results apply to the actual order of the method and are, in some cases, sharper.

The case where

$$\begin{aligned} & (1 + z^2 b^T (I + z^2 A)^{-1} (\vec{\theta} - z^2 \vec{\beta}) + \tilde{\beta} z^2) \\ & \neq (1 + z^2 b^T (I + z^2 A)^{-1} (\vec{\alpha} - z^2 \vec{\sigma}) + \tilde{\sigma} z^2) \end{aligned}$$

is partially covered in "Unconditionally Stable Methods for Second Order Differential Equations" [17] by E. Hairer. The roots to our characteristic equation are also roots to the following equation

$$\begin{aligned} & ((1 + \tilde{\beta} z^2) \det(I + z^2 A) + z^2 b^T (I + z^2 A)^{-1} (\vec{\theta} - z^2 \vec{\beta}) \det(I + z^2 A)) \xi^2 \\ & + ((-2 + \tilde{\delta} z^2) \det(I + z^2 A) + z^2 b^T (I + z^2 A)^{-1} (\vec{\gamma} - z^2 \vec{\delta}) \det(I + z^2 A)) \xi \\ & + ((1 + \tilde{\sigma} z^2) \det(I + z^2 A) + z^2 b^T (I + z^2 A)^{-1} (\vec{\alpha} - z^2 \vec{\sigma}) \det(I + z^2 A)) = 0 \end{aligned}$$

This equation is in the form of

$$Q(z, \xi) = Q_0(z^2) \xi^2 + Q_1(z^2) \xi + Q_2(z^2) = 0.$$

In [17] Hairer uses the following definition for order.

DEFINITION 3.2: The solution of $Q(z, \xi) = 0$ is said to be of order p ($p \geq 1$), if and only if one of the principal roots (say R_1) satisfies

$$e^z - R_1(z) = C z^{p+1} + \mathcal{O}(z^{p+2}) \quad \text{for } z \rightarrow 0, \quad \text{with } C \neq 0$$

Using this definition of order p the following result was proved in [17].

Corollary 5 in [17] says if $Q(z, \xi)$ satisfies the following:

- I) is irreducible
- II) $Q_0(0) \neq 0$
- III) $Q(0, 1) = 0, \frac{\partial Q}{\partial R}(0, 1) = 0, \frac{\partial^2 Q}{\partial R^2}(0, 1) \neq 0$

then if the method is unconditionally stable, that is, the roots ξ_i are of modulus less than or equal to one for all real z , then

$$p \leq 2 \deg Q_0 .$$

If the method is of order p in our sense, then it is also of order p in this weaker sense, so this gives us the following result. If our method is unconditionally stable then

$$\text{order} \leq 2 \deg Q_0 \leq 2(s+1) .$$

It is very easy to show the $Q(z, \xi)$ for our method satisfies conditions II and III so the only condition in question is I. Therefore, in conclusion, if $Q(z, \xi)$ is irreducible and the method is unconditionally stable, then the order is less than or equal to $2(s+1)$.

§ 3.1 Methods with one intermediate stage: $s = 1$.

In this section we explore the limitations of order for methods of the form (2.8) when $s = 1$. When $s = 1$ the method takes the following form

$$\begin{aligned} y^{n,i} &= \alpha_1 y^{n-1} + \gamma_1 y^n + \theta_1 y^{n+1} + h^2 \sigma_1 f^{n-1} + h^2 \delta_1 f^n \\ &\quad + h^2 \beta_1 f^{n+1} + h^2 a_{11} f(t^n + c_1 h, y^{n,1}) \\ y^{n+1} &= -y^{n-1} + 2y^n + h^2 b_1 f(t^n + c_1 h, y^{n,1}) + h^2 \tilde{\sigma} f^{n-1} \\ &\quad + h^2 \tilde{\delta} f^n + h^2 \tilde{\beta} f^{n+1} \end{aligned} \tag{3.1}$$

THEOREM 3.1. *A method of the form (3.1) cannot have order greater than 4.*

PROOF: Say the method has order greater than 4; then by Theorem(2.6) property

$B(6)$ holds. If so, the following equations hold

$$\tilde{\sigma} + \tilde{\delta} + \tilde{\beta} + b_1 = 1 \quad (3.2)$$

$$-\tilde{\sigma} + \tilde{\beta} + b_1 c_1 = 0 \quad (3.3)$$

$$\tilde{\sigma} + \tilde{\beta} + b_1 c_1^2 = \frac{1}{6} \quad (3.4)$$

$$-\tilde{\sigma} + \tilde{\beta} + b_1 c_1^3 = 0 \quad (3.5)$$

$$\tilde{\sigma} + \tilde{\beta} + b_1 c_1^4 = \frac{1}{15} . \quad (3.6)$$

By subtracting (3.3) from (3.5) and then factoring we obtain

$$b_1 c_1 (c_1 - 1)(c_1 + 1) = 0 .$$

Therefore at least one of the following equations holds

$$b_1 = 0, \quad c_1 = 0, \quad c_1 = 1, \quad \text{or} \quad c_1 = -1 .$$

If $b_1 = 0$ or $c_1 = 0$ then by (3.4) and (3.6) we have

$$\tilde{\sigma} + \tilde{\beta} = \frac{1}{6} \quad \text{and} \quad \tilde{\sigma} + \tilde{\beta} = \frac{1}{15}$$

which is a contradiction.

If $c_1 = \pm 1$ then by (3.4) and (3.6) we get

$$\tilde{\sigma} + \tilde{\beta} + b_1 = \frac{1}{6} \quad \text{and} \quad \tilde{\sigma} + \tilde{\beta} + b_1 = \frac{1}{15}$$

which again is a contradiction. Therefore there is no solution to these equations, so there does not exist a 5th order method in the form of (3.1).

A method is 4th order if and only if it obeys $A(5)$, which by Theorems (2.12) , (2.6) and (2.10) happens if and only if properties $B(5)$ and $C(3)$ hold. Therefore

the method (3.1) has order 4 if and only if it obeys equations (3.2) through (3.5) and the following equations

$$\delta_1 + \beta_1 + \sigma_1 + a_{11} = \frac{c_1^2 + c_1 - 2\theta_1}{2} \quad (3.7)$$

and

$$\beta_1 - \sigma_1 + a_{11} = \frac{c_1^3 - c_1}{6} . \quad (3.8)$$

Also the compatibility conditions are

$$\alpha_1 + \gamma_1 + \theta_1 = 1 \quad (3.9)$$

$$\theta_1 - \alpha_1 = c_1 . \quad (3.10)$$

By subtracting (3.3) from (3.5) and then factoring we obtain

$$b_1 c_1 (c_1 - 1)(c_1 + 1) = 0 .$$

Therefore one of the following must hold

$$b_1 = 0, \text{ or } c_1 = 0, \text{ or } c_1 = 1 \text{ or } c_1 = -1 .$$

If $b_1 = 0$ then the method is really just a linear multistep method. If $c_1 = 1$, then by using this value of c_1 in equations (3.2) through (3.5) and equations (3.7)

through (3.10) we obtain the following set of equations

$$\begin{aligned}
 \tilde{\sigma} + \tilde{\delta} + \tilde{\beta} + b_1 &= 1 \\
 -\tilde{\sigma} + \tilde{\beta} + b_1 &= 0 \\
 \tilde{\sigma} + \tilde{\beta} + b_1 &= \frac{1}{6} \\
 -\tilde{\sigma} + \tilde{\beta} + b_1 &= 0 \\
 \delta_1 + \beta_1 + \sigma_1 + a_{11} &= 1 - \theta_1 \\
 \beta_1 - \sigma_1 + a_{11} &= 0 \\
 \alpha_1 - \gamma_1 + \theta_1 &= 1 \\
 \theta_1 - \alpha_1 &= 1 \quad .
 \end{aligned} \tag{3.11}$$

The second equation gives us $\tilde{\beta} = \tilde{\sigma} - b_1$; using this result in the third equation gives us

$$2\tilde{\sigma} = \frac{1}{6}$$

therefore $\tilde{\sigma} = \frac{1}{12}$.

Using this value of $\tilde{\sigma}$ gives us

$$\tilde{\beta} = \frac{1}{12} - b_1 .$$

Using these two results in the first equation of (3.11) gives us

$$\frac{1}{12} + \tilde{\delta} + \frac{1}{12} - b_1 + b_1 = 1$$

therefore $\tilde{\delta} = \frac{5}{6}$.

The equation $\beta_1 - \sigma_1 + a_{11} = 0$ implies $\beta_1 = \sigma_1 - a_{11}$. Using this result in the equation

$$\delta_1 + \beta_1 + \sigma_1 + a_{11} = 1 - \theta_1$$

gives us $\delta_1 + \sigma_1 - a_{11} + \sigma_1 + a_{11} = 1 - \theta_1$.

Using this formula for α_1 in the equation

$$\alpha_1 + \gamma_1 + \theta_1 = 1 \quad \text{we get}$$

$$\theta_1 - 1 + \gamma_1 + \theta_1 = 1$$

therefore $\gamma_1 = 2 - 2\theta_1$.

So for $c_1 = 1$ all solutions to (3.11) can be expressed in terms of b_1, θ_1, σ_1 , and a_{11} in the following manner

$$\begin{aligned} c_1 = 1 \quad \tilde{\sigma} &= \frac{1}{12} \quad \tilde{\beta} = -b_1 + \frac{1}{12} \\ \tilde{\delta} &= \frac{5}{6} \quad \beta_1 = \sigma_1 - a_{11} \quad \delta_1 = 1 - \theta_1 - 2\sigma_1 \\ \alpha_1 &= \theta_1 - 1 \quad \gamma_1 = 2 - 2\theta_1 \end{aligned} \quad (3.12)$$

In a similar manner the solutions to equations (3.2) through (3.5) and (3.7) through (3.10) can be solved in terms of $b_1, \sigma_1, \theta_1, a_{11}$ for $c_1 = 0$ and $c_1 = -1$. For $c_1 = 0$ the solutions will obey the following equations

$$\begin{aligned} c_1 = 0 \quad \tilde{\beta} = \tilde{\sigma} &= \frac{1}{12} \quad \tilde{\delta} = \frac{5}{6} - b_1 \\ \beta_1 &= \sigma_1 - a_{11} \quad \delta_1 = -2\sigma_1 - \theta_1 \quad \alpha_1 = \theta_1 \quad \text{and} \quad \gamma_1 = 1 - 2\theta_1 \end{aligned} \quad (3.13)$$

For the case $c_1 = -1$ the solutions will obey the following equations

$$\begin{aligned} c_1 = -1 \quad \tilde{\sigma} &= \frac{1}{12} - b_1 \quad \tilde{\beta} = \frac{1}{12} \quad \tilde{\delta} = \frac{5}{6} \\ \beta_1 &= \sigma_1 - a_{11} \quad \delta_1 = -2\sigma_1 - \theta_1 \\ \alpha_1 &= 1 + \theta_1 \quad \gamma_1 = -2\theta_1 \end{aligned} \quad (3.14)$$

We have thus exhibited many possibilities for methods of order 4. In particular, in [8] Chawla gives the following method

$$\begin{aligned} y^{n+1} - 2y^n + y^{n-1} &= \frac{h^2}{12}(f^{n+1} + 10\bar{f}^n + f^{n-1}) \\ \bar{y}^n &= y^n - \alpha h^2(f^{n+1} - 2f^n + f^{n-1}) \end{aligned} \quad (3.15)$$

where α is a free parameter, $\alpha > \frac{1}{120}$. This method is of the form (3.1) with

$$\begin{aligned} c_1 &= 0, & b_1 &= \frac{10}{12}, & \tilde{\beta} &= \tilde{\sigma} = \frac{1}{12}, & \tilde{\delta} &= 0 \\ \alpha_1 &= \theta_1 = 0, & \gamma_1 &= 1, & \sigma_1 &= \beta_1 = \alpha, & \delta_1 &= 2\alpha & a_{11} &= 0. \end{aligned}$$

This method has order 4 and is unconditionally stable so we know such a method exists.

§ 3.2. Methods with two intermediate stages: $s = 2$.

First we show there exists an 8th order method where $s = 2$.

THEOREM 3.2. *There exists an 8th order method of the form (2.8) with $s = 2$.*

PROOF: By Theorems (2.6) and (2.12) for $s = 2$ property $A(9)$ implies that properties $C(6)$ and $B(9)$ hold. If properties $B(9)$ and $C(6)$ hold, then by Theorem (2.10) $\Psi(t) = 1$ for all A trees t such that $\rho(t) \leq 9$ and t is of the form $t = [t_1, \dots, t_n]$ where $\rho(t_i) \leq 6$. The only A trees of order 9 or less not in this form are of the form $t = [\tilde{t}]$ where $\rho(\tilde{t}) = 7$. Note that for $\tilde{t} = [\tilde{t}_1, \dots, \tilde{t}_m]$ where $\rho(\tilde{t}_i) \leq 5$, if the property $C(6)$ holds then $a_i(\tilde{t}_j) = c^{\rho(\tilde{t}_j)}$ for $i = 1, 2, j = 1, \dots, m$. This means that

$$a_i(\tilde{t}) = \alpha_i(-1) + \theta_i - \sigma_i \cdot 7 \cdot 6 + \beta_i \cdot 7 \cdot 6 + 7 \cdot 6 \sum_{j=1}^2 a_{ij} c_j^5.$$

Thus $\Psi([t]) = 1 - 9 \cdot 8 \tilde{\sigma} + 9 \cdot 8 \tilde{\beta} + 9 \cdot 8 \sum_{i=1}^2 b_i (-\alpha_i + \theta_i - 42 \sigma_i + 42 \beta_i + 42 \sum_{j=1}^2 a_{ij} c_j^5)$
for any A tree of this form.

