Collocation methods for a class of second order initial value problems with oscillatory solutions

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Collocation Methods For A Class Of Second Order Initial Value Problems With Oscillatory Solutions

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Abstract

We derive and analyse two families of multistep collocation methods for periodic initial-value problems of the form

$$y'' = f(x, y); \quad y(x_0) = y_0, \quad y'(x_0) = z_0$$

involving ordinary differential equations of second order in which the first derivative does not appear explicitly.

A survey of recent results and proposed numerical methods is given in chapter 2. Chapter 3 is devoted to the analysis of a family of implicit Chebyshev methods proposed by Panovsky & Richardson. We show that for each non-negative integer r, there are two methods of order $2r$ from this family which possess non-vanishing intervals of periodicity. The equivalence of these methods with one-step collocation methods is also established, and these methods are shown to be neither P-stable nor symplectic.

In chapters 4 and 5, two families of multistep collocation methods are derived, and their order and stability properties are investigated. A detailed analysis of the two-step symmetric methods from each class is also given. The multistep Runge-Kutta-Nyström methods of chapter 4 are found to be difficult to analyse, and the specific examples considered are found to perform poorly in the areas of both accuracy and stability. By contrast, the two-step symmetric hybrid methods of chapter 5 are shown to have excellent stability properties, in particular we show that all two-step $2N$-point methods of this type possess non-vanishing intervals of periodicity, and we

give conditions under which these methods are almost P-stable. P-stable and efficient methods from this family are obtained and demonstrated in numerical experiments. A simple, cheap and effective error estimator for these methods is also given.

Acknowledgement

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Statement of originality

The work of chapters 4 and 5 is entirely my own. Chapter 3 contains the results of work undertaken by myself and my supervisor, in particular the work in sections 3.6-3.8 is my own.

No part of the material offered has been presented for any other degree in any other university.

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Chapter 1

Introduction

In recent years there has been considerable interest in direct methods for the numerical solution of initial-value problems of the form

$$y'' = f(x, y); \quad y(x_0) = y_0, \quad y'(x_0) = z_0 \tag{1.1}$$

involving ordinary differential equations of second order in which the first derivative does not appear explicitly. In this thesis we are concerned with problems of the form (1.1) whose solutions are oscillatory in nature. Such problems arise in a wide variety of physical applications including celestial mechanics and quantum scattering.

A survey of the numerical methods now available to solve problems of the form (1.1) can be found in chapter 2, along with a discussion of some of the concepts, such as periodicity, which have been introduced in order to give a deeper understanding of the behaviour of numerical solutions generated by these methods.

Chapter 3 is devoted to the analysis of a family of implicit Chebyshev methods for (1.1) proposed by Panovsky & Richardson [53]. In the first half of that chapter we show that these methods may be written as two-step hybrid methods, and we go on to derive results regarding their order and stability properties. In particular we show that for each non-negative integer r, there are two methods of order $2r$ from this family which possess non-vanishing intervals of periodicity. In the second half

of the chapter, the equivalence of the Panovsky-Richardson and one-step collocation methods is established. With the aid of this equivalence we are able to show that these methods are neither P-stable nor symplectic.

Aspects of one-step collocation methods for (1.1) have recently been investigated by a number of authors. In particular, Coleman [22] has shown that none of these methods is P-Stable. In an attempt to overcome this problem we have derived two new classes of multistep collocation methods for (1.1).

The methods from the first of these classes are natural generalisations of the collocation-based Runge-Kutta-Nyström methods. Each of these methods is based on a polynomial which interpolates to y and y' at the previous step-points $\{x_{n-k+1}, \ldots, x_n\}$ ($k \geq 2$) and which satisfies the differential equation under consideration at the points $\{x_{n+c_i}\}_{i=1}^{m}$ contained within $[x_{n-k+1}, x_{n+1}]$. The analysis of these methods turns out to be particularly complex in all but the simplest cases, and so in order to derive some meaningful results we concentrate on the two-step methods whose nodes are symmetrically distributed in the interval $[x_{n-1}, x_{n+1}]$. Examples of specific methods and numerical results comparing them with the Panovsky-Richardson methods are also given.

Methods from the second class differ from those mentioned above in that they, like the hybrid methods and the differential equations with which we are concerned here, contain no explicit derivative information. The construction of these methods is seen to be considerably simpler than that for the previous methods, as are the conditions under which these methods are defined. The lack of explicit derivative information does present some difficulties when investigating the order of these methods, and consequently we are forced to resort to arguments based on Taylor analysis. The most attractive feature of these methods is their stability properties. In particular we show that, for the examples considered, the conditions under which a two-step $2N$-point method from this family is almost P-stable are far less restrictive than those necessary to guarantee that a similar method from the previous class has a non-vanishing interval of periodicity. A simple and inexpensive local truncation error

estimator is also given, and its effectiveness is demonstrated for a number of test problems. Examples of P-stable methods and a sixth order method with order of dispersion eight are also given.

Chapter 2

The story so far ...

Recent years have seen a considerable increase in the number of authors researching into numerical methods for initial value problems of the form

$$y'' = f(x, y); \quad y(x_0) = y_0, \quad y'(x_0) = z_0, \tag{2.1}$$

involving second order differential equations in which the first derivative does not appear explicitly, and in particular, those problems (2.1) whose solutions are oscillatory in nature. In this chapter we give a brief account of the methods available and of the concepts, such as periodicity, which have been introduced in order to give us a deeper understanding of the behaviour of numerical solutions produced by these methods. In section 2.1 we look at the oldest of the classes of methods considered here, the linear multistep methods. Section 2.2 is concerned with one-step methods, including collocation methods. Finally, in section 2.3, we look at the newest class of methods, the hybrid methods, which combine features of the methods discussed in the previous sections.

2.1 Linear multistep methods

In this section we look at linear multistep methods for (2.1). We begin by looking at how such methods may be derived, and then move on to considerations of accuracy, stability, periodicity and dispersion.

Let $x_r = x_0 + rh$, for $h > 0$ and $r \in \mathbb{R}$, and let y_r and z_r denote numerical approximations to the exact solution of the differential equation under consideration, and its derivative, at the point x_r. A linear k-step method for (2.1) is a method of the form

$$\sum_{i=0}^{k} \alpha_i y_{n+i} = h^2 \sum_{i=0}^{k} \beta_i f_{n+i} \tag{2.2}$$

where $f_r = f(x_r, y_r)$. Throughout this section we will assume that the numbers $\{\alpha_i, \beta_i\}_{i=0}^{k}$ satisfy the conditions

$$\alpha_k = 1; \quad |\alpha_0| + |\beta_0| > 0 \quad \text{and} \quad \sum_{i=0}^{k} |\beta_i| > 0, \tag{2.3}$$

which simply ensure that the method (2.2) does not degenerate.

A common procedure for deriving linear multistep methods (2.2) has as its starting point the identity

$$y(x+\delta) - y(x) = \delta y'(x) + \int_x^{x+\delta} (x + \delta - \tau) y''(\tau) d\tau. \tag{2.4}$$

The first derivative term can be made to vanish by combining this formula with the formula obtained by replacing δ by $-\delta$, giving

$$y(x+\delta) - 2y(x) + y(x-\delta) = \int_x^{x+\delta} (x + \delta - \tau)(y''(\tau) + y''(2x - \tau)) d\tau. \tag{2.5}$$

Individual methods are now obtained by replacing y'' in the above integral by a polynomial interpolating to y'' at previous step points, and by choosing x and δ appropriately. A notable example of methods derived in this way is the family of Störmer-Cowell methods (see Henrici [38] p291), which takes its name from the work

of Störmer in 1907 and Cowell & Crommelin in 1910. These methods have remained popular and have been used successfully in a wide range of applications for a great many years. For example, with $k = 2$ we obtain the explicit method

$$y_{n+1} - 2y_n + y_{n-1} = h^2 f_n$$

and the implicit method

$$y_{n+1} - 2y_n + y_{n-1} = \frac{h^2}{12}(f_{n+1} + 10f_n + f_{n-1}) \tag{2.6}$$

which is attributed to Numerov.

Other linear multistep methods have been derived by choosing the numbers $\{\alpha_i, \beta_i\}_{i=0}^{k}$ so as to satisfy certain order and stability conditions.

2.1.1 Order and stability

Following Henrici [38] p295, we associate with each method of the form (2.2) the linear functional

$$\mathcal{L}[y(x), h] = \sum_{i=0}^{k} \alpha_i y(x + ih) - h^2 \sum_{i=0}^{k} \beta_i y''(x + ih). \tag{2.7}$$

This functional can act on any function $y(x)$ which possesses a second derivative, but in what follows we will assume that $y(x)$ will be as differentiable as we please. By expanding the terms $y(x + ih)$ and $y''(x + ih)$ as Taylor series about the point x we may write

$$\mathcal{L}[y(x), h] = C_0 y(x) + C_1 y'(x) + C_2 y''(x) + \ldots + C_r y^{(r)}(x) + \ldots \tag{2.8}$$

where the C_r are constants.