All of this leads to the following simplifying statement. For $s = 2$

$$A(9) \Leftrightarrow B(9) + C(6) + \Psi([t]) = 1 \quad \text{where} \quad \rho(\tilde{t}) = 7 .$$

For $s = 2$ property $B(9)$ implies

$$\tilde{\sigma} + \tilde{\delta} + \tilde{\beta} + b_1 + b_2 = 1 \quad (3.16)$$

$$-\tilde{\sigma} + \tilde{\beta} + b_1 c_1 + b_2 c_2 = 0 \quad (3.17)$$

$$\tilde{\sigma} + \tilde{\beta} + b_1 c_1^2 + b_2 c_2^2 = \frac{1}{6} \quad (3.18)$$

$$-\tilde{\sigma} + \tilde{\beta} + b_1 c_1^3 + b_2 c_2^3 = 0 \quad (3.19)$$

$$\tilde{\sigma} + \tilde{\beta} + b_1 c_1^4 + b_2 c_2^4 = \frac{1}{15} \quad (3.20)$$

$$-\tilde{\sigma} + \tilde{\beta} + b_1 c_1^5 + b_2 c_2^5 = 0 \quad (3.21)$$

$$\tilde{\sigma} + \tilde{\beta} + b_1 c_1^6 + b_2 c_2^6 = \frac{1}{28} \quad (3.22)$$

$$-\tilde{\sigma} + \tilde{\beta} + b_1 c_1^7 + b_2 c_2^7 = 0 \quad (3.23)$$

Here is a solution to equations (3.16) through (3.23):

$$\begin{aligned} c_1 &= \sqrt{\frac{\frac{1}{28} - \frac{1}{15}}{\frac{1}{15} - \frac{1}{6}}} = \sqrt{\frac{13}{42}} \cong .556348640 = -c_2 , \\ b_1 &= \frac{\frac{1}{15} - \frac{1}{6}}{2c_1^2(c_1^2 - 1)} = \frac{441}{1885} \cong .233952255 = b_2 , \\ \tilde{\beta} = \tilde{\sigma} &= \frac{1}{12} - b_1 c_1^2 = \frac{247}{22620} \cong .010919540 , \\ \tilde{\delta} &= 1 - 2\tilde{\sigma} - 2b_1 = \frac{5771}{11310} \cong .510256410 . \end{aligned}$$

Recall that for $s = 2$ if the property $C(6)$ holds then

$$\begin{aligned} \delta_i(0)^{k-2} + \beta_i(1)^{k-2} + \sigma_i(-1)^{k-2} + a_{i1}c_1^{k-2} + a_{i2}c_2^{k-2} \\ = \frac{c_i^k - (-1)^k c_i - \theta_i(1 + (-1)^k)}{(k)(k-1)} \end{aligned}$$

for $i = 1, 2$ and $2 \leq k \leq 6$.

Taking into account $c_1 = -c_2$, property $C(6)$ holding means the following equations hold.

$$\delta_1 + \beta_1 + \sigma_1 + a_{11} + a_{12} = \frac{c_1^2 + c_1 - 2\theta_1}{2} \quad (3.24)$$

$$\delta_2 + \beta_2 + \sigma_2 + a_{21} + a_{22} = \frac{c_1^2 - c_1 - 2\theta_2}{2} \quad (3.25)$$

$$\beta_1 - \sigma_1 + a_{11}c_1 - a_{12}c_1 = \frac{c_1^3 - c_1}{6} \quad (3.26)$$

$$\beta_2 - \sigma_2 + a_{21}c_1 - a_{22}c_1 = \frac{-c_1^3 + c_1}{6} \quad (3.27)$$

$$\beta_1 + \sigma_1 + a_{11}c_1^2 + a_{12}c_1^2 = \frac{c_1^4 + c_1 - 2\theta_1}{12} \quad (3.28)$$

$$\beta_2 + \sigma_2 + a_{21}c_1^2 + a_{22}c_1^2 = \frac{c_1^4 - c_1 - 2\theta_2}{12} \quad (3.29)$$

$$\beta_1 - \sigma_1 + a_{11}c_1^3 - a_{12}c_1^3 = \frac{c_1^5 - c_1}{20} \quad (3.30)$$

$$\beta_2 - \sigma_2 + a_{21}c_1^3 - a_{22}c_1^3 = \frac{-c_1^5 + c_1}{20} \quad (3.31)$$

$$\beta_1 + \sigma_1 + a_{11}c_1^4 + a_{12}c_1^4 = \frac{c_1^6 + c_1 - 2\theta_1}{30} \quad (3.32)$$

$$\beta_2 + \sigma_2 + a_{21}c_1^4 + a_{22}c_1^4 = \frac{c_1^6 - c_1 - 2\theta_2}{30} \quad (3.33)$$

These equations are easily manipulated, to first obtain, letting $\Delta = 60(c_1^2 - 1)$,

$$a_{11} - a_{12} = (3c_1^4 - 10c_1^2 + 7) / \Delta$$

$$a_{21} - a_{22} = (-3c_1^4 + 10c_1^2 - 7) / \Delta$$

$$a_{11} + a_{12} = (2c_1^6 - 5c_1^4 - 3c_1 + 6\theta_1) / (c_1^2 \Delta)$$

$$a_{21} + a_{22} = (2c_1^6 - 5c_1^4 + 3c_1 + 6\theta_2) / (c_1^2 \Delta)$$

from which we determine, upon setting $c_1 = \sqrt{\frac{13}{42}}$, the expressions

$$a_{11} = \frac{-5003}{146160} - \frac{147}{3770} \left(6\theta_1 - 3\sqrt{\frac{13}{42}} \right)$$

$$a_{12} = \frac{9787}{146160} - \frac{147}{3770} \left(6\theta_1 - 3\sqrt{\frac{13}{42}} \right)$$

$$a_{21} = \frac{9787}{146160} - \frac{147}{3770} \left(6\theta_2 + 3\sqrt{\frac{13}{42}} \right)$$

$$a_{22} = \frac{-5003}{146160} - \frac{147}{3770} \left(6\theta_2 + 3\sqrt{\frac{13}{42}} \right)$$

The other coefficients are then determined, approximately as

$$\sigma_1 = \frac{1}{2} \left(-(a_{11} + a_{12})c_1^2 + (a_{11} - a_{12})c_1 + \frac{c_1^4 + c_1 - 2\theta_1}{12} - \frac{c_1^3 - c_1}{6} \right)$$

$$= \frac{1}{2} (.0116548 - .0218391 \theta_1)$$

$$\sigma_2 = \frac{1}{2} \left(-(a_{21} + a_{22})c_1^2 + (a_{21} - a_{22})c_1 + \frac{c_1^4 - c_1 - 2\theta_2}{12} - \frac{-c_1^3 + c_1}{6} \right)$$

$$= \frac{1}{2} (-.0159495 - .0218391 \theta_2)$$

$$\beta_1 = \frac{c_1^3 - c_1}{6} - (a_{11} - a_{12})c_1 + \sigma_1 = -.0018997 - .0109196 \theta_1$$

$$\beta_2 = \frac{-c_1^3 + c_1}{6} - (a_{21} - a_{22})c_1 + \sigma_2 = -.0002477 - .0109196 \theta_2$$

$$\begin{aligned}
\delta_1 &= \frac{c_1^2 + c_1 - 2\theta_1}{2} - (a_{11} + a_{12}) - \sigma_1 - \beta_1 \\
&= .2661183 - .5102549 \theta_1 \\
\delta_2 &= \frac{c_1^2 - c_1 - 2\theta_2}{2} - (a_{21} + a_{22}) - \sigma_2 - \beta_2 \\
&= -.0177622 - .5102549 \theta_2 .
\end{aligned}$$

The requirement that $\Psi([\tilde{t}]) = 1$ where $\rho(\tilde{t}) = 7$ is equivalent to requiring

$$- \tilde{\sigma} + \tilde{\beta} + \sum_{i=1}^2 b_i(-\alpha_i + \theta_i - 42\sigma_i + 42\beta_i + 42 \sum_{j=1}^2 a_{ij}c_j^5) = 0 \quad (3.34)$$

Recall that the compatibility conditions from Chapter 2 give us $\alpha_i - \theta_i = c_i$; using this in (3.34) gives us

$$- \tilde{\sigma} + \tilde{\beta} + \sum_{i=1}^2 b_i(-\theta_i + c_i + \theta_i - 42\sigma_i + 42\beta_i + 42 \sum_{j=1}^2 a_{ij}c_j^5) = 0 . \quad (3.35)$$

The condition $B(9)$ gives us $-\tilde{\sigma} + \tilde{\beta} + \sum_{i=1}^2 b_i c_i = 0$, so using this, (3.35) becomes

$$\sum_{i=1}^2 b_i(-\sigma_i + \beta_i + \sum_{j=1}^2 a_{ij}c_j^5) = 0 . \quad (3.36)$$

Since $c_1 = -c_2$ and $b_1 = b_2$ (3.36) becomes

$$b_1(-\sigma_1 + \beta_1 - \sigma_2 + \beta_2 + ((a_{11} - a_{12}) + (a_{21} - a_{22}))c_1^5) = 0 \quad (3.37)$$

Summing (3.26) and (3.27) we get

$$\beta_1 - \sigma_1 + a_{11}c_1 - a_{12}c_1 + \beta_2 - \sigma_2 + a_{21}c_1 - a_{22}c_1 = 0$$

thus

$$-\sigma_1 + \beta_1 - \sigma_2 + \beta_2 = -c_1((a_{11} - a_{12}) + (a_{21} - a_{22})) = 0 \quad (3.38)$$

Using (3.38) in (3.37) and factoring produces

$$b_1 c_1 (c_1^5 - 1)(a_{11} - a_{12} + a_{21} - a_{22}) = 0 . \quad (3.39)$$

The condition $C(6)$ holding gives us

$$a_{11} - a_{12} + a_{21} - a_{22} = -.1011905 + .1011905 = 0$$

so equation (3.39) and thus equation (3.34) hold. ■

This shows there exists a two-parameter family of methods of order 8 for $s = 2$. We intend to pursue at a later date some ways to choose these parameters to see what type of effective methods might be generated. As is well known, though, we must still address the question of stability. Unfortunately next we will show that for $s = 2$ any method of order 6 or greater will not be unconditionally stable.

THEOREM 3.3. *There does not exist an unconditionally stable method of the form (2.8) with $s = 2$ of order 6 or greater.*

Proof: If a method has order 6 then it satisfies property A(7). By Theorems (2.6) and (2.12) for $s = 2$ property A(7) implies properties C(4) and B(7) hold. If properties B(7) and C(4) hold then by Theorem (2.10) $\Psi(t) = 1$ for all $t \in AT$ $\rho(t) \leq 7$ and $t = [t_1, \dots, t_n]$ where $\rho(t_i) \leq 4$. The only A trees of order 7 or less not in the above form are of the form $t = [\tilde{t}]$ where $\rho(\tilde{t}) = 5$. Note that this tree $\tilde{t}$ can be decomposed in the following manner

$$\tilde{t} = [t_1, \dots, \tilde{t}_m] \quad \text{where} \quad \rho(\tilde{t}_i) \leq 3 ,$$

so by C(4) we get $a_i(\tilde{t}_j) = c_i^{\rho(\tilde{t}_j)}$.

Using this we get

$$a_i(\tilde{t}) = \alpha_i(-1) + \theta_i + \sigma_i \cdot 5 \cdot 4 + \beta_i \cdot 5 \cdot 4 + \sum_{j=1}^2 a_{ij} \cdot 5 \cdot 4 \cdot c_j^3$$

thus

$$\begin{aligned} \Psi([\tilde{t}]) = 1 - 7 \cdot 6 \tilde{\sigma} + 7 \cdot 6 \tilde{\beta} + 7 \cdot 6 \sum_{i=1}^2 b_i(-\alpha_i + \theta_i - \sigma_i \cdot 5 \cdot 4 \\ + \beta_i \cdot 5 \cdot 4 + \sum_{j=1}^2 a_{ij} \cdot 5 \cdot 4 \cdot c_j^3) . \end{aligned} \quad (3.40)$$

All of this leads to the following simplifying statement. For $s = 2$

$$A(7) \iff B(7) + C(4) + \Psi([\tilde{t}]) = 1 \quad \text{where} \quad \rho(\tilde{t}) = 5 .$$

For $s = 2$ a method obeys B(7) if and only if equations (3.16) through (3.21) hold.