Definition 2.1 *A linear multistep method (2.2) is said to be of* **order p** *if, for all sufficiently differentiable functions $y(x)$, we have*

$$\mathcal{L}[y(x), h] = O(h^{p+2})$$

The method is said to be **consistent** *if it has order at least 1.*

With each linear multistep method (2.2) we associate the polynomials $\rho(\xi)$ and $\sigma(\xi)$ defined as follows:

$$\rho(\xi) = \sum_{i=0}^{k} \alpha_i \xi^i, \quad \sigma(\xi) = \sum_{i=0}^{k} \beta_i \xi^i. \tag{2.9}$$

For the methods considered in this section it will be assumed that $\rho(\xi)$ and $\sigma(\xi)$ have no common factors. In what follows we shall refer to (2.2) as the method (ρ, σ). We may now write the conditions for the method (ρ, σ) to be consistent in terms of these polynomials, giving

$$\rho(1) = \rho'(1) = 0 \quad \text{and} \quad \rho''(1) = 2\sigma(1) \tag{2.10}$$

We will assume that all methods considered in this section satisfy these conditions and so are consistent. The roots of $\rho(\xi)$ we denote by ξ_i, for $i = 1, \ldots, k$, where $\xi_1 = \xi_2 = 1$ are called the *principal roots*, and ξ_i, for $i = 3, \ldots, k$ are called *spurious roots.*

Definition 2.2 *The method (ρ, σ) is said to be* **zero stable** *if all roots of $\rho(\xi)$ lie in the unit disc $\{z \in \mathbb{C} : |z| \leq 1\}$, and any roots that lie on the unit circle $\{z \in \mathbb{C} : |z| = 1\}$ have multiplicity at most 2.*

It can be shown (e.g. Henrici [38] pp300-303) that consistency and zero stability are necessary and sufficient conditions for the method (ρ, σ) to be convergent. Since we have $2k + 2$ parameters in the method (ρ, σ) we might hope that its order could be raised to $2k$. However this is not possible if in addition we require the method to

be zero stable. The maximum order of a zero stable k-step method turns out to be $k+2$ if k is even, and $k+1$ if k is odd. Henrici [38] p311 gives examples of optimal order methods with $k = 2$,4 and 6.

When the method (ρ, σ) is applied to the scalar linear test equation

$$y'' = -\omega^2 y \tag{2.11}$$

we obtain the recurrence relation

$$\sum_{i=0}^{k} (\alpha_i + \nu^2 \beta_i) y_{n+i} = 0,$$

where $\nu = \omega h$, whose characteristic equation is

$$\pi(\xi, \nu^2) = \rho(\xi) + \nu^2 \sigma(\xi) = 0. \tag{2.12}$$

This polynomial $\pi(\xi, \nu^2)$ has roots r_i, for $i = 1, \ldots, k$, which are perturbations of the roots ξ_i of $\rho(\xi)$.

Definition 2.3 *A linear multistep method (ρ, σ) is said to be* **absolutely stable** *for $\nu^2 = \nu_0^2$ if all roots of $\pi(\xi, \nu^2)$ lie in the unit disc, and any roots that lie on the unit circle have multiplicity no greater than 2. A method is said to have an* **interval of absolute stability** *$(0, \beta^2)$ if it is absolutely stable for each $\nu^2 \in (0, \beta^2)$. If a method is absolutely stable for all positive values of ν^2 then it is said to be* **unconditionally stable** *(Dahlquist [26]).*

The investigation of the stability properties of a method can be simplified with the aid of the Routh-Hurwitz transformation (Lambert [45] p80)

$$\xi = \frac{1+z}{1-z},$$

which maps the unit disc onto the half-plane Re $z \leq 0$, and the unit circle onto the imaginary axis. Applying this transformation to equation (2.12) and multiplying

throughout by $(1-z)^k$ we obtain the polynomial equation

$$a_0 z^k + a_1 z^{k-1} + \ldots + a_{k-1} z + a_k = 0. \tag{2.13}$$

Then, for example, with $k = 2$, the necessary and sufficient conditions for the roots of (2.12) to have modulus less than 1, i.e. for the roots of (2.13) to have negative real parts, are that a_0, a_1 and a_2 be positive.

2.1.2 Periodicity and dispersion

Consider the scalar test equation (2.11). With x interpreted as time, this equation represents motion in a circular orbit in the complex plane. If Numerov's method is applied to this problem with a sufficiently small steplength, then the computed numerical solution stays on the orbit, though it does suffer an error in phase. However if a Störmer-Cowell method with $k > 2$ is used, then the numerical solution spirals inwards. Stiefel & Bettis [58] call these phenomena *orbital stability* and *orbital instability* respectively.

The investigation of these phenomena was continued by Lambert & Watson [46]. In that paper they introduce the notions of periodicity and P-stability, and give necessary and sufficient conditions under which a method (ρ, σ) is periodic for ν^2 sufficiently small. The following definitions and results are taken from that paper.

Definition 2.4 *The method (ρ, σ) is said to have an* **interval of periodicity** $(0, \beta^2)$ *if for all $\nu^2 \in (0, \beta^2)$, the roots r_i of $\pi(\xi, \nu^2)$ satisfy*

$$r_1 = e^{i\theta(\nu)}, \quad r_2 = e^{-i\theta(\nu)}, \quad |r_i| \leq 1, \text{ for } i = 3, \ldots, k$$

Theorem 2.1 *Let the method (ρ, σ) have a non-empty interval of periodicity. Then (ρ, σ) is a symmetric method, i.e.*

$$\alpha_i = \alpha_{k-i} \quad \text{and} \quad \beta_i = \beta_{k-i}, \quad \text{for } i = 0, \ldots, k$$

In particular, this means that the Störmer-Cowell methods with $k > 2$ possess no intervals of periodicity, since they are not symmetric.

Theorem 2.2 *Let the method (ρ, σ) be symmetric, and let $\rho(\xi)$ have no double roots on the unit circle other than the principal roots ξ_1 and ξ_2. Then (ρ, σ) has a non-vanishing interval of periodicity.*

Definition 2.5 *A method (ρ, σ) is said to be* **P-stable** *if its interval of periodicity is $(0, \infty)$.*

Theorem 2.3 *Let (ρ, σ) be a P-stable method. Then (i) (ρ, σ) is implicit, (ii) all roots of $\sigma(\xi)$ lie on the unit circle, and (iii) the order of (ρ, σ) is at most 2.*

Dahlquist [26] further showed that the order of an unconditionally stable method cannot exceed 2.

Lambert & Watson [46] give examples of methods of orders up to 8 which possess non-empty intervals of periodicity, higher order methods were derived by Quinlan & Tremaine [54]. Jeltsch [42] uses the *growth parameters* $\mu_i = 2\sigma(\xi_i)/\xi_i^2\rho''(\xi_i)$ associated with each root of $\pi(\xi, \nu^2)$ of modulus 1 to provide a complete characterisation of linear multistep methods with an a non-empty interval of periodicity.

Definition 2.6 *(van der Houwen & Sommeijer [65]) Assuming that the principal roots of $\pi(\xi, \nu^2)$ are of the form*

$$\xi_1 = a(\nu)e^{i\theta(\nu)} and \quad \xi_2 = a(\nu)e^{-i\theta(\nu)}$$

with $a, \theta > 0$, then the quantities

$$1 - a(\nu) \quad and \quad |\theta(\nu) - \nu|$$

are respectively called the **dissipation error** *and* **phase error**. *A linear multistep method is said to have* **order of dispersion** *q if $|\theta(\nu) - \nu| = O(\nu^{q+1})$ as $\nu^2 \to 0$.*

(Note: we have altered the original definition of the phase error in order to make it consistent with the rest of this thesis.)

Observe that if the method (ρ, σ) is periodic then it has zero dissipation error. Van der Houwen & Sommeijer [65] have constructed predictor-corrector methods of algebraic orders 4 and 6, and orders of dispersion of up to 10, which possess non-empty intervals of periodicity.

2.1.3 Rounding error

Henrici [38] p327 shows that convergent linear multistep methods for (2.1) are more sensitive to the build-up of rounding errors than the corresponding methods for first order equations. The main reason for this is that for very small h, the double root $\xi_{1,2} = 1$ of ρ causes the recurrence relation (2.2) to become unstable. To overcome this difficulty, Henrici presents an alternative formulation of (2.2) which he called the *summed form*, obtained, as its name suggests, by summing (2.2) for $n = 0, 1, \ldots, N$. The resulting method then takes the form of a one-step method, and the problem of the double root at 1 is removed. Hairer et al. [35] p425 discuss a further reformulation of (2.1) which proceeds by factorising the polynomial $\rho(\xi)$ in order to separate the roots at 1. For example, the method

$$y_{n+1} - 2y_n + y_{n-1} = h^2 f_n$$

can be reformulated as

$$\begin{aligned} w_{n+1} &= w_n + h f_n \\ y_{n+1} &= y_n + h w_{n+1} \end{aligned}$$

We shall return to the subject of rounding error in section 3.10.

2.2 One-step methods

The most important class of one-step methods is that of the Runge-Kutta-Nyström methods. As in the previous section we begin by showing how these methods were first derived, and by defining the concepts of order and stability. With these definitions under our belt we give a brief account of the way in which research into these methods has progressed over the years. Section 2.2.4 is concerned with the one-step collocation methods, which are a sub-class of the implicit Runge-Kutta-Nyström methods.

2.2.1 The first Runge-Kutta-Nyström methods

The first RKN methods were derived with the purpose of reducing the computational costs involved in numerically solving the general second order differential equation

$$y'' = f(x, y, y'); \quad y(x_0) = y_0,\ y'(x_0) = z_0 \tag{2.14}$$

by attacking it directly, rather than first splitting it into a higher dimensional system of coupled first order differential equations and then applying a conventional Runge-Kutta or linear multistep method.

To begin with we suppose that (2.14) has been split into the pair of coupled first order equations

$$\begin{pmatrix} y \\ z \end{pmatrix}' = \begin{pmatrix} z \\ f(x, y, z) \end{pmatrix} \quad \begin{matrix} y(x_0) = y_0 \\ z(x_0) = z_0. \end{matrix} \tag{2.15}$$

If we now apply a Runge-Kutta method to this problem we obtain

$$\begin{aligned} K_i &= z_n + h\sum_j a_{ij} L_j \\ L_i &= f(x_n + c_i h, y_n + h\sum_j a_{ij} K_j, z_n + h\sum_j a_{ij} L_j) \\ y_{n+1} &= y_n + h\sum_j b_j K_j \\ z_{n+1} &= z_n + h\sum_j b_j L_j \end{aligned}$$

By inserting the first of these formulae into the others we can eliminate the K_i quantities to get

$$\begin{aligned} L_i &= f(x_n + c_i h, y_n + c_i h z_n + h^2 \sum_j \bar{a}_{ij} L_j, z_n + \sum_j a_{ij} L_j) \\ y_{n+1} &= y_n + h z_n + h^2 \sum_j \bar{b}_j L_j \\ z_{n+1} &= z_n + h \sum_j b_j L_j \end{aligned} \tag{2.16}$$

where the constants $\bar{a}_{ij}$ and $\bar{b}_j$ are given by

$$\bar{a}_{ij} = \sum_k a_{ik} a_{kj}, \quad \bar{b}_j = \sum_k b_k a_{kj}. \tag{2.17}$$

In 1925, Nyström proposed the first methods of the form (2.16) whose coefficients violated conditions (2.17), which we now know as Runge-Kutta-Nyström methods. He claimed that his methods were more efficient from a computational point of view than 'the' Runge-Kutta method (see Hairer et al. [35], p137), though this does not appear to be the case. However his methods do have the advantage of a 25%-50% saving in storage requirements over the Runge-Kutta methods applied to the corresponding first order system.

Where Nyström's methods do lead to a very real decrease in computational costs is in the special case when the function f in (2.14) does not depend on y', which is of particular interest to us in this thesis. In this case we may write the RKN method as

$$y_{n+c_i} = y_n + c_i h z_n + h^2 \sum_j B_{ij} f_{n+c_j}, \tag{2.18}$$

$$y_{n+1} = y_n + h z_n + h^2 \sum_j b_j f_{n+c_j} \tag{2.19}$$

$$z_{n+1} = z_n + h \sum_j d_j f_{n+c_j} \tag{2.20}$$

Nyström's methods were explicit, but in the same way as for Runge-Kutta methods we can define implicit methods (the matrix $B = (B_{ij})$ is full), diagonally implicit

methods (the matrix B is lower triangular), etc. In this section we will assume that (2.18)-(2.20) is a fully implicit method with m stages, so that all the summations in those formulae should run from 1 to m.

2.2.2 Order, stability and dispersion

The following definition is taken from Hairer et al. [35] p261:

Definition 2.7 *A Runge-Kutta-Nystrom method (2.18)-(2.20) is said to have* **(algebraic) order** p *if, given that* $y(x_n) = y_n$ *and* $y'(x_n) = z_n$, *the numerical solution* (y_{n+1}, z_{n+1}) *satisfies*

$$\begin{aligned} y(x_{n+1}) - y_{n+1} &= O(h^{p+1}) \\ y'(x_{n+1}) - z_{n+1} &= O(h^{p+1}) \end{aligned}$$

for y *sufficiently smooth.*

As with Runge-Kutta methods, it is possible to identify the order conditions for explicit methods with relatively few stages using a bare-hands Taylor series approach, however this approach is unsuitable for most methods due to the complexity and number of the computations involved. A far more elegant approach has been derived by Hairer and Wanner [36], which is an extension of Butcher's tree-based approach used for Runge-Kutta methods (see e.g. Hairer et al. [35] pp142-153). Using this approach, numerous explicit methods of order 8 have been derived, and Hairer [34] has derived an explicit RKN method of order 10 which requires 35% fewer function evaluations per step than Runge-Kutta methods of the same order. In addition, a number of embedded methods have been derived of orders as high as 11(10) (see e.g. Filipi & Gräf [29]). We will see later that in the case of collocation-based RKN methods the order conditions can be identified by considering a simple interpolatory quadrature problem.

The stability of a Runge-Kutta-Nyström method is investigated by applying it to the standard scalar test problem (2.11). Once again setting $\nu = \omega h$ and applying the

RKN method (2.18)-(2.20) to (2.11) we obtain

$$\mathbf{y}_{n+1} = A(\nu^2)\mathbf{y}_n, \tag{2.21}$$

where $\mathbf{y}_n = (y_n, hz_n)^{\mathrm{T}}$,

$$A(\nu^2) = \begin{pmatrix} 1 - \nu^2\mathbf{b}^{\mathrm{T}}(1+\nu^2 B)^{-1}\mathbf{e} & 1 - \nu^2\mathbf{b}^{\mathrm{T}}(1+\nu^2 B)^{-1}\mathbf{c} \\ -\nu^2\mathbf{d}^{\mathrm{T}}(1+\nu^2 B)^{-1}\mathbf{e} & 1 - \nu^2\mathbf{d}^{\mathrm{T}}(1+\nu^2 B)^{-1}\mathbf{c} \end{pmatrix},$$

$\mathbf{b}^{\mathrm{T}} = (b_1, \ldots, b_m)$, $\mathbf{d}^{\mathrm{T}} = (d_1, \ldots, d_m)$, $\mathbf{c}^{\mathrm{T}} = (c_1, \ldots, c_m)$ and $\mathbf{e}^{\mathrm{T}} = (1, \ldots, 1)$. Let $\lambda_1(\nu^2)$ and $\lambda_2(\nu^2)$ be the eigenvalues of $A(\nu^2)$ with $|\lambda_1(\nu^2)| \geq |\lambda_2(\nu^2)|$, then we adopt the following definitions.

Definition 2.8 *A Runge-Kutta-Nyström method (2.18)-(2.20) is said to be* **absolutely stable** *for $\nu^2 = \nu_0^2$ if the eigenvalues $\lambda_1(\nu_0^2)$ and $\lambda_2(\nu_0^2)$ lie in the closed unit disc $\{z \in \mathbb{C} : |z| \leq 1\}$, and $\lambda_1(\nu_0^2) \neq \lambda_2(\nu_0^2)$ if $|\lambda_1(\nu_0^2)| = 1$. The RKN method is said to have an* **interval of absolute stability** *$(0, \beta^2)$ if it is absolutely stable for all $\nu^2 \in (0, \beta^2)$, and is said to be* **unconditionally stable** *if it is absolutely stable for all $\nu^2 > 0$.*

Definition 2.9 *A Runge-Kutta-Nyström method (2.18)-(2.20) is said to be* **periodic** *for $\nu^2 = \nu_0^2$ if the eigenvalues $\lambda_1(\nu_0^2)$ and $\lambda_2(\nu_0^2)$ lie on the unit circle $\{z \in \mathbb{C} : |z| = 1\}$, and $\lambda_1(\nu_0^2) \neq \lambda_2(\nu_0^2)$. The RKN method is said to have an* **interval of periodicity** *$(0, \beta^2)$ if it is periodic for all $\nu^2 \in (0, \beta^2)$, and is said to be* **P-stable** *if it is periodic for all $\nu^2 > 0$.*

For brevity we will suppress the argument of A in what follows. Employing the Routh-Hurwitz criterion once again we can obtain stability conditions in terms of the trace and determinant of the matrix A. The RKN method (2.18)-(2.20) will be absolutely stable for $\nu^2 = \nu_0^2$ if

$$|\det A| \leq 1 \quad \text{and} \quad |tr(A)| \leq |1 + \det A|,$$

and periodic for $\nu^2 = \nu_0^2$ if

$$\det A = 1 \quad \text{and} \quad |tr(A)| < 2.$$

Several authors have investigated the stability properties of explicit and diagonally implicit methods with relatively few stages, (see e.g. Chawla & Sharma [19] and Sharp et al. [56]). With the problem of solving large systems of semi-discretised hyperbolic equations in mind, van der Houwen [63] has derived a number of methods with extended stability intervals obtained by restricting their order to 1 or 2 and then using the remaining free parameters to improve the stability properties of the methods. Chawla [12] shows that the maximum length of the periodicity interval for these methods is bounded above by $4m^2$ and that this bound can only be attained if the method has order no greater than 2. Jain et al [40] investigates implicit RKN methods and has succeeded in deriving a family of P-stable formulae based on Lobatto quadrature.