Next we show that if a method obeys property B(7) where $s = 2$ then $b_1 = b_2 \neq 0$, $\tilde{\sigma} = \tilde{\beta}$, and $c_1 = -c_2 \neq 0, \pm 1$. Subtracting equation (3.17) from equation (3.19) yields

$$b_1(c_1^3 - c_1) + b_2(c_2^3 - c_2) = 0$$

which implies

$$b_2 c_2 (c_2^2 - 1) = -b_1 c_1 (c_1^2 - 1) . \quad (3.41)$$

Subtracting equation (3.19) from (3.21) and factoring gives us

$$b_1 c_1^2 c_1 (c_1^2 - 1) + b_2 c_2^2 c_2 (c_2^2 - 1) = 0 . \quad (3.42)$$

By using equation (3.41) in (3.42) we obtain

$$b_1 c_1^3 (c_1^2 - 1) + c_2^2 b_1 c_1 (c_1^2 - 1) = 0 .$$

Factoring this gives us

$$b_1 c_1 (c_1^2 - 1)(c_1^2 - c_2^2) = 0 .$$

Therefore one of the following must be true

$$b_1 = 0 \quad \text{or} \quad c_1 = 0 \quad \text{or} \quad c_1 = \pm 1 \quad \text{or} \quad c_1^2 = c_2^2 .$$

If $b_1 = 0$ or $c_1 = 0$ or $c_1 = \pm 1$ then (3.41) becomes

$$b_2 c_2 (c_2^2 - 1) = 0$$

therefore one of the following must hold

$$b_2 = 0 \quad \text{or} \quad c_2 = 0 \quad \text{or} \quad c_2 = \pm 1 .$$

By subtracting (3.18) from (3.20) we get

$$b_1(c_1^4 - c_1^2) + b_2(c_2^4 - c_2^2) = \frac{1}{15} - \frac{1}{16} \quad (3.43)$$

if $b_1 = 0$ or $c_1 = 0$ or $c_1 = \pm 1$ and $b_2 = 0$ or $c_2 = 0$ or $c_2 = \pm 1$

then the left hand side of this equation is zero which leads to a contradiction. So

$b_1 = 0, c_1 = 0$ and $c_1 = \pm 1$ are not possible and therefore $c_1^2 = c_2^2$ must hold.

If $c_1 = c_2$ then equation (3.41) becomes

$$b_2 c_1 (c_1^2 - 1) = -b_1 c_1 (c_1^2 - 1)$$

therefore one of the following must hold

$$b_1 = -b_2 \quad \text{or} \quad c_1 = 0 \quad \text{or} \quad c_1 = \pm 1 .$$

It was shown that $c_1 = 0$ or ± 1 is not possible. If $b_1 = -b_2$ then equation (3.43) becomes

$$b_1(c_1^4 - c_1^2) - b_1(c_1^4 - c_1^2) = \frac{1}{15} - \frac{1}{6}$$

which is impossible since the left hand side is zero so $c_1 \neq c_2$.

The only possible left is $c_1 = -c_2$; then (3.41) becomes

$$-b_2c_1(c_1^2 - 1) = -b_1c_1(c_1^2 - 1), \quad \text{and}$$

therefore $b_1 = b_2$ since $c_1 \neq 0, \pm 1$. Using this in (3.17) gives

$$-\tilde{\sigma} + \tilde{\beta} = 0$$

and therefore $\tilde{\sigma} = \tilde{\beta}$.

Using the results $b_1 = b_2, \tilde{\sigma} = \tilde{\beta}$, and $c_1 = -c_2$ in equations (3.16), (3.18) and (3.20) we obtain

$$\begin{aligned} \tilde{\delta} + 2\tilde{\beta} + 2b_1 &= 1 \\ 2\tilde{\beta} + 2b_1c_1^2 &= \frac{1}{6} \\ 2\tilde{\beta} + 2b_1c_1^4 &= \frac{1}{15} \end{aligned}$$

Therefore the following holds

$$2b_1c_1^4 - 2b_1c_1^2 = \frac{1}{15} - \frac{1}{6} = \frac{-1}{10}.$$

Since $c_1 \neq \pm 1, 0$ we obtain

$$b_1 = \frac{-1}{20c_1^2(c_1^2 - 1)} \tag{3.44}$$

Simple algebra gives us

$$\tilde{\beta} = \frac{1}{2} \left(\frac{1}{6} - 2b_1c_1^2 \right). \tag{3.45}$$

By using (3.44) in (3.43) and simplifying we get

$$\tilde{\beta} = \frac{1}{2} \left(\frac{1}{6} + \frac{1}{10(c_1^2 - 1)} \right) . \quad (3.46)$$

Since

$$\tilde{\delta} = 1 - 2\tilde{\beta} - 2b_1 \quad (3.47)$$

by using (3.43) and (3.44) we get the following equation

$$\tilde{\delta} = 1 - \left(\frac{1}{6} + \frac{1}{10(c_1^2 - 1)} \right) + \frac{1}{20c_1^2(c_1^2 - 1)} . \quad (3.48)$$

So this solves equations (3.16) through (3.21), thus the equations for the B(7) condition are solved.

The condition C(4) holds if equations (3.24) through (3.29) hold.

Equations (3.24) and (3.25) imply

$$\delta_1 = \frac{c_1^2 + c_1 - 2\theta_1}{2} - \beta_1 - \sigma_1 - a_{11} - a_{12} \quad (3.49)$$

and

$$\delta_2 = \frac{c_1^2 - c_1 - 2\theta_2}{2} - \beta_2 - \sigma_2 - a_{21} - a_{22} . \quad (3.50)$$

By adding (3.26) to (3.28) and doing some simple algebra we obtain

$$\beta_1 = \frac{1}{2} \left(\frac{c_1^4 + c_1 - 2\theta_1}{12} + \frac{c_1^3 - c_1}{6} - (a_{11} - a_{12})c_1 - (a_{11} + a_{12})c_1^2 \right) . \quad (3.51)$$

A similar calculation involving equations (3.27) and (3.29) produces the following formula for β_2

$$\beta_2 = \frac{1}{2} \left(\frac{c_1^4 - c_1 - 2\theta_2}{12} + \frac{-c_1^3 + c_1}{6} - (a_{21} + a_{22})c_1^2 - (a_{21} - a_{22})c_1 \right) . \quad (3.52)$$

By subtracting (3.26) from (3.28) and doing some algebra we obtain

$$\sigma_1 = \frac{1}{2} \left(-(a_{11} + a_{12})c_1^2 + (a_{11} - a_{12})c_1 + \frac{c_1^4 - c_1 - 2\theta_1}{12} - \frac{c_1^3 - c_1}{6} \right) . \quad (3.53)$$

A similar calculation involving equations (3.27) and (3.29) produces the following equation

$$\sigma_2 = \frac{1}{2} \left(-(a_{11} + a_{12})c_1^2 + (a_{11} - a_{12})c_1 + \frac{c_1^4 + c_1 - 2\theta_1}{12} - \frac{c_1^3 - c_1}{6} \right) . \quad (3.54)$$

Using the results $b_1 = b_2, \tilde{\sigma} = \tilde{\beta}$ and $c_1 = -c_2$ the requirement $\Psi([\tilde{t}]) = 1$ where $\rho(\tilde{t}) = 5$ becomes

$$\begin{aligned} 1 - 7 \cdot 6 \tilde{\beta} + 7 \cdot 6 \tilde{\beta} + 7 \cdot 6 (b_1(-\alpha_1 + \theta_1 - 5 \cdot 4 \sigma_1 + 5 \cdot 4 \beta_1 \\ + 5 \cdot 4(a_{11}c_1^3 - a_{12}c_1^3)) + b_1(-\alpha_2 + \theta_2 - 5 \cdot 4 \sigma_2 + 5 \cdot 4 \beta_2 \\ + 5 \cdot 4(a_{21}c_1^3 - a_{22}c_1^3))) = 1 . \end{aligned} \quad (3.55)$$

By considering the compatibility condition $\theta_i - \alpha_i = c_i$ in (3.55) we obtain

$$\begin{aligned} b_1(c_1 - 20 \sigma_1 + 20 \beta_1 + 20(a_{11}c_1^3 - a_{12}c_1^3)) \\ + b_1(-c_1 - 20 \sigma_2 + 20 \beta_2 + 20(a_{21}c_1^3 - a_{22}c_1^3)) = 0 . \end{aligned} \quad (3.56)$$

Since $b_1 \neq 0$ (3.56) is true if and only if

$$-\sigma_1 + \beta_1 - \sigma_2 + \beta_2 + (a_{11} - a_{12})c_1^3 + (a_{21} - a_{22})c_1^3 = 0 . \quad (3.57)$$

Adding equations (3.26) and (3.27) yields

$$\begin{aligned} \beta_1 - \sigma_1 + \beta_2 - \sigma_2 &= \frac{c_1^3 - c_1}{6} - \frac{c_1^3 + c_1}{6} - (a_{11} - a_{12})c_1 - (a_{21} - a_{22})c_1 \\ &= -(a_{11} - a_{12} + a_{21} - a_{22})c_1 \end{aligned} \quad (3.58)$$

By using this result in (3.57) and factoring we obtain

$$(a_{11} - a_{12} + a_{21} - a_{22})(c_1^3 - c_1) = 0 .$$

Since $c_1 \neq \pm 1, 0$ $c_1^3 - c_1 \neq 0$, so we must have

$$a_{11} - a_{12} + a_{21} - a_{22} = 0 \quad (3.59)$$

To summarize this work for $s = 2$ our method has order 6 if and only if its parameters satisfy equations (3.44), (3.46), (3.48), (3.49), (3.50), (3.51), (3.52), (3.53), (3.54), (3.59) and $b_1 = b_2$, $\tilde{\sigma} = \tilde{\beta}$, and $c_1 = -c_2$. Using this information we next show that such a method cannot be unconditionally stable.

The usual linear stability analysis goes as follows. We apply our method (for $s = 2$) to the problem $y'' = -\lambda^2 y$, (y here is in $\mathbf{IR}^1$), where $\lambda \in \mathbf{IR}$, to obtain

$$\begin{aligned} y^{n,1} &= \alpha_1 y^{n-1} + \gamma_1 y^n + \theta_1 y^{n+1} - (\lambda h)^2 \sigma_1 y^{n-1} - (\lambda h)^2 \delta_1 y^n \\ &\quad - (\lambda h)^2 \beta_1 y^{n+1} - (\lambda h)^2 a_{11} y^{n,1} - (\lambda h)^2 a_{12} y^{n,2} \\ y^{n,2} &= \alpha_2 y^{n-1} + \gamma_2 y^n + \theta_2 y^{n+1} - (\lambda h)^2 \sigma_2 y^{n-1} - (\lambda h)^2 \delta_2 y^n \\ &\quad - (\lambda h)^2 \beta_2 y^{n+1} - (\lambda h)^2 a_{21} y^{n,1} - (\lambda h)^2 a_{22} y^{n,2} \end{aligned}$$

and

$$\begin{aligned} y^{n+1} &= -y^{n-1} + 2y^n - (\lambda h)^2 (b_1 y^{n,1} + b_2 y^{n,2}) \\ &\quad - (\lambda h)^2 \tilde{\sigma} y^{n-1} - (\lambda h)^2 \tilde{\delta} y^n - (\lambda h)^2 \tilde{\beta} y^{n+1} . \end{aligned}$$

If we let $\vec{Y}^n$ be the vector $\begin{bmatrix} y^{n,1} \\ y^{n,2} \end{bmatrix}$ then we have

$$\begin{aligned} \vec{Y}^n &= \vec{\alpha} y^{n-1} + \vec{\gamma} y^n + \vec{\theta} y^{n+1} - (\lambda h)^2 \vec{\sigma} y^{n-1} - (\lambda h)^2 \vec{\delta} y^n \\ &\quad - (\lambda h)^2 \vec{\beta} y^{n+1} - (\lambda h)^2 A \vec{Y}^n \end{aligned}$$

and

$$y^{n+1} = -y^{n-1} + 2y^n - (\lambda h)^2 b^T \vec{Y}^n - (\lambda h)^2 \tilde{\sigma} y^{n-1} - (\lambda h)^2 \tilde{\delta} y^n - (\lambda h)^2 \tilde{\beta} y^{n+1}$$

where $A = \begin{bmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{bmatrix}$, $\vec{b} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$, $\vec{\alpha} = \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix}$ etc. By setting $z^2 = (\lambda h)^2$ and doing some algebra we obtain

$$\vec{Y}^n + z^2 A \vec{Y}^n = (\vec{\alpha} - z^2 \vec{\sigma}) y^{n-1} + (\vec{\gamma} - z^2 \vec{\delta}) y^n + (\vec{\theta} - z^2 \vec{\beta}) y^{n+1} \quad (3.60)$$

$$y^{n+1} = -y^{n-1} + 2y^n - z^2 b^T \vec{Y}^n - z^2 \tilde{\sigma} y^{n-1} - z^2 \tilde{\delta} y^n - z^2 \tilde{\beta} y^{n+1}.$$