Van der Houwen & Sommeijer [66] define the phase error or dispersion of a Runge-Kutta-Nyström method to be

$$\phi(\nu) = \nu - \cos^{-1}\left(\frac{tr(A)}{\sqrt{2\det A}}\right) \tag{2.22}$$

assuming A has complex conjugate eigenvalues for sufficiently small ν^2. Order of dispersion is then defined as follows.

Definition 2.10 *A Runge-Kutta-Nyström method (2.18)-(2.20) is said to have* **order of dispersion** q *if the quantity $\phi(\nu)$ given by (2.22) satisfies $\phi(\nu) = O(h^{q+1})$ as $\nu \to 0$.*

Explicit and diagonally implicit Runge-Kutta-Nyström methods whose order of dispersion is higher than their algebraic order have been discussed by Chawla & Rao [18], Sharp et al. [56] and by van der Houwen & Sommeijer [64] and [66]. In particular, van der Houwen & Sommeijer [66] have derived diagonally implicit methods with a

relatively low algebraic order (2 or 3) but with orders of dispersion as high as 10. Their numerical experiments show that for linear oscillation problems the higher order of dispersion can be a considerable advantage, however for non-linear problems and large stepsizes this advantage may be lost.

2.2.3 Symplecticness

A Hamiltonian system with N degrees of freedom is a system of ordinary differential equations of the form

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}, \quad \frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \quad \text{for } i = 1, \ldots, N \tag{2.23}$$

where the Hamiltonian $H = H(p_1, \ldots, p_N, q_1, \ldots, q_N)$ is a sufficiently differentiable real-valued function. The flow of this system, $\phi_{t,H}$, is a transformation of the phase space such that

$$(\mathbf{p}, \mathbf{q}) = \phi_{t,H}(\mathbf{p_0}, \mathbf{q_0})$$

is the solution at time t given that $\mathbf{p}(0) = \mathbf{p_0}$ and $\mathbf{q}(0) = \mathbf{q_0}$. For each value of t, $\phi_{t,H}$ is a symplectic transformation. This means that for any bounded two-dimensional surface $\mathcal{S}$ in phase space, the sum of the two-dimensional areas of the N projections of $\mathcal{S}$ onto the planes (p_i, q_i) is the same as the sum of the areas of the N projections of $\phi_{t,H}(\mathcal{S})$ onto those planes. In particular when $N = 1$, $\phi_{t,H}$ is area-preserving.

A one-step numerical method defines a transformation $\psi_{t,H}$ such that

$$(\mathbf{p^{n+1}}, \mathbf{q^{n+1}}) = \psi_{t,H}(\mathbf{p^n}, \mathbf{q^n}).$$

A symplectic method is one for which $\psi_{t,H}$ is a symplectic transformation for all Hamiltonians H and all steplengths h. According to Channell & Scovel [8] the first symplectic methods were discovered in 1956 by De Vogalaére in a series of unpublished reports, however it was not until 1983 that the first work involving these methods was published. To begin with, symplectic methods were derived using generating

functions, but more recent work has shown that there are symplectic Runge-Kutta and Runge-Kutta-Nyström methods. In particular Sanz-Serna [55] has shown that there exist no explicit symplectic RK methods, but that those based on Gauss-Legendre quadrature are symplectic.

The autonomous second order system

$$\frac{d^2\mathbf{q}}{dt^2} = \mathbf{f}(\mathbf{q}) \tag{2.24}$$

may be rewritten as

$$\frac{d\mathbf{p}}{dt} = \mathbf{f}(\mathbf{q}), \quad \frac{d\mathbf{q}}{dt} = \mathbf{p}.$$

If $\mathbf{f}$ is the gradient of a scalar function $-V$ then this is a Hamiltonian system with the Hamiltonian

$$H(\mathbf{p},\mathbf{q}) = \tfrac{1}{2}\mathbf{p}^T\mathbf{p} + V(\mathbf{q}).$$

A Runge-Kutta-Nyström method (2.18)-(2.20) is symplectic if the following conditions, attributed to Suris (see Suris [59] or Okunbor & Skeel [52]), are satisfied:

$$\begin{aligned} b_i &= (1-c_i)d_i, && \text{for } i = 1,\ldots,m \\ d_j(b_i - B_{ji}) &= d_i(b_j - B_{ij}), && \text{for } i,j = 1,\ldots,m \end{aligned}$$

Calvo & Sanz-Serna [4] found that these conditions led to a simplification of the order conditions for such methods. Explicit symplectic RKN methods exist and have been investigated in several papers by Calvo, Sanz-Serna, Okunbor & Skeel and others. Calvo & Sanz-Serna [5] have shown that for Kepler's two-body problem their fourth order symplectic methods are more efficient than the standard variable-stepsize codes, this is primarily due to the fact that the global error exhibits a linear dependence on the number of orbits in the case of their methods, while for the standard methods this dependence is quadratic. Encouraged by these results they implemented a variable-stepsize symplectic method in the hope of combining the advantages of symplecticness and stepsize control, however they found that this was not possible, and that their

new method was less efficient than its fixed stepsize counterparts.

2.2.4 Collocation methods

In the same way as for first order systems, a collocation method for (2.1) proceeds by approximating the solution on the interval $[x_n, x_{n+1}]$ by a polynomial which satisfies the differential equation at a number of specified points contained within that interval. Let $\{c_i\}_{i=1}^m$ be a set of distinct real numbers with $0 \leq c_1 < c_2 < \ldots < c_m \leq 1$, then an m-point one-step collocation method for (2.1) is defined as follows: find $u \in \mathcal{P}_{m+1}$ such that

$$\begin{aligned} u(x_n) &= y_n \\ u'(x_n) &= z_n \\ u''(x_n + c_i h) &= f(x_n + c_i h, u(x_n + c_i h)) \quad \text{for } i = 1, \ldots, m \end{aligned}$$

then take $u(x_{n+1})$ and $u'(x_{n+1})$ as approximations to $y(x_{n+1})$ and $z(x_{n+1})$ respectively.

The third of the above conditions may be satisfied by a polynomial of the form

$$u''(x) = \sum_{j=1}^{m} l_j(x) f(x_{n+c_j}, y_{n+c_j})$$

where $l_j(x)$ is the j^{th} fundamental Lagrange basis function based on the collocation nodes $\{x_{n+c_i}\}_{i=1}^m$, and where we have set $y_{n+c_i} = u(x_{n+c_i})$, for $i = 1, \ldots, m$. Integrating this twice and using the remaining conditions we obtain

$$u(x) = u(x_n) + (x - x_n)u'(x_n) + \sum_{i=1}^{m} f_{n+c_i} \int_{x_n}^{x} \int_{x_n}^{\tau} l_j(\sigma) d\sigma d\tau.$$

Using this, and changing variable to $s = (x - x_n)/h$, we may rewrite our collocation method as an implicit Runge-Kutta-Nyström method of the form (2.18)-(2.20) with the coefficients of the method given by

$$B_{ij} = \int_0^{c_i} (c_i - \tau) l_j(\tau) d\tau,$$

$$b_j = \int_0^1 (1-\tau) l_j(\tau) d\tau,$$
$$d_j = \int_0^1 l_j(\tau) d\tau,$$

for $i, j = 1, \ldots, m$.

By construction, an m-point one-step collocation method has order at least m. However, by choosing the collocation nodes $\{x_{n+c_i}\}_{i=1}^m$ appropriately, it is possible to increase the order to as much as $2m$ (superconvergence at the step-points). Using a modified version of the Gröbner-Alekseev formula it can be shown that the method will have order $m + r$ if

$$\int_{x_n}^{x_{n+1}} \tau^j \prod_{i=1}^{m} (\tau - x_{n+c_i}) d\tau = 0, \quad \text{for } i = 0, \ldots, r$$

(see e.g. van der Houwen et al. [68]).

The polynomial $u''(x) + \omega^2 u(x)$ on the interval $[x_n, x_{n+1}]$ has degree at most $m+1$, and has simple zeros at the collocation nodes $\{x_{n+c_i}\}_{i=1}^m$. Hence we can write

$$u''(x) = -\omega^2 u(x) + R(x) \prod_{i=1}^{m} (x - x_{n+c_i})$$

where $R(x)$ is a polynomial of degree at most 1. Kramarz [44] uses this expression to derive a simpler method of constructing the matrix A for any one-step collocation method than that given in section 2.2.2. He further shows that the method must be symmetric (i.e. the collocation nodes must be distributed symmetrically in the interval $[x_n, x_{n+1}]$) in order for it to possess a non-empty interval of periodicity. Van der Houwen et al. [67], [68] analyse the attainable order and stability properties of both direct (see above) and indirect (collocation-based Runge-Kutta methods applied to the equivalent first order system) collocation methods for (2.1). They show that while direct methods can have higher stage orders than indirect methods, their stability properties are not as good. Kramarz and van der Houwen et al. were unsuccessful in deriving P-stable collocation methods, and both pose the question of whether such

methods do exist. The answer to this question was provided by Coleman [22] who showed that there do not exist any P-stable one-step collocation methods. In an attempt to improve the stability properties of their methods, van der Houwen et al. [67], [68] introduce a stabilisation technique based on preconditioning, and, using this technique, they succeed in deriving a number of P-stable and A-stable formulae.

By considering collocation over the interval $[x_{n+k-1}, x_{n+1}]$ $(k \geq 2)$, Norsett and Lie [50], [47] have derived and investigated multistep collocation methods for first order systems. This work provides a basis for the work contained in chapters 4 and 5.

2.3 Hybrid methods

In 1955, De Vogalaere [28] introduced a fourth order method which combined features of one-step and multistep methods. This method is explicit and is given by

$$\begin{aligned} y_{n+1} &= y_n + hz_n + \frac{h^2}{12}(4f_{n+1/2} + 2f_n) \\ z_{n+1} &= z_n + \frac{h}{6}(f_{n+1} + 4f_{n+1/2} + 2f_n) \\ y_{n+1/2} &= y_n + \frac{h}{2}z_n + \frac{h^2}{24}(4f_n - f_{n-1/2}). \end{aligned}$$

The first two equations are obtained by approximating the integral (2.4) and the corresponding integral for y'. These equations are similar to those arising in an RKN method, however in this case, information from the previous step is required in order to generate the off-step value $y_{n+1/2}$. Procedures to start the method were also given. Although this method is designed for general second order differential equations, it is of interest to us since it is believed to be the first of the hybrid methods for second order problems.

Coleman & Mohamed [24] analysed De Vogalaere's method in detail, and in particular found that it possesses no interval of periodicity. Subsequently Coleman [20] proposed a modification of the method which resulted in a method which was peri-

odic in $(0, 2.4)$. A further modification proposed by Kambo et al. [43] resulted in a P-stable method.

There has been considerable interest in the development of hybrid methods in recent years. This interest stems mainly from the fact that hybrid methods do not suffer the conflict between high order and P-stability which affects linear multistep methods. These methods also score over Runge-Kutta-Nyström methods in that they can achieve high order of convergence and P-stability with relatively few implicit stages. In the remainder of this section we will outline some of the hybrid methods which are available and some of the motivating factors behind their derivation. In the next section we will look at a way of studying the stability properties and orders of dispersion of many of these methods, and all Runge-Kutta-Nyström methods, investigated by Coleman [21].

One family of methods which has received particular attention is that derived by Cash [6]. Methods from this family take the form

$$y_{n+1} - 2y_n + y_{n-1} = h^2(\beta_0(f_{n+1} + f_{n-1}) + \gamma f_n + \beta_1(f_{n+\alpha_1} + f_{n-\alpha_1})) \tag{2.25}$$

$$y_{n\pm\alpha_1} = A_\pm y_{n+1} + B_\pm y_n + C_\pm y_{n-1} + h^2(s_\pm f_{n+1} + t_\pm f_n + u_\pm f_{n-1})) \tag{2.26}$$

Cash [6] has derived a three-parameter family of P-stable methods of order four from this family. Chawla [9] independently derived methods from a subclass of the methods (2.25)-(2.26) obtained by imposing the symmetry conditions

$$A_\pm = C_\mp \quad \text{and} \quad s_\pm = u_\mp$$

and found a two-parameter family of fourth order P-stable methods of this type. The fourth order P-stable methods of Costabile & Costabile [25] also fall into the class of methods (2.25)-(2.26).

Cash [6] further showed that even if this family is extended to include approximations $y_{n\pm\alpha_2}$ at a second pair of off-step points, generated in the same way as (2.26),

then one cannot obtain a method of this form which is both sixth order and P-stable. However it is possible to derive sixth order P-stable methods if approximations to y at two pairs of off-step points are included and if in addition the approximations $y_{n\pm\alpha_2}$ are allowed to depend on $y_{n\pm\alpha_1}$, i.e.

$$\begin{aligned} y_{n+1} - 2y_n + y_{n-1} &= h^2(\beta_0(f_{n+1} + f_{n-1}) + \gamma f_n + \beta_1(f_{n+\alpha_1} + f_{n-\alpha_1}) \\ &\quad +\beta_2(f_{n+\alpha_2} + f_{n-\alpha_2})) \end{aligned} \tag{2.27}$$

$$\begin{aligned} y_{n\pm\alpha_2} &= R_\pm y_{n+1} + S_\pm y_n + T_\pm y_{n-1} + h^2(U_\pm f_{n+1} + V_\pm f_n + W_\pm f_{n-1} \\ &\quad +X_\pm f_{n-\alpha_1} + Z_\pm f_{n+\alpha_1}) \end{aligned} \tag{2.28}$$

with $y_{n\pm\alpha_1}$ determined from (2.26) as before.

The fourth order methods of Cash [6] and Chawla [9], and Cash's sixth order methods require three and five (new) function evaluations per step respectively. Cash [7], Chawla & Neta [14] and Thomas [60], [61] have derived methods from these classes which require only two and four (new) function evaluations per step respectively, and Thomas [62] has derived sixth order methods which require only three (new) function evaluations per step. If these methods are to be implemented using a modified Newton iteration scheme, then another way in which their efficiency can be improved is to force the iteration matrix to be a perfect square/cube. Methods which possess this property are derived by Thomas [61], [62].

The possibility of increasing the order of dispersion of these methods was investigated by Thomas [60], who showed that this could only be done by sacrificing P-stability. However the author does succeed in deriving fourth order methods with order of dispersion six and sixth order methods with order of dispersion eight which are *almost P-stable* in the sense that they are periodic for both small and very large values of ν^2, or more accurately:

Definition 2.11 *(Thomas) A method is said to be* **almost P-stable** *if it is periodic*

for all $\nu^2 \in (0, \beta^2)$ *and for* $\nu^2 \in (\gamma^2, \infty)$, *with* $0 < \beta^2 < \gamma^2$.

Another approach used by many authors to derive hybrid methods is to take an existing linear multistep method, and replace some of the function values required by that method by those generated in additional implicit or explicit stages. One method which has been used as a starting point for many methods derived in this way is the popular Numerov method (2.6).

By introducing the stage

$$\bar{y}_n = y_n - \alpha h^2 (f_{n+1} - 2f_n + f_{n-1})$$

where α is a parameter, and replacing (2.6) by

$$y_{n+1} - 2y_n + y_{n-1} = \frac{h^2}{12}(f_{n+1} + 10\bar{f}_n + f_{n-1}),$$

Chawla [10] obtained a family of unconditionally stable methods ($\alpha > 1/120$), and Chawla & Rao [15] obtained a method with order of dispersion six and a slightly longer interval of periodicity than Numerov's method. Chawla [11], [13] then went on to consider the more general family of *explicit* methods given by

$$y_n^{(i)} = y_n - \alpha_i h^2 f_n^{(i-1)}$$

$$y_{n+1}^* = 2y_n - y_{n-1} + h^2 f_n^{(m)}$$

$$y_{n+1} - 2y_n + y_{n-1} = \frac{h^2}{12}(f_{n+1}^* + 10f_n + f_{n-1}),$$

for $i = 1, \ldots, m$ with $f_n^{(0)} = f_n$. Methods from this family which possess periodicity intervals of length nearly $2((m+1)(m+3))^{1/2}$ have been derived. A further modification suggested by Chawla & Rao [17] produced an explicit method with an even smaller phase lag and a slightly larger interval of periodicity.

A number of methods, based on different linear multistep methods, have been derived in this way by Jain et al. [41], Chawla & Rao [16], Ananthakrishnaiah [1],

Simos [57] and others.

All the methods discussed so far have been designed to be exact when the solution to the differential equation under consideration is a polynomial of sufficiently low degree. However, if the differential equation describes orbital or oscillatory motion, then its solution is more likely to be a linear combination of exponential functions with complex arguments than a polynomial. It is for this reason that the so-called *exponential fitting* methods were developed by Gautschi [31]. As their name suggests, these methods are designed to be exact for polynomials in $e^{\pm i\omega h}$, or Fourier polynomials, of sufficiently low degree, where ω is a given (fixed) frequency. Stiefel & Bettis [58] extended this idea and derived methods which are exact for products of ordinary and Fourier polynomials; since then, a great many of these methods have been proposed by numerous authors. A further discussion of exponential fitting methods is beyond the scope of this thesis; we mention them here for completeness only.