Multiplying both sides of (3.60) by $(I + z^2 A)^{-1}$ produces

$$\begin{aligned} \vec{Y}^n &= (I + z^2 A)^{-1} (\vec{\alpha} - z^2 \vec{\sigma}) y^{n-1} + (I + z^2 A)^{-1} (\vec{\gamma} - z^2 \vec{\delta}) y^n \\ &\quad + (I + z^2 A)^{-1} (\vec{\theta} - z^2 \vec{\beta}) y^{n+1}. \end{aligned}$$

Thus

$$\begin{aligned} y^{n+1} &= -y^{n-1} + 2y^n - z^2 b^T \{ (I + z^2 A)^{-1} (\vec{\alpha} - z^2 \vec{\sigma}) y^{n-1} \\ &\quad + (I + z^2 A)^{-1} (\vec{\gamma} - z^2 \vec{\delta}) y^n + (I + z^2 A)^{-1} (\vec{\theta} - z^2 \vec{\beta}) y^{n+1} \} \\ &\quad - z^2 \tilde{\sigma} y^{n-1} - z^2 \tilde{\delta} y^n - z^2 \tilde{\beta} y^{n+1}. \end{aligned}$$

Therefore

$$\begin{aligned} &(1 + z^2 b^T (I + z^2 A)^{-1} (\vec{\theta} - z^2 \vec{\beta}) + \tilde{\beta} z^2) y^{n+1} \\ &+ (-2 + z^2 b^T (I + z^2 A)^{-1} (\vec{\gamma} - z^2 \vec{\delta}) + \tilde{\delta} z^2) y^n \\ &+ (1 + z^2 b^T (I + z^2 A)^{-1} (\vec{\alpha} - z^2 \vec{\sigma}) + \tilde{\sigma} z^2) y^{n-1} = 0. \end{aligned} \quad (3.61)$$

The solution to the difference equation (3.61) is in the form $y^n = \xi^n$ with ξ a root of the quadratic

$$\begin{aligned} &(1 + z^2 b^T (I + z^2 A)^{-1} (\vec{\theta} - z^2 \vec{\beta}) + \tilde{\beta} z^2) \xi^2 \\ &+ (-2 + z^2 b^T (I + z^2 A)^{-1} (\vec{\gamma} - z^2 \vec{\delta}) + \tilde{\delta} z^2) \xi \\ &+ (1 + z^2 b^T (I + z^2 A)^{-1} (\vec{\alpha} - z^2 \vec{\sigma}) + \tilde{\sigma} z^2) = 0. \end{aligned} \quad (3.62)$$

The method is unconditionally stable if the roots ξ_i of (3.62) obey $|\xi_i| \leq 1$ for $i = 1, 2$ for all real z . In analyzing stability, our task is simplified by showing that for $s = 2$, if our method has order 6 or greater, then

$$\begin{aligned} & (1 + z^2 b^T (I + z^2 A)^{-1} (\vec{\theta} - z^2 \vec{\beta}) + \tilde{\beta} z^2) \\ &= (1 + z^2 b^T (I + z^2 A)^{-1} (\vec{\alpha} - z^2 \vec{\sigma}) + \tilde{\sigma} z^2). \end{aligned}$$

Since $\tilde{\beta} = \tilde{\sigma}$ all that is needed to show us that

$$b^T (I + z^2 A)^{-1} (\vec{\theta} - z^2 \vec{\beta}) = b^T (I + z^2 A)^{-1} (\vec{\alpha} - z^2 \vec{\sigma}).$$

Since

$$(I + z^2 A)^{-1} = \frac{1}{(1 + z^2 a_{11})(1 + z^2 a_{22}) - z^4 a_{12} a_{21}} \begin{bmatrix} 1 + z^2 a_{22} & -z^2 a_{12} \\ -z^2 a_{21} & 1 + z^2 a_{11} \end{bmatrix}$$

and $b_1 = b_2$ and by equation (3.59) $a_{11} - a_{12} = a_{22} - a_{21}$ the following equation holds for a vector $\vec{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$

$$\begin{aligned} b^T (I + z^2 A)^{-1} \vec{x} &= \frac{[b_1, b_1]}{(1 + z^2 a_{11})(1 + z^2 a_{22}) - z^4 a_{12} a_{21}} \times \\ &\quad \begin{bmatrix} 1 + z^2 a_{22} & -z^2 a_{12} \\ -z^2 a_{21} & 1 + z^2 a_{11} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \\ &= \frac{b_1 \{(1 + z^2 a_{22})x_1 - z^2 a_{12} x_2\} + b_1 \{-z^2 a_{21} x_1 + (1 + z^2 a_{11})x_2\}}{(1 + z^2 a_{11})(1 + z^2 a_{22}) - z^4 a_{12} a_{21}} \\ &= \frac{b_1 \{(x_1 + x_2) + z^2((a_{22} - a_{21})x_1 + (-a_{12} + a_{11})x_2)\}}{(1 + z^2 a_{11})(1 + z^2 a_{22}) - z^4 a_{12} a_{21}} \\ &= \frac{b_1 \{(x_1 + x_2) + z^2((a_{11} - a_{12})(x_1 + x_2))\}}{(1 + z^2 a_{11})(1 + z^2 a_{22}) - z^4 a_{12} a_{21}}. \end{aligned} \tag{3.63}$$

Using this fact we have

$$b^T (I + z^2 A)^{-1} (\vec{\theta} - z^2 \vec{\beta}) = \frac{b_1((\theta_1 + \theta_2) - z^2(\beta_1 + \beta_2))(1 + (a_{11} - a_{12})z^2)}{(1 + z^2 a_{11})(1 + z^2 a_{22}) - z^4 a_{12} a_{21}}$$

and

$$b^T(I + z^2 A)^{-1}(\vec{\alpha} - z^2 \vec{\sigma}) = \frac{b_1((\alpha_1 + \alpha_2) - z^2(\sigma_1 + \sigma_2))(1 + (a_{11} - a_{12})z^2)}{(1 + z^2 a_{11})(1 + z^2 a_{22}) - z^4 a_{12} a_{21}}.$$

So all that is left to show is that $\theta_1 + \theta_2 = \alpha_1 + \alpha_2$ and $\beta_1 + \beta_2 = \sigma_1 + \sigma_2$. The compatibility conditions give us

$$\alpha_i = \theta_i - c_i \quad \text{so} \quad \alpha_1 + \alpha_2 = \theta_1 + \theta_2 - (c_1 + c_2) = \theta_1 + \theta_2.$$

By using equation (3.59) in equation (3.58) we obtain

$$\beta_1 - \sigma_1 + \beta_2 - \sigma_2 = 0$$

thus

$$\beta_1 + \beta_2 = \sigma_1 + \sigma_2, \quad (3.64)$$

which gives us the desired equality.

The roots of an equation of the form

$$a\xi^2 + 2b\xi + a = 0$$

are less than or equal to one in magnitude if and only if

$$\left| \frac{b}{a} \right| \leq 1.$$

So the roots of (3.62) are less than or equal to one in magnitude if and only if

$$\begin{aligned} & \left| \frac{-\frac{1}{2}(-2 + z^2 \vec{b}^T(I + z^2 A)^{-1}(\vec{\gamma} - z^2 \vec{\delta}) + \tilde{\delta}z^2)}{1 + z^2 \vec{b}^T(I + z^2 A)^{-1}(\vec{\theta} - z^2 \vec{\beta}) + \tilde{\beta}z^2} \right| \leq 1 \\ \Leftrightarrow & \left| \frac{-\frac{1}{2}(\tilde{\delta}z^2 - 2)((1 + z^2 a_{11})(1 + z^2 a_{22}) - z^4 a_{12} a_{21})}{(\tilde{\beta}z^2 + 1)((1 + z^2 a_{11})(1 + z^2 a_{22}) - z^4 a_{12} a_{21})} \right. \\ & \left. \frac{+ z^2 b_1(\gamma_1 + \gamma_2 - z^2(\delta_1 + \delta_2))(1 + z^2(a_{11} - a_{12}))}{+ z^2 b_1(\theta_1 + \theta_2 - z^2(\beta_1 + \beta_2))(1 + z^2(a_{11} - a_{12}))} \right| \leq 1. \end{aligned} \quad (3.65)$$

The following calculations shows that $(1 + (a_{11} - a_{12})z^2)$ is a factor of both the numerator and the denominator of the left hand side of the inequality (3.65), by establishing that $(1 + (a_{11} - a_{12})z^2)$ is a factor of $(1 + z^2 a_{11})(1 + z^2 a_{22}) - z^4 a_{12} a_{21}$.

Equation (3.59) gives us $a_{22} = a_{11} - a_{12} + a_{21}$ so the following two equations will hold

$$a_{11} + a_{22} = (a_{11} - a_{12}) + (a_{21} + a_{11}) \quad (3.66)$$

and

$$\begin{aligned} a_{11} a_{22} - a_{12} a_{21} &= a_{11}(a_{11} - a_{12} + a_{21}) - a_{12} a_{21} \\ &= (a_{11} + a_{21})(a_{11} - a_{12}) . \end{aligned} \quad (3.67)$$

Simple algebra and equations (3.66) and (3.67) give us

$$\begin{aligned} (1 + z^2 a_{11})(1 + z^2 a_{22}) - z^4 a_{12} a_{21} &= 1 + (a_{11} + a_{22})z^2 + (a_{11} a_{22} - a_{12} a_{21})z^4 \\ &= 1 + ((a_{11} - a_{12}) + (a_{21} + a_{11}))z^2 + (a_{11} + a_{21})(a_{11} - a_{12})z^4 \\ &= (1 + (a_{11} - a_{12})z^2)(1 + (a_{21} + a_{11})z^2) \end{aligned} \quad (3.68)$$

which gives us the factorization we wanted.

Using this result we have our method is unconditionally stable if and only if

$$\begin{aligned} |R(z)| &= \left| \frac{P(z)}{Q(z)} \right| \\ &= \left| \frac{-\frac{1}{2}\{(\tilde{\delta}z^2 - 2)(1 + (a_{21} + a_{11})z^2) + z^2 b_1(\gamma_1 + \gamma_2 - z^2(\delta_1 + \delta_2))\}}{(\tilde{\beta}z^2 + 1)(1 + (a_{21} + a_{11})z^2) + z^2 b_1(\theta_1 + \theta_2 - z^2(\beta_1 + \beta_2))} \right| \leq 1 . \end{aligned} \quad (3.69)$$

The inequality $-1 \leq \frac{P(z)}{Q(z)} \leq 1$ holds for all real z if and only if

$$\begin{cases} 0 \leq Q(z) - P(z) \\ \text{and} \\ 0 \leq Q(z) + P(z) \end{cases} \quad \text{where } Q(z) > 0$$

$$\begin{cases} 0 \geq Q(z) - P(z) \\ \text{and} \\ 0 \geq Q(z) + P(z) \end{cases} \quad \text{where } Q(z) < 0$$

$$P(z) = Q(z) \quad \text{where } Q(z) = 0 .$$

The following calculations will help put the coefficients of $Q(z) + P(z)$ and $Q(z) - P(z)$ in terms of the variables $a_{11} + a_{21}$, c_1 , $\theta_1 + \theta_2$. Recall that the compatibility conditions give us

$$\alpha_i + \theta_i + \gamma_i = 1 \quad \text{and} \quad \theta_i - \alpha_i = c_i$$

therefore

$$\begin{aligned} \gamma_1 + \gamma_2 &= 2 - (\theta_1 + \theta_2) - (\alpha_1 + \alpha_2) \\ &= 2 - (\theta_1 + \theta_2) - (\theta_1 + \theta_2 - (c_1 + c_2)) \\ &= 2 - 2(\theta_1 + \theta_2) . \end{aligned} \tag{3.70}$$

Equation (3.59) gives us

$$a_{11} + a_{12} + a_{22} + a_{21} = 2(a_{11} + a_{21}) . \tag{3.71}$$

By adding equations (3.51) and (3.52) and using equations (3.59) and (3.71) we

obtain

$$\begin{aligned}
\beta_1 + \beta_2 &= \frac{1}{2} \left(\frac{2c_1^4 - 2(\theta_1 + \theta_2)}{12} - (a_{11} - a_{12} + a_{21} - a_{22})c_1 \right. \\
&\quad \left. - (a_{11} + a_{12} + a_{22} + a_{21})c_1^2 \right) \\
&= \frac{1}{2} \left(\frac{c_1^4 - (\theta_1 + \theta_2)}{6} - 2(a_{11} + a_{21})c_1^2 \right). \tag{3.72}
\end{aligned}$$

Summing equations (3.49) and (3.50) and using equations (3.71) and (3.64) produces

$$\delta_1 + \delta_2 = c_1^2 - (\theta_1 + \theta_2) - 2(\beta_1 + \beta_2) - 2(a_{11} + a_{21}). \tag{3.73}$$

By using equation (3.72) in (3.73) we get

$$\begin{aligned}
\delta_1 + \delta_2 &= c_1^2 - (\theta_1 + \theta_2) - \frac{c_1^4 - (\theta_1 + \theta_2)}{6} + 2(a_{11} + a_{21})c_1^2 - 2(a_{11} + a_{21}) \\
&= c_1^2 + \frac{5}{6}(\theta_1 + \theta_2) - \frac{c_1^4}{6} + 2(a_{11} + a_{21})(c_1^2 - 1). \tag{3.74}
\end{aligned}$$

Equation (3.70), (3.73), (3.47) and (3.44) will enable us to do the following calculation

$$\begin{aligned}
Q(z) - P(z) &= z^2(\tilde{\delta}/2 + \tilde{\beta})(1 + (a_{21} + a_{11})z^2) \\
&\quad + z^2b_1\{\theta_1 + \theta_2 + \frac{1}{2}(2 - 2(\theta_1 + \theta_2)) \\
&\quad - z^2[\beta_1 + \beta_2 + \frac{1}{2}(c_1^2 - (\theta_1 + \theta_2) - 2(\beta_1 + \beta_2) - 2(a_{11} + a_{21}))]\} \\
&= z^2(\frac{1}{2} - b_1)(1 + (a_{21} + a_{11})z^2) \\
&\quad + z^2b_1\{1 - \frac{z^2}{2}[c_1^2 - (\theta_1 + \theta_2) - 2(a_{11} + a_{21})]\} \\
&= \frac{z^2}{2}\{1 + ((a_{21} + a_{11}) + \frac{1}{20(c_1^2 - 1)} - \frac{(\theta_1 + \theta_2)}{20c_1^2(c_1^2 - 1)})z^2\}. \tag{3.75}
\end{aligned}$$

By using equations (3.70), (3.47), (3.73), (3.72), (3.46) and (3.44) we obtain

$$Q(z) + P(z) = (2 + (\tilde{\beta} - \frac{\tilde{\delta}}{2})z^2)(1 + (a_{21} + a_{11})z^2)$$

$$\begin{aligned}
& + z^2 b_1 \left\{ \theta_1 + \theta_2 - \frac{\gamma_1 + \gamma_2}{2} - z^2 [(\beta_1 + \beta_2) - \frac{1}{2}(\delta_1 + \delta_2)] \right\} \\
& = (2 + (\tilde{\beta} - (\frac{1}{2} - \tilde{\beta} - b_1))) z^2 [1 + (a_{21} + a_{11}) z^2] \\
& + z^2 b_1 \left\{ \theta_1 + \theta_2 - (1 - (\theta_1 + \theta_2)) - z^2 [\beta_1 + \beta_2 \right. \\
& \quad \left. - (\frac{c_1^2}{2} - \frac{\theta_1 + \theta_2}{2} - (\beta_1 + \beta_2) - (a_{11} + a_{21})) \right\} \\
& = (2 + (2\tilde{\beta} - \frac{1}{2} + b_1) z^2) [1 + (a_{21} + a_{11}) z^2] \\
& + z^2 b_1 \left\{ 2(\theta_1 + \theta_2) - 1 - z^2 [2(\beta_1 + \beta_2) - \frac{c_1^2}{2} + \frac{\theta_1 + \theta_2}{2} + (a_{11} + a_{21})] \right\} \\
& = 2 + \{ 2\tilde{\beta} - \frac{1}{2} + b_1 + 2(a_{21} + a_{11}) - b_1 + 2b_1(\theta_1 + \theta_2) \} z^2 \\
& + \{ (a_{21} + a_{11})(2\tilde{\beta} - \frac{1}{2} + b_1) - 2b_1(\beta_1 + \beta_2) + \frac{b_1 c_1^2}{2} - \frac{b_1(\theta_1 + \theta_2)}{2} \\
& \quad - b_1(a_{11} + a_{21}) \} z^4 \\
& = 2 + \{ 2\tilde{\beta} - \frac{1}{2} + 2(a_{21} + a_{11}) + 2b_1(\theta_1 + \theta_2) \} z^2 \\
& + \{ (a_{21} + a_{11})(2\tilde{\beta} - \frac{1}{2}) - 2b_1(\beta_1 + \beta_2) + \frac{b_1 c_1^2}{2} - \frac{b_1(\theta_1 + \theta_2)}{2} \} z^4 \\
& = 2 + \left\{ \frac{1}{6} - \frac{1}{2} + \frac{1}{10(c_1^2 - 1)} + 2(a_{21} + a_{11}) - \frac{(\theta_1 + \theta_2)}{10c_1^2(c_1^2 - 1)} \right\} z^2 \\
& + \{ (a_{21} + a_{11}) \left(\frac{1}{6} + \frac{1}{10(c_1^2 - 1)} - \frac{1}{2} \right) + \frac{1}{20c_1^2(c_1^2 - 1)} \left[\frac{c_1^4 - (\theta_1 + \theta_2)}{6} \right. \right. \\
& \quad \left. \left. - 2(a_{11} + a_{21})c_1^2 \right] - \frac{c_1^2}{40c_1^2(c_1^2 - 1)} + \frac{\theta_1 + \theta_2}{40c_1^2(c_1^2 - 1)} \right\} z^4 \\
& = 2 + \left\{ 2(a_{11} + a_{21}) - \frac{1}{3} + \frac{1}{10(c_1^2 - 1)} - \frac{\theta_1 + \theta_2}{10c_1^2(c_1^2 - 1)} \right\} z^2 \\
& + \left\{ \frac{-2}{3}(a_{21} + a_{11}) + \frac{2(\theta_1 + \theta_2)}{60c_1^2(c_1^2 - 1)} + \frac{c_1^2}{60(c_1^2 - 1)} - \frac{1}{20(c_1^2 - 1)} \right\} z^4. \quad (3.76)
\end{aligned}$$

If the method is unconditionally stable then $Q(z) - P(z)$, $Q(z) + P(z)$, and $Q(z)$ must agree in sign for all real z . If these three polynomials agree in sign for all real z then their leading coefficients must agree in sign. If the leading coefficients are all

less than or equal to zero then

$$a_{11} + a_{21} + \frac{1}{20(c_1^2 - 1)} - \frac{(\theta_1 + \theta_2)}{20c_1^2(c_1^2 - 1)} \leq 0$$

and

$$-\frac{2}{3}(a_{11} + a_{21}) + \frac{2(\theta_1 + \theta_2)}{20c_1^2(c_1^2 - 1)} + \frac{c_1^2}{60(c_1^2 - 1)} - \frac{1}{20(c_1^2 - 1)} \leq 0$$

therefore

$$a_{11} + a_{21} \leq \frac{-1}{20(c_1^2 - 1)} + \frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)}$$

and

$$a_{11} + a_{21} \geq \frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)} + \frac{c_1^2}{40(c_1^2 - 1)} - \frac{3}{40(c_1^2 - 1)} .$$

For these two inequalities to be true the following must hold

$$\frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)} + \frac{c_1^2}{40(c_1^2 - 1)} - \frac{3}{40(c_1^2 - 1)} \leq \frac{-1}{20c_1^2(c_1^2 - 1)} + \frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)}$$

which is true if and only if

$$\frac{c_1^2 - 1}{40(c_1^2 - 1)} \leq 0$$

which is not possible.

Therefore if the three leading coefficients agree in sign they must all be positive.

For this to happen the following three inequalities must hold

$$\frac{1}{2}(a_{11} + a_{21}) + \frac{1}{20c_1^2(c_1^2 - 1)} \left(\frac{c_1^4 - (\theta_1 + \theta_2)}{12} \right) > 0$$

and

$$-\frac{2}{3}(a_{11} + a_{21}) + \frac{2(\theta_1 + \theta_2)}{20c_1^2(c_1^2 - 1)} + \frac{c_1^2}{60(c_1^2 - 1)} - \frac{1}{20(c_1^2 - 1)} > 0$$

and

$$(a_{11} + a_{21}) + \frac{1}{20(c_1^2 - 1)} - \frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)} > 0 .$$

These three inequalities are true if and only if the following three inequalities hold

$$a_{11} + a_{21} > \frac{-c_1^2}{20(c_1^2 - 1)} + \frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)}$$

and

$$a_{11} + a_{21} < \frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)} + \frac{c_1}{40(c_1^2 - 1)} - \frac{3}{40(c_1^2 - 1)}$$

and

$$a_{11} + a_{21} > \frac{-1}{20(c_1^2 - 1)} + \frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)}.$$

Note that

$$\frac{-c_1^2}{20(c_1^2 - 1)} + \frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)} < \frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)} - \frac{1}{20(c_1^2 - 1)}$$

since

$$\frac{c_1^2}{20(c_1^2 - 1)} > \frac{1}{20(c_1^2 - 1)} \quad \text{for } c_1^2 \neq 1$$

(recall the order conditions require $c_1^2 \neq 1$). Therefore the three leading coefficients are positive if and only if

$$\frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)} - \frac{1}{20(c_1^2 - 1)} < a_{11} + a_{21} < \frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)} + \frac{c_1^2 - 3}{40(c_1^2 - 1)}$$

To get stability at infinity it was shown that $a_{11} + a_{21}$ must be in the interval

$$\left(\frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)} - \frac{1}{20(c_1^2 - 1)}, \frac{-3}{40(c_1^2 - 1)} + \frac{c_1^2}{40(c_1^2 - 1)} + \frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)} \right)$$

so

$$\begin{aligned} a_{11} + a_{12} + \frac{1}{20(c_1^2 - 1)} - \frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)} \\ \geq \left(\frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)} - \frac{1}{20(c_1^2 - 1)} + \frac{1}{20(c_1^2 - 1)} - \frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)} \right) \end{aligned}$$

therefore

$$a_{11} + a_{12} + \frac{1}{20(c_1^2 - 1)} - \frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)} \geq 0.$$

Now $Q(z) - P(z) = \frac{1}{2}(z^2 + \left[(a_{11} + a_{21}) + \frac{1}{20(c_1^2 - 1)} - \frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)} \right] z^4)$ so $Q(z) - P(z) \geq 0$ for all real z . Therefore to get unconditional stability $Q(z) + P(z)$ must be positive for all z .

To look at the sign of $Q(z) + P(z)$ consider the case if

$$a_{11} + a_{21} \in \left(\frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)} - \frac{1}{20(c_1^2 - 1)}, \frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)} + \frac{c_1^2 - 5}{80(c_1^2 - 1)} \right)$$

then

$$\begin{aligned} Q(z) + P(z) &= \frac{1}{2} \left(4 + (4(a_{11} + a_{21}) - \frac{2}{3} + \frac{1}{5(c_1^2 - 1)} - \frac{4(\theta_1 + \theta_2)}{20c_1^2(c_1^2 - 1)})z^2 \right. \\ &\quad \left. + (-\frac{2}{3}(a_{11} + a_{21}) + \left(\frac{2}{3}\right)\frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)} + \frac{c_1^2}{60(c_1^2 - 1)} - \frac{1}{20(c_1^2 - 1)})z^4 \right) \\ &\leq \frac{1}{2} \left(4 + (4(\frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)} + \frac{c_1^2 - 5}{80(c_1^2 - 1)}) - \frac{2}{3} + \frac{1}{5(c_1^2 - 1)} - \frac{4(\theta_1 + \theta_2)}{20c_1^2(c_1^2 - 1)})z^2 \right. \\ &\quad \left. + (\frac{-2}{3}(\frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)} - \frac{1}{20(c_1^2 - 1)}) + \left(\frac{2}{3}\right)\frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)} + \frac{c_1^2 - 3}{60(c_1^2 - 1)})z^4 \right) \\ &= \frac{1}{2} \left(4 + \left(\frac{c_1^2 - 5 + 4}{40(c_1^2 - 1)} - \frac{2}{3} \right) z^2 + \left(\frac{2 + c_1^2 - 3}{60(c_1^2 - 1)} \right) z^4 \right) \\ &= \frac{1}{2} \left(4 + \left(\frac{c_1^2 - 1}{20(c_1^2 - 1)} - \frac{2}{3} \right) z^2 + \frac{c_1^2 - 1}{60(c_1^2 - 1)} z^4 \right) \\ &= 2 - \frac{37}{120} z^2 + \frac{1}{120} z^4. \end{aligned}$$

Using this polynomial inequality and evaluating it at $z = 4$ gives us

$$Q(z) + P(z) \big|_{z=4} \leq \left(2 - \frac{37}{120} z^2 + \frac{1}{120} z^4 \right) \big|_{z=4} = -.8 < 0.$$

So in this case $Q(z) - P(z)$ and $Q(z) + P(z)$ differ in sign at $z = 4$. Therefore the method is not unconditionally stable for $a_{11} + a_{21}$ in this subinterval.