2.3.1 Periodicity and dispersion

When any of the two-step hybrid methods mentioned in the previous section, or the methods of Ananthakrishnaiah [2] or Meneguette [49], are applied to the scalar test equation (2.11) we obtain a recurrence relation of the form

$$y_{n+1} - 2R_{\lambda\mu}(\nu^2)y_n + y_{n-1} = 0 \tag{2.29}$$

where $\nu = \omega h$ and $R_{\lambda\mu}(\nu^2)$ is a rational function with numerator of degree λ and denominator of degree μ. In what follows we will refer to $R_{\lambda\mu}(\nu^2)$ as the *stability function* of the method. The solutions of (2.29) are determined by the roots of the characteristic equation

$$\xi^2 - 2R_{\lambda\mu}(\nu^2)\xi + 1 = 0. \tag{2.30}$$

Observe that the same type of equation occurs when analysing the stability properties of Runge-Kutta-Nyström methods (2.18)-(2.20). The exact solution to (2.11) satisfies

$$y(x_{n+1}) - 2\cos(\nu)y(x_n) + y(x_{n-1}) = 0$$

hence $R_{\lambda\mu}(\nu^2)$ may be regarded as a rational approximation for $\cos(\nu)$.

For a method whose characteristic equation is of the form (2.30) to be periodic (Lambert & Watson [46]) for $\nu^2 = \nu_0^2$, the roots of that equation must lie on the unit circle $\{z \in \mathbb{C} : |z| = 1\}$, or equivalently, $R_{\lambda\mu}(\nu_0^2)$ must be less than or equal to one in modulus. When $|R_{\lambda\mu}(\nu_0^2)| = 1$, then the stability of numerical solutions depends on details of the method, for example Hairer [33] presents two methods which have the same stability function, but one is P-stable, while the other is periodic for all ν^2 except $\nu^2 = 12$. Consequently, since in this section we seek to draw conclusions regarding the stability properties of methods solely based on investigations of the characteristic equation (2.30), we take $|R_{\lambda\mu}(\nu_0^2)| < 1$ as our condition for periodicity.

Definition 2.12 *(van der Houwen & Sommeijer) For any method corresponding to the characteristic equation (2.30), the quantity*

$$\phi(\nu) = \nu - \cos^{-1}[R_{\lambda\mu}(\nu^2)]$$

is called the dispersion (or phase-lag). If $\phi(\nu) = O(\nu^{q+1})$ as $\nu \to 0$ the order of dispersion is q.

From this it can easily be deduced that if the method has order of dispersion $q = 2r$ then

$$\cos(\nu) - R_{\lambda\mu}(\nu^2) = O(\nu^{2r+2})$$

By investigating the properties of $R_{\lambda\mu}(\nu^2)$, Coleman [21] determines the attainable orders of dispersion and stability properties of a range of methods, and also discovers a conflict between the requirements of P-stability and high order of dispersion. We close this section with some of the main results from that paper.

Theorem 2.4 *For given values of λ and μ, the maximum order of dispersion is $2\lambda + 2\mu$. That order is attained when $R_{\lambda\mu}(\nu^2)$ is the $[2\lambda/2\mu]$ Padé approximant for $\cos(\nu)$.*

Theorem 2.5 *If an explicit method with stability function $R_{\lambda 0}(\nu^2)$ possesses an interval of periodicity $(0, \beta^2)$ and order of dispersion 2λ, then $\beta < \pi$ when λ is odd, and $\beta < 2\pi$ when λ is even.*

Theorem 2.6 *A P-stable method with stability function $R_{\lambda\mu}(\nu^2)$ has order of dispersion at most 2μ.*

Chapter 3

Analysis of the methods of Panovsky & Richardson

Panovsky & Richardson [53] proposed a family of implicit methods for initial value problems of the form

$$y'' = f(x, y); \quad y(x_0) = y_0, \quad y'(x_0) = z_0, \tag{3.1}$$

involving second order differential equations in which the first derivative does not appear explicitly. Each method from this family is based on a polynomial approximation of degree n for the function f whose interpolation nodes are determined by the extrema of the Chebyshev polynomial of degree n. The derivation of these methods is summarised in section 3.1.

In section 3.2 we show that these methods may be expressed as two-step symmetric hybrid methods and we derive expressions for the coefficients involved. The accuracy of these methods is investigated in section 3.3, and we show that the methods have order $n + 1$ if n is odd, and $n + 2$ if n is even.

In section 3.4 we show that the stability properties of methods from this family are determined by the roots of a quadratic equation, $\lambda^2 - 2\alpha_n(\nu^2)\lambda + 1 = 0$, where $\alpha_n(\nu^2)$ is a rational approximation for $\cos(\nu)$. We also show that each Panovsky-

Richardson method possesses a non-vanishing interval of periodicity, and we tabulate the periodicity intervals for methods of degrees 1 to 10. These results suggest some conjectures for which we do not yet have proof.

Implementation considerations are discussed in section 3.5, and the results of numerical experiments are given in section 3.6.

A generalisation of the methods of Panovsky & Richardson is introduced in section 3.7 with a view to extending the applicability and simplifying the derivation of the main result of section 3.8. In section 3.8 we show that these generalised Panovsky-Richardson methods are equivalent to certain collocation-based Runge-Kutta-Nyström methods in the sense that, in the absence of rounding errors, they would produce identical numerical results from the same starting values.

With the aid of the equivalence established in section 3.8, we are able to show in section 3.9 that the Panovsky-Richardson methods are neither P-stable nor symplectic

Finally, in section 3.10 we investigate the effect of rounding errors on these methods in both the original and the RKN formulations.

3.1 The methods of Panovsky and Richardson

Integrating (3.1) twice gives:

$$y(x \pm \xi h) - y(x) = \pm \xi h y'(x) + \int_x^{x \pm \xi h} (x \pm \xi h - \tau) f(\tau) d\tau \tag{3.2}$$

where for notational convenience we have temporarily suppressed the second argument of f. Adding these expressions we obtain the identity

$$y(x + \xi h) - 2y(x) + y(x - \xi h) = \int_x^{x + \xi h} (x + \xi h - \tau)[f(\tau) + f(2x - \tau)] d\tau \tag{3.3}$$

As noted in section 2.1, this identity provides a starting point for the derivation of a number of methods for (3.1) which do not require an approximation for the first derivative of the solution. Let $x_m = x_0 + mh$ for $m = 0, 1, 2, \ldots$ and where the

steplength h is assumed to be fixed. Introducing a new variable α defined by the relation

$$\tau = x_m + \tfrac{1}{2}h(1+\alpha)$$

and taking $x = x_m$, we can write (3.3) as

$$y(x+\xi h) - 2y(x) + y(x-\xi h) = \tfrac{1}{4}h^2 \int_{-1}^{2\xi-1} (2\xi - 1 - \alpha)[f^+(\alpha) + f^-(\alpha)]d\alpha \quad (3.4)$$

with

$$f^{\pm}(\alpha) = f(x_m \pm \tfrac{1}{2}h(1+\alpha))$$

The Störmer-Cowell methods are derived from this identity by replacing $f^{\pm}$ by interpolating polynomials based on previous grid points and taking $\xi = 1$ (see e.g. Hairer et al. [35] p422 or Henrici [38] p290). Panovsky and Richardson [53] also replace $f^{\pm}$ by interpolating polynomials, but their interpolation nodes include off-step points which are the extrema of a Chebyshev polynomial.

The Chebyshev polynomial of degree n, T_n, takes its extreme values on the interval $[-1,1]$ at the points

$$\alpha_j = \cos\theta_j \qquad \text{where} \qquad \theta_j = \frac{(n-j)\pi}{n}, \qquad j = 0,1,\ldots,n \quad (3.5)$$

The polynomial of degree n which interpolates to a function g at the points α_j is

$$p_n(\alpha) = \sum_{k=0}^{n}{}'' C_k T_k(\alpha) \quad (3.6)$$

where

$$C_k = \frac{2}{n}\sum_{j=0}^{n}{}'' g(\alpha_j)T_k(\alpha_j)$$

where the double prime on the sum indicates that the first and last terms are to be halved (see e.g. Fox & Parker [30] p32).

Let

$$\xi_j = \tfrac{1}{2}(1+\alpha_j) \qquad \text{and} \qquad x_{m\pm\xi_j} = x_m \pm \xi_j h, \qquad j = 0,\ldots,n \tag{3.7}$$

Then the corresponding expressions for $f^{\pm}$ are

$$f^{\pm}(\alpha) = {\sum_{k=0}^{n}}'' a_k^{\pm} T_k(\alpha) \tag{3.8}$$

with

$$\begin{bmatrix} a_k^+ \\ a_k^- \end{bmatrix} = \frac{2}{n} {\sum_{k=0}^{n}}'' \begin{bmatrix} f_{m+\xi_j} \\ f_{m-\xi_j} \end{bmatrix} T_k(\alpha_j) \tag{3.9}$$

where

$$f_{m\pm\xi_j} = f(x_{m\pm\xi_j}, y_{m\pm\xi_j}), \qquad j = 0,\ldots,n$$

and where $y_{m\pm\xi_j}$ is an approximation for $y(x_{m\pm\xi_j})$. By substituting these approximations for $f^{\pm}$ into (3.4), Panovsky and Richardson obtain the formulae

$$y_{m+\xi_j} - 2y_m + y_{m-\xi_j} = \tfrac{1}{4}h^2 {\sum_{k=0}^{n}}''(a_k^+ + a_k^-)R_{jk} \tag{3.10}$$

for $j = 1,\ldots,n$, where

$$\begin{aligned} R_{jk} &= \int_{-1}^{2\xi_j - 1} (2\xi_j - 1 - \alpha) T_k(\alpha)\, d\alpha \\ &= \int_{-1}^{\alpha_j} \int_{-1}^{\alpha} T_k(\beta)\, d\beta\, d\alpha \end{aligned} \tag{3.11}$$