If

$$a_{11} + a_{12} \in \left(\frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)} + \frac{c_1^2 - 5}{80(c_1^2 - 1)}, \frac{c_1^2 - 3}{40(c_1^2 - 1)} + \frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)} \right)$$

then

$$\begin{aligned} Q(z) + P(z) &\leq \frac{1}{2} \left(4 + \left(4 \left(\frac{c_1^2 - 3}{40(c_1^2 - 1)} + \frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)} \right) - \frac{2}{3} \right. \right. \\ &\quad \left. \left. + \frac{1}{5(c_1^2 - 1)} - \frac{4(\theta_1 + \theta_2)}{20c_1^2(c_1^2 - 1)} \right) z^2 + \left(\frac{-2}{3} \left(\frac{\theta_1 + \theta_2}{20c_1^2(c_1^2 - 1)} + \frac{c_1^2 - 5}{80(c_1^2 - 1)} \right) \right. \right. \\ &\quad \left. \left. + \frac{2(\theta_1 + \theta_2)}{60c_1^2(c_1^2 - 1)} + \frac{c_1^2}{60(c_1^2 - 1)} - \frac{1}{20(c_1^2 - 1)} \right) z^4 \right) \\ &= \frac{1}{2} \left(4 + \left(\frac{c_1^2 - 3 + 2}{10(c_1^2 - 1)} - \frac{2}{3} \right) z^2 + \left(\frac{c_1^2 - 1}{120(c_1^2 - 1)} \right) z^4 \right) = 2 - \frac{17}{60} z^2 + \frac{1}{240} z^4. \end{aligned}$$

Therefore in this case

$$Q(z) + P(z) \big|_{z=4} \leq \left(2 - \frac{17}{60} z^2 + \frac{1}{240} z^4 \right) \big|_{z=4} = -1.466665$$

Therefore at $z = 4$ the signs of $Q(z) + P(z)$ and $Q(z) - P(z)$ are different, so the method is not unconditionally stable for $a_{11} + a_{21}$ in this subinterval.

Therefore there is no way to pick $a_{11} + a_{21}$ and have an unconditionally stable method. Thus for $s = 2$ if the method has order 6 or more it will not be unconditionally stable.

Even so, with the flexibility afforded by the two-parameter family of eighth order methods, it may yet be of interest to consider them for problems in which conditional stability is acceptable. For the coefficients we have determined it can be shown after some calculation that the associated rational function is

$$R(z) = \frac{1 - \frac{115}{252} z^2 + \frac{313}{15120} z^4}{1 + \frac{11}{252} z^2 + \frac{13}{15120} z^4}$$

(which is, indeed, the (4.4) Padé approximation to $\cos z$). It is then simple to show that $|R(z)| \leq 1$ if and only if $z^2 = |h\lambda|^2 \leq \frac{126}{5}$, thus giving the stability limit.

CHAPTER 4

IMPLEMENTATION AND SOME CONCLUSIONS

§ 4.0 General Strategy.

This chapter is concerned with developing methods that are easy to implement. When our method is implemented at each step the following equation must be solved.

$$\begin{aligned}
 \begin{bmatrix} y^{n,1} \\ \vdots \\ y^{n,s} \\ y^{n+1} \end{bmatrix} &= \begin{bmatrix} \alpha_1 y^{n-1} \\ \vdots \\ \alpha_s y^{n-1} \\ -y^{n-1} \end{bmatrix} + \begin{bmatrix} \gamma_1 y^n \\ \vdots \\ \gamma_s y^n \\ 2y^n \end{bmatrix} + \begin{bmatrix} \theta_1 y^{n+1} \\ \vdots \\ \theta_s y^{n+1} \\ 0y^{n+1} \end{bmatrix} \\
 &+ h^2 \begin{bmatrix} \sigma_1 f(y^{n-1}) \\ \vdots \\ \sigma_s f(y^{n-1}) \\ \tilde{\sigma} f(y^{n-1}) \end{bmatrix} + h^2 \begin{bmatrix} \delta_1 f(y^n) \\ \vdots \\ \delta_s f(y^n) \\ \tilde{\delta} f(y^n) \end{bmatrix} \\
 &+ h^2 \left(\begin{bmatrix} a_{11} & \dots & a_{1s} & \beta_1 \\ \vdots & & \vdots & \vdots \\ a_{s1} & \dots & a_{ss} & \beta_s \\ b_1 & \dots & b_s & \tilde{\beta} \end{bmatrix} \otimes I_m \right) \begin{bmatrix} f(y^{n,1}) \\ f(y^{n,s}) \\ f(y^{n+1}) \end{bmatrix}. \quad (4.1)
 \end{aligned}$$

where $y(t) \in \mathbf{IR}^m$ so $y^{n,i}, y^{n+1}, y^n, y^{n-1}, f(y^{n,i}), f(y^{n+1}), f(y^n)$, and $f(y^{n-1})$ are m dimensional real column vectors and where $\otimes$ is the direct product.

Since

$$\begin{aligned}
 \begin{bmatrix} \theta_1 y^{n+1} \\ \vdots \\ \theta_s y^{n+1} \\ 0y^{n+1} \end{bmatrix} &= \left(\begin{bmatrix} 0 & \dots & 0 & \theta_1 \\ \vdots & & \vdots & \vdots \\ 0 & \dots & 0 & \theta_s \\ 0 & \dots & 0 & 0 \end{bmatrix} \otimes I_m \right) \begin{bmatrix} y^{n,1} \\ \vdots \\ y^{n,s} \\ y^{n+1} \end{bmatrix} \\
 \text{and } \begin{bmatrix} y^{n,1} \\ \vdots \\ y^{n,s} \\ y^{n+1} \end{bmatrix} &= I_{(s+1)m} \begin{bmatrix} y^{n,1} \\ \vdots \\ y^{n,s} \\ y^{n+1} \end{bmatrix} = (I_{(s+1)} \otimes I_m) \begin{bmatrix} y^{n,1} \\ \vdots \\ y^{n,s} \\ y^{n+1} \end{bmatrix}
 \end{aligned}$$

solving (4.1) is equivalent to solving

$$\begin{aligned}
 & \left((I_{s+1} \otimes I_m) - \left(\begin{bmatrix} 0 & \dots & 0 & \theta_1 \\ \vdots & & \vdots & \vdots \\ 0 & \dots & 0 & \theta_s \\ 0 & \dots & 0 & 0 \end{bmatrix} \otimes I_m \right) \right) \begin{bmatrix} y^{n,1} \\ \vdots \\ y^{n,s} \\ y^{n+1} \end{bmatrix} \\
 &= \begin{bmatrix} \alpha_1 y^{n-1} \\ \vdots \\ \alpha_s y^{n-1} \\ -y^{n-1} \end{bmatrix} + \begin{bmatrix} \gamma_1 y^n \\ \vdots \\ \gamma_s y^n \\ 2y^n \end{bmatrix} + h^2 \left(\begin{bmatrix} a_{11} & \dots & a_{1s} & \beta_1 \\ \vdots & & \vdots & \vdots \\ a_{s1} & \dots & a_{ss} & \beta_s \\ b_1 & \dots & b_s & \tilde{\beta} \end{bmatrix} \otimes I_m \right) \\
 & \times \begin{bmatrix} f(y^{n,1}) \\ \vdots \\ f(y^{n,s}) \\ f(y^{n+1}) \end{bmatrix} + h^2 \begin{bmatrix} \sigma_1 f(y^{n-1}) \\ \vdots \\ \sigma_s f(y^{n-1}) \\ \tilde{\sigma} f(y^{n-1}) \end{bmatrix} + h^2 \begin{bmatrix} \delta_1 f(y_n) \\ \vdots \\ \delta_s f(y_n) \\ \tilde{\delta} f(y_n) \end{bmatrix}. \quad (4.2)
 \end{aligned}$$

Since in [20] Lancaster shows $(A + B) \otimes C = (A \otimes C) + (B \otimes C)$ and $(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}$ for any three square matrices A, B , and C , we have

$$\begin{aligned}
 & \left((I_{s+1} \otimes I_m) - \left(\begin{bmatrix} 0 & \dots & 0 & \theta_1 \\ \vdots & & \vdots & \vdots \\ 0 & \dots & 0 & \theta_s \\ 0 & \dots & 0 & 0 \end{bmatrix} \otimes I_m \right) \right)^{-1} \\
 &= \begin{bmatrix} 1 & 0 & \dots & 0 & \theta_1 \\ 0 & 1 & & \vdots & \\ \vdots & & \ddots & 0 & \\ \vdots & & & 1 & \theta_s \\ 0 & 0 & \dots & 0 & 1 \end{bmatrix} \otimes I_m.
 \end{aligned}$$

In [20] Lancaster showed that if A, C are square matrices of dimension s and B, D are square matrices of dimension m then

$$(A \otimes B) (C \otimes D) = (AC) \otimes (BD).$$

By using this fact and multiplying both sides of (4.2) by

$$\begin{bmatrix} 1 & 0 & \dots & 0 & \theta_1 \\ 0 & 1 & & & \vdots \\ \vdots & & \ddots & & 0 \\ \vdots & & & 1 & \theta_s \\ 0 & 0 & \dots & 0 & 1 \end{bmatrix} \otimes I_m .$$

this produces the following equation

$$\begin{aligned} \begin{bmatrix} y^{n,1} \\ \vdots \\ y^{n,s} \\ y^{n+1} \end{bmatrix} &= \left(\begin{bmatrix} 1 & 0 & \dots & 0 & \theta_1 \\ 0 & 1 & & & \vdots \\ \vdots & & \ddots & & 0 \\ \vdots & & & 1 & \theta_s \\ 0 & 0 & \dots & 0 & 1 \end{bmatrix} \otimes I_m \right) \\ &\quad \left(\begin{bmatrix} \alpha_1 y^{n-1} \\ \vdots \\ \alpha_s y^{n-1} \\ -y^{n-1} \end{bmatrix} + \begin{bmatrix} \gamma_1 y^n \\ \vdots \\ \gamma_s y^n \\ 2 y^n \end{bmatrix} + h^2 \begin{bmatrix} \sigma_1 f(y^{n-1}) \\ \vdots \\ \sigma_s f(y^{n-2}) \\ \tilde{\sigma} f(y^{n-1}) \end{bmatrix} + h^2 \begin{bmatrix} \delta_1 f(y^n) \\ \vdots \\ \delta_s f(y^n) \\ \tilde{\delta} f(y^n) \end{bmatrix} \right) \\ &\quad + h^2 \left(\begin{bmatrix} 1 & 0 & \dots & 0 & \theta_1 \\ 0 & 1 & & & \vdots \\ \vdots & & \ddots & & 0 \\ \vdots & & & 1 & \theta_s \\ 0 & 0 & \dots & 0 & 1 \end{bmatrix} \begin{bmatrix} a_{11} & \dots & a_{1s} & \beta_1 \\ \vdots & & \vdots & \vdots \\ a_{s1} & \dots & a_{ss} & \beta_s \\ b_1 & \dots & b_s & \tilde{\beta} \end{bmatrix} \otimes I_m \right) \begin{bmatrix} f(y^{n,1}) \\ \vdots \\ f(y^{n,s}) \\ f(y^{n+1}) \end{bmatrix} . \quad (4.3) \end{aligned}$$

Since when calculating y^{n+1} , the terms y^n and y^{n-1} have already been calculated,

when solving the equation (4.3) we can set

$$\begin{aligned} &\left(\begin{bmatrix} 1 & 0 & \dots & 0 & \theta_1 \\ 0 & 1 & & & \vdots \\ \vdots & & \ddots & & 0 \\ \vdots & & & 1 & \theta_s \\ 0 & 0 & \dots & 0 & 1 \end{bmatrix} \otimes I_m \right) \left(\begin{bmatrix} \alpha_1 y^{n-1} \\ \vdots \\ \alpha_s y^{n-1} \\ -y^{n-1} \end{bmatrix} + \begin{bmatrix} \gamma_1 y^n \\ \vdots \\ \gamma_s y^n \\ 2 y^n \end{bmatrix} \right. \\ &\quad \left. + h^2 \begin{bmatrix} \sigma_1 f(y^{n-1}) \\ \vdots \\ \sigma_s f(y^{n-1}) \\ \tilde{\sigma} f(y^{n-1}) \end{bmatrix} + h^2 \begin{bmatrix} \delta_1 f(y^n) \\ \vdots \\ \delta_s f(y^n) \\ \tilde{\delta} f(y^n) \end{bmatrix} \right) = k^n \end{aligned}$$

a constant vector.

Let

$$M = [m_{ij}] = \begin{bmatrix} 1 & 0 & \dots & 0 & \theta_1 \\ 0 & 1 & & \vdots & \\ \vdots & & \ddots & 0 & \\ \vdots & & & 1 & \theta_s \\ 0 & 0 & \dots & 0 & 1 \end{bmatrix} \begin{bmatrix} a_{11} & \dots & a_{1s} & \beta_1 \\ \vdots & & \vdots & \vdots \\ a_{s1} & \dots & a_{ss} & \beta_s \\ b_1 & \dots & b_s & \tilde{\beta} \end{bmatrix}.$$

With this new notation equation (4.3) becomes

$$\begin{bmatrix} y^{n,1} \\ \vdots \\ y^{n,s} \\ y^{n+1} \end{bmatrix} = h^2(M \otimes I_m) \begin{bmatrix} f(y^{n,1}) \\ \vdots \\ f(y^{n,s}) \\ f(y^{n+1}) \end{bmatrix} + k^n \quad (4.4)$$

The question explored in this chapter is how might the parameters of our method be chosen so that M will be in a form that will facilitate solving equation (4.4). For example if M is diagonal then equation (4.4) will be much easier to solve, and, in fact, the stages can be done in parallel. Several authors (c.f. [13], [14]) discuss ways in which M might be diagonalized by similarity transformations. While this indeed may be possible for our case, we have chosen instead to look for schemes which avoid such transformations and yet admit a sort of decoupling of the stages. Work involving similarity transformations will be reported on at a later date.

We first attempt this for the case $s = 2$. Then,

$$M = \begin{bmatrix} a_{11} + \theta_1 b_1 & a_{12} + \theta_1 b_1 & \beta_1 + \theta_1 \tilde{\beta} \\ a_{21} + \theta_2 b_1 & a_{22} + \theta_2 b_2 & \beta_2 + \theta_2 \tilde{\beta} \\ b_1 & b_2 & \tilde{\beta} \end{bmatrix}$$

is diagonal if and only if

$$b_1 = b_2 = a_{12} = a_{21} = 0$$

and

$$\beta_1 + \theta_1 \tilde{\beta} = \beta_2 + \theta_2 \tilde{\beta} = 0.$$

If the method also has order 3 then the property $B(4)$ must hold, so the following must hold

$$\begin{aligned}\tilde{\sigma} + \tilde{\delta} + \tilde{\beta} + b_1 + b_2 &= 1 \\ -\tilde{\sigma} + \tilde{\beta} + b_1 c_1 + b_2 c_2 &= 0 \\ \tilde{\sigma} + \tilde{\beta} + b_1 c_1^2 + b_2 c_2^2 &= \frac{1}{6}.\end{aligned}$$

Taking into account the assumption that M is diagonal the following must hold:

$$\tilde{\sigma} = \tilde{\beta}, \quad \tilde{\beta} = \frac{1}{12}, \quad \tilde{\delta} = \frac{5}{6}.$$

The stability polynomial is

$$\begin{aligned}& (1 + z^2 b^T (I + z^2 A)^{-1} (\vec{\theta} - z^2 \vec{\beta}) + \tilde{\beta} z^2) \xi^2 \\ & + (-2 + z^2 b^T (I + z^2 A)^{-1} (\vec{\gamma} - z^2 \vec{\delta}) + (\tilde{\delta} z^2) \xi \\ & + (1 + z^2 b^T (I + z^2 A)^{-1} (\vec{\alpha} - z^2 \vec{\sigma}) + \tilde{\sigma} z^2) = 0.\end{aligned}\tag{4.5}$$

Since $b_1 = b_2 = 0$ the stability polynomial will be

$$(1 + \frac{1}{12} z^2) \xi^2 + (-2 + \frac{5}{6} z^2) \xi + (1 + \frac{1}{12} z^2) = 0.$$

The modulus of the roots of the stability polynomial is less than one if and only if

$$\left| \frac{1 - (\frac{5}{12}) z^2}{1 + (\frac{1}{12}) z^2} \right| \leq 1 \quad \text{for all } z$$

which is obviously not true. Hence the possibility of a diagonal M for this case has been ruled out.

§ 4.1 A Specific Class of Fourth-Order, Unconditionally Stable Schemes.

Our next approach is to look for schemes in which M is lower triangular. In that case, it is possible to solve $(s + 1)$ systems of size m in a sequential manner. Further, if the diagonal entries are distinct, indeed, this will lead to schemes for which the stages may be solved in parallel following a similarity transformation. We concentrate here only on the first phase of this problem.

That is, next a method will be developed that has implementation matrix M lower triangular with distinct entries on the diagonal, is unconditionally stable and has order 4 with $s = 2$. We remark that the methods of Cash [6], Chawla [8] and Hairer [17] achieve order 4 and unconditional stability with $s = 1$ but in each case, M is not lower triangular and has complex eigenvalues, ruling out a similarity transformation to diagonal form with real diagonal entries. Here, our approach is to avoid such transformations, anyway.

By the same argument used in Chapter 3, Theorems (2.3) and (2.7) give us that for $s = 2$ a method has order 4 if and only if conditions $B(5), C(2)$ hold and $\Psi([\cdot]) = 1$.

Condition $B(5)$ holds if and only if

$$\begin{aligned}\tilde{\sigma} + \tilde{\delta} + \tilde{\beta} + b_1 + b_2 &= 1 \\ -\tilde{\sigma} + \tilde{\beta} + b_1 c_1 + b_2 c_2 &= 0 \\ \tilde{\sigma} + \tilde{\beta} + b_1 c_1^2 + b_2 c_2^2 &= \frac{1}{6} \\ -\tilde{\sigma} + \tilde{\beta} + b_1 c_1^3 + b_2 c_2^3 &= 0.\end{aligned}$$

Condition $C(2)$ holds if and only if

$$\delta_1 + \beta_1 + \sigma_1 + a_{11} + a_{12} = \frac{c_1^2 + c_1 - 2\theta_1}{2}$$

and

$$\delta_2 + \beta_2 + \sigma_2 + a_{21} + a_{22} = \frac{c_2^2 + c_2 - 2\theta_2}{2}$$

The requirement $\Psi([[.]]) = 1$ implies

$$b_1(-\sigma_1 + \beta_1 + (a_{11}c_1 + a_{12}c_2)) + b_2(-\sigma_2 + \beta_2 + (a_{21}c_1 + a_{22}c_2)) = 0$$

since it is already assumed that

$$-\tilde{\sigma} + \tilde{\beta} + b_1c_1 + b_2c_2 = 0.$$

Since

$$M = \begin{bmatrix} a_{11} + \theta_1 b_1 & a_{12} + \theta_1 b_1 & \beta_1 + \theta_1 \tilde{\beta} \\ a_{21} + \theta_2 b_1 & a_{22} + \theta_2 b_2 & \beta_2 + \theta_2 \tilde{\beta} \\ b_1 & b_2 & \tilde{\beta} \end{bmatrix}$$

M is lower triangular if and only if

$$a_{12} + \theta_1 b_1 = 0$$

$$\beta_1 + \theta_1 \tilde{\beta} = 0$$

$$\beta_2 + \theta_2 \tilde{\beta} = 0.$$

The compatibility conditions imply

$$\alpha_i = \theta_i - c_i \quad \text{and} \quad \gamma_i = 1 - 2\theta_i + c_i \quad i = 1, 2.$$

If $\tilde{\sigma} = \tilde{\beta}$, $c_1 = -c_2$, $b_1 = b_2$, $\sigma_1 + \sigma_2 = \beta_1 + \beta_2$ and $a_{11} - a_{12} = a_{22} - a_{21}$ then the second and fourth equations of the B condition hold and $\Psi([[.]]) = 1$ is also true.

By the same calculations done in Chapter 3 we obtain

$$\begin{aligned} & 1 + z^2 b^T (I + z^2 A)^{-1} (\vec{\theta} - z^2 \vec{\beta}) + \tilde{\beta} z^2 \\ &= 1 + z^2 b^T (I + z^2 A)^{-1} (\vec{\alpha} - z^2 \vec{\sigma}) + \tilde{\sigma} z^2. \end{aligned} \tag{4.6}$$

Since (4.6) holds, by the same argument used in Chapter 3 the roots of the stability polynomial (4.5) have modulus less than or equal to one if and only if

$$|R(z)| = \left| \frac{P(z)}{Q(z)} \right| = \left| \frac{-\frac{1}{2}(-2 + z^2 b^T (I + z^2 A)^{-1} (\vec{\gamma} - z^2 \vec{\delta}) + \tilde{\delta} z^2)}{(1 + z^2 b^T (I + z^2 A)^{-1} (\vec{\theta} - z^2 \vec{\beta}) + \tilde{\beta} z^2)} \right| \leq 1.$$

Now

$$(I + z^2 A)^{-1} = \frac{\begin{bmatrix} 1 + z^2 a_{22} & -z^2 a_{12} \\ -z^2 a_{21} & 1 + z^2 a_{11} \end{bmatrix}}{(1 + (a_{11} + a_{22})z^2 + (a_{11}a_{22} - a_{12}a_{21})z^4)}$$

so for any vector $\vec{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$

$$[1, 1] (I + z^2 A)^{-1} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \frac{(1 + z^2(a_{11} - a_{12})) (x_1 + x_2)}{1 + (a_{11} + a_{22})z^2 + (a_{11}a_{22} - a_{12}a_{21})z^4}$$

since $a_{11} - a_{12} = a_{22} - a_{21}$.

Therefore

$$\begin{aligned} & \frac{1}{2}(-2 + z^2 b^T (I + z^2 A)^{-1} (\vec{\gamma} - z^2 \vec{\delta}) + \tilde{\delta} z^2) \\ &= -1 + \frac{\frac{z^2}{2} b_1 (1 + (a_{11} - a_{12})z^2)(\gamma_1 + \gamma_2 - (\delta_1 + \delta_2)z^2)}{1 + (a_{11} + a_{22})z^2 + (a_{11}a_{22} - a_{12}a_{21})z^4} + \frac{\tilde{\delta}}{2} z^2 \\ &= \{(-1 + \frac{\tilde{\delta}}{2} z^2)(1 + (a_{11} + a_{22})z^2 + (a_{11}a_{22} - a_{12}a_{21})z^4)\} \\ &+ \frac{b_1}{2} z^2 (1 + (a_{11} - a_{12})z^2)(\gamma_1 + \gamma_2 - (\delta_1 + \delta_2)z^2) \\ &\quad \times \left(\frac{1}{1 + (a_{11} + a_{22})z^2 + (a_{11}a_{22} - a_{12}a_{21})z^4} \right). \end{aligned}$$

As in Chapter 3, since $a_{11} - a_{12} = a_{22} - a_{21}$ the following equations hold

$$a_{11} + a_{22} = (a_{11} - a_{12}) + (a_{11} + a_{21})$$

and

$$a_{11}a_{22} - a_{12}a_{21} = (a_{11} + a_{21})(a_{11} - a_{12})$$

and

$$a_{11} + a_{12} + a_{21} + a_{22} = 2(a_{11} + a_{21}) .$$

By compatibility, $\gamma_1 + \gamma_2 = 2 - 2(\theta_1 + \theta_2)$. The condition B(5) holding implies

$$\tilde{\delta} = 1 - 2b_1 - 2\tilde{\beta} .$$

Since M is lower triangular

$$\beta_1 + \beta_2 = -\tilde{\beta}(\theta_1 + \theta_2) .$$

Since $\sigma_1 + \sigma_2 = \beta_1 + \beta_2$, the C(2) condition implies

$$\begin{aligned} \delta_1 + \delta_2 &= -2(\beta_1 + \beta_2) - (a_{11} + a_{12} + a_{21} + a_{22}) + c_1^2 - (\theta_1 + \theta_2) \\ &= 2\tilde{\beta}(\theta_1 + \theta_2) - 2(a_{11} + a_{21}) + c_1^2 - (\theta_1 + \theta_2) . \end{aligned}$$

Using these results we obtain

$$\begin{aligned} &\frac{1}{2}(-2 + z^2 b^T(I + z^2 A)^{-1}(\vec{\gamma} - z^2 \vec{\delta}) + \tilde{\delta} z^2) \\ &= \{(-1 + (\frac{1}{2} - b_1 - \tilde{\beta})z^2) \times \\ &\quad [1 + ((a_{11} - a_{12}) + (a_{11} + a_{21}))z^2 + (a_{11} - a_{12})(a_{11} + a_{21})z^4] \\ &\quad + \frac{z^2 b_1}{2}(1 + (a_{11} - a_{12})z^2) [2 - 2(\theta_1 + \theta_2) - (2\tilde{\beta}(\theta_1 + \theta_2) - 2(a_{11} + a_{21}) \\ &\quad + c_1^2 - (\theta_1 + \theta_2))z^2]\} \\ &\quad \times \left(\frac{1}{1 + ((a_{11} + a_{21}) + (a_{11} - a_{12}))z^2 + (a_{11} - a_{12})(a_{11} + a_{21})z^4} \right) . \end{aligned}$$

Factoring yields

$$\begin{aligned}
& \frac{1}{2} \{-2 + z^2 b^T (I + z^2 A)^{-1} (\vec{\gamma} - z^2 \vec{\delta}) + \tilde{\delta} z^2\} \\
&= [1 + (a_{11} - a_{12})z^2] \left\{ \left[-1 + \left(\frac{1}{2} - b_1 - \tilde{\beta} \right) z^2 \right] [1 + (a_{11} + a_{21})z^2] \right. \\
&\quad \left. + z^2 b_1 [1 - (\theta_1 + \theta_2) - \left(\tilde{\beta}(\theta_1 + \theta_2) - (a_{11} + a_{21}) + \frac{c_1^2}{2} - \frac{(\theta_1 + \theta_2)}{2} \right) z^2] \right\} \\
&\quad \times \left(\frac{1}{[1 + (a_{11} - a_{12})z^2][1 + (a_{11} + a_{21})z^2]} \right).
\end{aligned}$$