Using the identities

$$\int T_k(\alpha)\, d\alpha = \frac{1}{2}\left(\frac{1}{k+1} T_{k+1}(\alpha) - \frac{1}{k-1} T_{k-1}(\alpha)\right), \quad k \geq 2, \tag{3.12}$$

$$\int T_1(\alpha)\, d\alpha = \tfrac{1}{4}(T_0(\alpha) + T_2(\alpha)), \tag{3.13}$$

$$\int T_0(\alpha)\, d\alpha = T_1(\alpha) \tag{3.14}$$

to evaluate the integrals (3.11) we can derive the following explicit expressions for

the R_{jk}:

$$R_{jk} = \frac{\cos[(k+2)\theta_j]}{4(k+1)(k+2)} - \frac{\cos k\theta_j}{2(k^2-1)} + \frac{\cos[(k-2)\theta_j]}{4(k-1)(k-2)} + (-1)^{k-1}\left[\frac{\cos\theta_j}{k^2-1} + \frac{1}{k^2-4}\right], \qquad k \geq 3 \tag{3.15}$$

$$R_{j2} = \frac{1}{48}(-9 - 16\cos\theta_j - 8\cos 2\theta_j + \cos 4\theta_j), \tag{3.16}$$

$$R_{j1} = \frac{1}{24}(-8 - 9\cos\theta_j + \cos 3\theta_j), \tag{3.17}$$

$$R_{j0} = \frac{1}{4}(3 + 4\cos\theta_j + \cos 2\theta_j). \tag{3.18}$$

Equation (3.15) corrects a misprint in the corresponding expression given in [53].

3.2 An alternative formulation

By substituting (3.9) into (3.10) and changing the order of the summations we can write

$$y_{m+\xi_i} - 2y_m + y_{m-\xi_i} = \frac{h^2}{2n}\sum_{j=0}^{n}{}''A_{ij}(f_{m+\xi_j} + f_{m-\xi_j}), \qquad i = 1,\ldots,n \tag{3.19}$$

with

$$A_{ij} = \sum_{k=0}^{n}{}''R_{ik}T_k(\alpha_j). \tag{3.20}$$

This simple rearrangement shows the methods of Panovsky and Richardson [53] as 2-step symmetric hybrid methods with $2n-2$ off-step points in the interval $[x_{m-1}, x_{m+1}]$ for each m. We will refer to the integer n, which is the degree of the polynomial approximations for $f^{\pm}(\alpha)$ in (3.8), as the **degree** of the method. Panovsky and Richardson call n the *order* of the method, but we prefer to reserve that word for its normal use (see the next section).

The first two methods from this family are given in the following examples

Example 1 $n = 1$

In this case there are no off-step points and (3.19) gives a single equation

$$y_{m+1} - 2y_m + y_{m-1} = \tfrac{1}{6}h^2(f_{m+1} + 4f_m + f_{m-1}) \tag{3.21}$$

as noted in [53]. This is a linear 2-step method of order 2.

Example 2 $n = 2$

The equations for this method are

$$\begin{aligned} y_{m+\frac{1}{2}} - 2y_m + y_{m-\frac{1}{2}} &= \tfrac{1}{48}h^2(7f_m + 3(f_{m+\frac{1}{2}} + f_{m-\frac{1}{2}}) \\ &\quad -\tfrac{1}{2}(f_{m+1} + f_{m-1})) \qquad (3.22) \\ y_{m+1} - 2y_m + y_{m-1} &= \tfrac{1}{3}h^2(f_m + f_{m+\frac{1}{2}} + f_{m-\frac{1}{2}}). \qquad (3.23) \end{aligned}$$

This method has order 4.

3.2.1 The coefficients A_{ij}

In this subsection we attempt to find explicit expressions for the coefficients A_{ij} in terms of the numbers α_j.

Combining equations (3.20) and (3.11) we obtain

$$A_{ij} = \int_{-1}^{\alpha_j}\int_{-1}^{\alpha}{\sum_{k=0}^{n}}'' T_k(\alpha_j)T_k(\beta)\,d\beta d\alpha \tag{3.24}$$

Let $\beta = \cos\phi$, then we may rewrite the sum in the above integral as

$$\begin{aligned} {\sum_{k=0}^{n}}'' \cos k\theta_j \cos k\phi &= \tfrac{1}{2}{\sum_{k=0}^{n}}'' (\cos[k(\phi+\theta_j)] + \cos[k(\phi-\theta_j]) \\ &= \tfrac{1}{4}(-1)^{n-j}\sin n\phi\left(\cot[\tfrac{1}{2}(\phi+\theta_j)] + \cot[\tfrac{1}{2}(\phi-\theta_j)]\right) \\ &= \frac{(-1)^{n-j}\sin n\phi\ \sin\phi}{2(\cos\theta_j - \cos\phi)} \qquad (3.25) \end{aligned}$$

Using this result we may re-express A_{ij} in the following forms:

$$A_{ij} = \frac{(-1)^{n-j}}{2} \int_{-1}^{\alpha_i} \int_{-1}^{\alpha} \frac{\sin n\phi \ \sin \phi}{(\cos \theta_j - \cos \phi)} d(\cos \phi) d\alpha \tag{3.26}$$

$$= \frac{(-1)^{n-j}}{2n} \int_{-1}^{\alpha_i} \int_{-1}^{\alpha} \frac{(1-\beta^2) T_n'(\beta)}{(\alpha_j - \beta)} d\beta d\alpha \tag{3.27}$$

$$= \frac{(-1)^{n-j}}{2n} \int_{-1}^{\alpha_i} \frac{(\alpha_j - \alpha)(1-\alpha^2) T_n'(\alpha)}{(\alpha_j - \alpha)} d\alpha \tag{3.28}$$

Now $T_n'(\alpha)$ is a polynomial of degree $n-1$ which has zeros on the open interval $(-1,1)$ at the points α_j, for $j = 1, \ldots, n-1$. We can thus write

$$T_n'(\alpha) = K \prod_{j=1}^{n-1} (\alpha - \alpha_j)$$

for some constant K. By looking at the limit of $T_n'(\alpha)$ as α tends to 1, we can determine the value of this constant, and hence obtain the following expression for $T_n'(\alpha)$:

$$T_n'(\alpha) = n^2 \prod_{j=1}^{n-1} \left(\frac{\alpha - \alpha_j}{1 - \alpha_j} \right)$$

Using this it is easy to show that $(1-\alpha^2) T_n'(\alpha)/(\alpha_j - \alpha)$ is a polynomial for each $j = 0, \ldots, n$. It is not yet clear if A_{ij} can be expressed in a simple closed form for all $i, j \leq n$ and n arbitrary, but we have found explicit formulae for A_{jj}, A_{i0} and for A_{in}.

The special cases $i = j$

$$A_{jj} = \frac{(-1)^{n-j}}{2n} \int_{-1}^{\alpha_j} (1-\alpha^2) T_n'(\alpha) d\alpha$$

$$= \frac{(-1)^{n-j}}{2n} \left\{ \left[(1-\alpha^2) T_n(\alpha) \right]_{-1}^{\alpha_j} + 2 \int_{-1}^{\alpha_j} \alpha T_n(\alpha) d\alpha \right\}$$

Using

$$\int \alpha T_k(\alpha) d\alpha = \frac{1}{4} \left[\frac{1}{k+2} T_{k+2}(\alpha) - \frac{1}{k-2} T_{k-2}(\alpha) \right], \qquad k \geq 3 \tag{3.29}$$

to evaluate the above integral we obtain

$$A_{jj} = \frac{(-1)^{n-j}}{2n}\left[(1-\alpha_j^2)T_n(\alpha_j) + \frac{T_{n+2}(\alpha_j)}{2(n+2)} - \frac{T_{n-2}(\alpha_j)}{2(n-2)} + \frac{2(-1)^n}{n^2-4}\right], \quad n \geq 3.$$

Furthermore, since

$$T_n(\alpha_j) = \cos n\theta_j = (-1)^{n-j} \quad \text{and} \quad T_{n\pm r}(\alpha_j) = (-1)^{n-j}\cos r\theta_j, \quad r \geq 0 \tag{3.30}$$

this can be reduced to

$$A_{jj} = \frac{(1-\alpha_j^2)n^2 - 2(1-(-1)^j)}{2n(n^2-4)}, \qquad n \geq 3. \tag{3.31}$$

The coefficients A_{jj} are defined only for $j \leq n$ where n is the degree of the method. For $n = 1$ the only coefficient of this form is $A_{11} = \frac{2}{3}$. When $n = 2$ the relevant coefficients are $A_{11} = \frac{1}{4}$ and $A_{22} = 0$.