Doing the same type of calculation again we obtain

$$\begin{aligned}
& 1 + z^2 b^T (I + z^2 A)^{-1} (\vec{\theta} - z^2 \vec{\beta}) + \tilde{\beta} z^2 \\
&= [1 + (a_{11} - a_{12})z^2] \{ [1 + z^2 \tilde{\beta}] [1 + (a_{11} + a_{21})z^2] \\
&\quad + b_1(\theta_1 + \theta_2) z^2 + b_1 \tilde{\beta}(\theta_1 + \theta_2) z^4 \} \left(\frac{1}{[1 + (a_{11} - a_{12})z^2][1 + (a_{11} + a_{21})z^2]} \right).
\end{aligned}$$

Since $R(z) = \frac{P(z)}{Q(z)}$ using the previous calculations we can write $P(z)$ and $Q(z)$ as

$$\begin{aligned}
Q(z) &= (1 + (a_{11} - a_{12})z^2) \{ [1 + \tilde{\beta} z^2] [1 + (a_{11} + a_{21})z^2] \\
&\quad + b_1(\theta_1 + \theta_2) z^2 + b_1 \tilde{\beta}(\theta_1 + \theta_2) z^4 \} \\
P(z) &= (1 + (a_{11} - a_{12})z^2) \left(1 + \left(-\frac{1}{2} + b_1 + \tilde{\beta} \right) z^2 \right) (1 + (a_{11} + a_{21})z^2) \\
&\quad - z^2 b_1 (1 - (\theta_1 + \theta_2)) + z^4 b_1 (\tilde{\beta}(\theta_1 + \theta_2) \\
&\quad - (a_{11} + a_{21}) + \frac{c_1^2}{2} - \frac{\theta_1 + \theta_2}{2}) \\
&= Q(z) - (1 + (a_{11} - a_{12})z^2) \left(\left(\frac{1}{2} - b_1 \right) z^2 (1 + (a_{11} + a_{21})z^2) \right. \\
&\quad \left. + z^2 b_1 - z^4 b_1 \left(-(a_{11} + a_{21}) + \frac{c_1^2}{2} - \frac{(\theta_1 + \theta_2)}{2} \right) \right) \\
&= Q(z) - [1 + (a_{11} - a_{12})z^2] z^2 \left\{ \left(\frac{1}{2} - b_1 \right) + \left(\frac{1}{2} - b_1 \right) (a_{11} + a_{21}) z^2 \right\}
\end{aligned}$$

$$\begin{aligned}
& + b_1 - b_1[-(a_{11} + a_{21}) + \frac{c_1^2}{2} - \frac{\theta_1 + \theta_2}{2}]z^2\} \\
& = Q(z) - (1 + (a_{11} - a_{12})z^2)z^2 \\
& \quad \times \left\{ \frac{1}{2} + \left[\frac{a_{11} + a_{21}}{2} - \frac{b_1 c_1^2}{2} + \frac{b_1(\theta_1 + \theta_2)}{2} \right] z^2 \right\}.
\end{aligned}$$

Therefore

$$\begin{aligned}
R(z) &= \frac{P(z)}{Q(z)} \\
&= \frac{Q(z) - \frac{1}{2}(1 + (a_{11} - a_{12})z^2)z^2\{1 + [(a_{11} + a_{21}) - b_1 c_1^2 + b_1(\theta_1 + \theta_2)]z^2\}}{Q(z)} \\
&= 1 - \frac{\frac{1}{2}z^2[1 + ((a_{11} + a_{21}) - b_1 c_1^2 + b_1(\theta_1 + \theta_2))z^2]}{(1 + \tilde{\beta}z^2)[1 + (a_{11} + a_{21})z^2 + b_1(\theta_1 + \theta_2)z^2]} \\
&= 1 - \frac{\frac{1}{2}z^2\{1 + [(a_{11} + a_{21}) - b_1 c_1^2 + b_1(\theta_1 + \theta_2)]z^2\}}{(1 + \tilde{\beta}z^2)(1 + [(a_{11} + a_{21}) + b_1(\theta_1 + \theta_2)]z^2)}.
\end{aligned}$$

If $\tilde{\beta} > 0$ and $(a_{11} + a_{21}) + b_1(\theta_1 + \theta_2) > 0$ then $(1 + \tilde{\beta}z^2)$ and $(1 + ((a_{11} + a_{21}) + b_1(\theta_1 + \theta_2))z^2) > 0$ for all real z . Under these conditions

$$\begin{aligned}
R(z) &\leq 1 \\
&\Leftrightarrow 1 - \frac{\frac{1}{2}z^2\{1 + [(a_{11} + a_{21}) + b_1(\theta_1 + \theta_2) - b_1 c_1^2]z^2\}}{(1 + \tilde{\beta}z^2)\{1 + [(a_{11} + a_{21}) + b_1(\theta_1 + \theta_2)]z^2\}} \leq 1 \\
&\Leftrightarrow -\frac{1}{2}z^2\{1 + [(a_{11} + a_{21}) + b_1(\theta_1 + \theta_2) - b_1 c_1^2]z^2\} \leq 0 \\
&\Leftrightarrow 1 + [(a_{11} + a_{21}) + b_1(\theta_1 + \theta_2) - b_1 c_1^2]z^2 \geq 0.
\end{aligned}$$

This last inequality holds for all real z if and only if

$$(a_{11} + a_{21}) + b_1(\theta_1 + \theta_2) - b_1 c_1^2 \geq 0.$$

$$\begin{aligned}
& -1 \leq R(z) \quad \text{also holds for all real } z \\
& \Leftrightarrow -1 \leq 1 - \frac{\frac{1}{2}z^2(1 + [(a_{11} + a_{21}) + b_1(\theta_1 + \theta_2) - b_1c_1^2]z^2)}{(1 + z^2\tilde{\beta})\{1 + [(a_{11} + a_{21}) + b_1(\theta_1 + \theta_2)]z^2\}} \\
& \Leftrightarrow -2 \leq \frac{-\frac{1}{2}z^2\{1 + [(a_{11} + a_{21}) + b_1(\theta_1 + \theta_2) - b_1c_1^2]z^2\}}{(1 + z^2\tilde{\beta})\{1 + [(a_{11} + a_{21}) + b_1(\theta_1 + \theta_2)]z^2\}} \\
& \Leftrightarrow 4(1 + z^2\tilde{\beta})(1 + [(a_{11} + a_{21}) + b_1(\theta_1 + \theta_2)]z^2) \\
& \quad \geq z^2\{1 + [a_{11} + a_{21}) + b_1(\theta_1 + \theta_2) - b_1c_1^2]z^2\} \\
& \Leftrightarrow 4 + 4(\tilde{\beta} + (a_{11} + a_{21}) + b_1(\theta_1 + \theta_2))z^2 \\
& \quad + 4\tilde{\beta}((a_{11} + a_{21}) + b_1(\theta_1 + \theta_2))z^4 \\
& \quad \geq z^2 + ((a_{11} + a_{21}) + b_1(\theta_1 + \theta_2) - b_1c_1^2)z^4 \\
& \Leftrightarrow 4 + (4[\tilde{\beta} + (a_{11} + a_{21}) + b_1(\theta_1 + \theta_2)] - 1)z^2 \\
& \quad + 4(\tilde{\beta}[(a_{11} + a_{21}) + b_1(\theta_1 + \theta_2)] - (a_{11} + a_{21}) - b_1(\theta_1 + \theta_2) + b_1c_1^2)z^4 > 0.
\end{aligned}$$

This last inequality is true for all real z if

$$\tilde{\beta} + (a_{11} + a_{21}) + b_1(\theta_1 + \theta_2) \geq \frac{1}{4}$$

and if

$$(4\tilde{\beta} - 1)((a_{11} + a_{21}) + b_1(\theta_1 + \theta_2)) + b_1c_1^2 \geq 0$$

Therefore if the parameters $a_{11} + a_{21}$, $\theta_1 + \theta_2$, c_1 , b_1 obey the following inequalities

$$\tilde{\beta} \geq 0$$

$$a_{11} + a_{21} + b_1(\theta_1 + \theta_2) \geq 0$$

$$(a_{11} + a_{21}) + b_1(\theta_1 + \theta_2) - b_1c_1^2 \geq \frac{1}{6}$$

$$\tilde{\beta} + (a_{11} + a_{21}) + b_1(\theta_1 + \theta_2) \geq \frac{1}{4}$$

and

$$(4\tilde{\beta} - 1)[(a_{11} + a_{21}) + b_1(\theta_1 + \theta_2)] + b_1c_1^2 \geq 0$$

where

$$\tilde{\beta} = \frac{1}{12} - b_1c_1^2$$

then the method is unconditionally stable.

One set of choices of parameters that obey the above inequalities is the following:

$$a_{11} + a_{21} = 1$$

$$\theta_1 + \theta_2 = \frac{1}{3}$$

$$c_1 = \frac{1}{\sqrt{2}}$$

$$b_1 = \frac{-1}{2}$$

With these choices

$$\tilde{\beta} = \frac{1}{12} - b_1c_1^2 = \frac{1}{12} - \frac{-1}{2} \cdot \frac{1}{2} = \frac{1}{3}$$

and the rational function $R(z)$ will be

$$\begin{aligned} R(z) &= 1 - \frac{\frac{1}{2}z^2[1 + (1 - \frac{1}{6} + \frac{1}{4})z^2]}{(1 + \frac{1}{3}z^2)(1 + (1 - \frac{1}{6})z^2)} \\ &= \frac{1 + \frac{4}{6}z^2 - \frac{19}{72}z^4}{1 + \frac{7}{6}z^2 + \frac{20}{72}z^4} \end{aligned}$$

So with these choices $|R(z)| \leq 1 \quad \forall z \in \mathbf{IR}$; therefore the method is unconditionally stable.

Therefore the following method will be unconditionally stable, have order 4 and have an implementation matrix M that is lower triangular with distinct entries on

the diagonal

$$\begin{aligned}
y^{n,1} &= \left(\frac{1}{3} - \frac{1}{\sqrt{2}}\right)y^{n-1} + \left(\frac{1}{3} + \frac{1}{\sqrt{2}}\right)y^n + \left(\frac{1}{3}\right)y^{n+1} \\
&\quad + h^2\left(\left(\frac{1}{2\sqrt{2}} - \frac{8}{9}\right)f^n - \frac{1}{9}f^{n+1} + \frac{3}{4}f^{n,1} + \frac{1}{6}f^{n,2}\right) \\
y^{n,2} &= \left(\frac{1}{\sqrt{2}}\right)y^{n-1} + \left(1 - \frac{1}{\sqrt{2}}\right)y^n \\
&\quad + h^2\left(-\frac{1}{9}f^{n-1} + \left(-\frac{1}{2\sqrt{2}} - \frac{13}{18}\right)f^n + \frac{1}{4}f^{n,1} + \frac{5}{6}f^{n,2}\right) \\
y^{n+1} &= -y^{n-1} + 2y^n + h^2\left(-\frac{1}{2}(f^{n,1} + f^{n,2}) + \frac{1}{3}(f^{n-1} + f^{n+1}) + \frac{4}{3}f^n\right).
\end{aligned} \tag{4.7}$$

We note that the order of dispersion of this scheme is also 4; we assert, without presenting here the proof, that it is not possible to elevate this order of dispersion to 6 while maintaining lower triangularity of M and unconditional stability.

§ 4.2 Conclusions.

We have provided a tree based framework for analyzing a broad class of numerical methods for second-order initial value problems. We have established a set of relationships among the parameters of the methods which aid in the determination of order. These relationships have been used in a positive sense to discover specific families of methods; they also serve to establish limitations on the possible order of methods with a given number of stages. In conjunction, the matter of unconditional stability has been weighed against attainable order. We intend to continue to pursue such theoretical connections.

We have suggested some classes of methods for which further study is possible. The eighth-order family in Chapter 3 is only conditionally stable. Nevertheless, with the freedom to choose its parameters, without effecting the stability limit we perceive the possibility of using them to find some easily implemented schemes or,

perhaps, schemes for which certain dominant terms in the local truncation error are eliminated. Likewise, for the fourth-order unconditionally stable schemes of this chapter, there may be other solutions which accomplish some specific goal with respect to local truncation error. Further, a comparison with methods which can be decoupled by similarity transformation is indicated.

Indeed, our framework will allow the analysis of other methods with more stages, not yet considered. One possible avenue, with parallel processing a goal, would be to increase s , but to attempt to find the parameters so that the implementation matrix is block diagonal, with blocks of at most size 2. In that case, each processor would effectively be working on a system like that which a method with just one internal stage produces.

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