In particular, when $j = n$ we have

$$A_{nn} = \begin{cases} \dfrac{(-1)^n - 1}{n(n^2-4)}, & \text{for } n > 2, \\ 0, & \text{for } n = 2, \\ \frac{2}{3}, & \text{for } n = 1. \end{cases}$$

The special cases $j = 0$

Once again the denominator of the integrand of (3.28) is a factor of the numerator and the integral is easily evaluated.

$$\begin{aligned} A_{i0} &= \frac{(-1)^{n+1}}{2n}\int_{-1}^{\alpha_i}(\alpha_i - \alpha)(1-\alpha)T_n'(\alpha)d\alpha \\ &= \frac{(-1)^{n+1}}{2n}\left\{[(\alpha_i - \alpha)(1-\alpha)T_n(\alpha)]_{-1}^{\alpha_i} + (1+\alpha_i)\int_{-1}^{\alpha_i} T_n(\alpha)d\alpha \right. \\ &\quad \left. -2\int_{-1}^{\alpha_i}\alpha T_n(\alpha)d\alpha\right\} \end{aligned}$$

Using the integration formulae (3.12)-(3.14) and (3.29) to evaluate the above integrals, and (3.30) to simplify the resulting expression, we obtain, for $n \geq 2$

$$A_{i0} = \frac{1}{2n}\left[2(1+\alpha_i) + \frac{(1+\alpha_i)(1+(-1)^i\alpha_i)}{n^2-1} + \frac{2\{1+(-1)^i(2\alpha_i^2-1)\}}{n^2-4}\right]. \quad (3.32)$$

When $n = 1$ the only relevant coefficient is $A_{10} = \frac{4}{3}$, and when $n = 2$, the coefficients of this form are $A_{10} = \frac{7}{12}$ and $A_{20} = \frac{4}{3}$.

The special cases $j = n$

In this case (3.28) becomes

$$A_{in} = \frac{1}{2n}\int_{-1}^{\alpha_i}(\alpha_i - \alpha)(1+\alpha)T_n'(\alpha)d\alpha$$

For $n \geq 2$ we obtain

$$A_{in} = \frac{(-1)^{n+1}}{2n}\left[\frac{2((-1)^i+1-2\alpha_i^2)}{n^2-4} - \frac{(1-\alpha_i)(\alpha_i+(-1)^i)}{n^2-1}\right]. \quad (3.33)$$

For $n = 1$ the only coefficient of this form is $A_{11} = \frac{2}{3}$, and when $n = 2$ the relevant coefficients are $A_{12} = \frac{-1}{12}$ and $A_{22} = 0$.

3.3 Order and local truncation error

In order to study the local truncation error of these methods we adopt the approach used by Lambert [45]. For y an arbitrary test function, assumed to be as differentable as we please, we define the linear functionals

$$\begin{aligned}\mathcal{L}_i[y(x),h] &= y(x+\xi_i h) - 2y(x) + y(x-\xi_i h) \\ &\quad -\frac{h^2}{2n}\sum_{j=0}^{n}{}''A_{ij}\left[y''(x+\xi_j h) + y''(x-\xi_j h)\right], \quad i = 1,\ldots,n. \quad (3.34)\end{aligned}$$

Expanding $y(x \pm \xi_i h)$ and $y''(x \pm \xi_j h)$ as Taylor series about x and collecting terms we obtain

$$\mathcal{L}_i[y(x), h] = 2 \sum_{q=0}^{r} \frac{h^{2q+2} y^{(2q+2)}(x)}{(2q+2)!} B_q^i + O(h^{2r+4}), \quad i = 1, \ldots, n. \tag{3.35}$$

where

$$B_q^i = \xi_i^{2q+2} - \frac{(2q+1)(2q+2)}{2n} \sum_{j=0}^{n}{}'' A_{ij} \xi_j^{2q}. \tag{3.36}$$

Denote by $\delta_i[y(x_m), h]$ the local truncation error in the approximation $y_{m+\xi_i}$ to $y(x_m + \xi_i)$, where y is a solution to the differential equation under consideration. Then it is easy to show that

$$\delta_i[y(x_m), h] = \mathcal{L}_i[y(x_m), h] + \frac{h^2}{2n} \frac{\partial f}{\partial y}(x_m, y(x_m)) \sum_{j=0}^{n}{}'' A_{ij} \mathcal{L}_j[y(x_m), h] + \ldots \tag{3.37}$$

From this we see that the following conditions are sufficient, but by no means necessary, for the method of advancing the solution from x_m to x_{m+1} to have order $2p$:

$$B_q^i = 0, \qquad i = 1, \ldots, n, \; q = 0, \ldots, p-1 \tag{3.38}$$

$$B_p^n \neq 0, \tag{3.39}$$

If these conditions are satisfied then the error constant for the method, which is the coefficient of the leading term in the expansion of the local truncation error at x_{m+1}, is given by

$$\frac{2}{(2p+2)!} B_p^n = \frac{2}{(2p+2)!} - \frac{1}{n(2p)!} \sum_{j=0}^{n}{}'' A_{nj} \left(\frac{1+\alpha_j}{2} \right)^{2p}. \tag{3.40}$$

The following theorem gives the order and error constant of the Panovsky-Richardson method of arbitrary degree n.

Theorem 3.1 *When n is odd, the Panovsky-Richardson method of degree n has order $n+1$ and its error constant is*

$$\frac{1}{2^{2n-1}n(n^2-4)(n+1)!}.$$

For even n the method has order $n+2$ and its error constant is

$$\frac{-1}{2^{2n}(n+2)(n^2-1)(n^2-9)(n-1)!}.$$

Proof For a suitable set of coefficients C_i^r we can write

$$\left(\frac{1+x}{2}\right)^r = \sum_{i=0}^{r} C_i^r T_i(x), \qquad \text{for } r \geq 0 \tag{3.41}$$

since the left-hand side is a polynomial of degree r in x. To prove this theorem we substitute the above expansion into (3.40), and then simplify the resulting expression using the following summation orthogonality property of the Chebyshev polynomials:

For $k \leq n$,

$$\sum_{j=0}^{n}{}'' T_i(\alpha_j)T_k(\alpha_j) = \begin{cases} n & \text{if } k=0 \text{ and } i = 0,\ 2n,\ 4n, \ldots \\ n & \text{if } k=n \text{ and } i = n,\ 3n,\ 5n, \ldots \\ \frac{1}{2}n & \text{if } k \neq 0 \text{ or } n \text{ and } i = k,\ 2n \pm k,\ 4n \pm k, \ldots \\ 0 & \text{otherwise.} \end{cases}$$

Case (i) $2q \leq n$

Combining (3.20) and (3.41) we have

$$\begin{aligned} \frac{1}{n}\sum_{j=0}^{n}{}'' A_{ij}\left(\frac{1+\alpha_j}{2}\right)^{2q} &= \frac{1}{n}\sum_{k=0}^{n}{}'' R_{ik}\sum_{l=0}^{2q} C_l^{2q}\sum_{j=0}^{n}{}'' T_l(\alpha_j)T_k(\alpha_j) \\ &= \frac{1}{2}\sum_{k=0}^{2q} C_k^{2q} R_{ik} \end{aligned}$$

$$\begin{aligned} &= \frac{1}{2}\int_{-1}^{\alpha_i}\int_{-1}^{\alpha}\sum_{k=0}^{2q} C_k^{2q} T_k(\beta)\,d\beta d\alpha \\ &= \frac{1}{2}\int_{-1}^{\alpha_i}\int_{-1}^{\alpha}\left(\frac{1+\beta}{2}\right)^{2q} d\beta d\alpha \\ &= \frac{\xi_i^{2q+2}}{(q+1)(2q+1)}. \end{aligned}$$

Hence $B_q^i = 0$ for $i = 0, \ldots, n$ when $2q \leq n$. It follows that the order of the method is at least $n+1$ when n is odd, and $n+2$ when n is even.

Case (ii) $2q > n$

With the convention that $C_i^{2q} = 0$ if $i > 2q$, we have in this case that

$$\frac{1}{n}{\sum_{j=0}^{n}}'' A_{ij}\left(\frac{1+\alpha_j}{2}\right)^{2q} = \frac{1}{2}\left[\sum_{k=0}^{n} C_k^{2q} R_{ik} + C_{n+1}^{2q} R_{i,n-1} + C_{n+2}^{2q} R_{i,n-2} + \ldots\right]$$

If n is odd and $2q = n+1$ then

$$\begin{aligned} B_q^i &= \xi_i^{2q+2} - \frac{(2q+2)(2q+1)}{4}\left[\sum_{k=0}^{n} C_k^{n+1} R_{ik} + C_{n+1}^{n+1} R_{i,n-1}\right] \\ &= \xi_i^{n+3} - \frac{(n+3)(n+2)}{4}\int_{-1}^{\alpha_i}\int_{-1}^{\alpha}\left(\tfrac{1}{2}(1+\beta)\right)^{n+1} d\beta d\alpha \\ &\quad + \frac{(n+3)(n+2)}{4}\int_{-1}^{\alpha_i}\int_{-1}^{\alpha} C_{n+1}^{n+1}\left[T_{n-1}(\beta) - T_{n+1}(\beta)\right] d\beta d\alpha \\ &= \frac{(n+3)(n+2)}{4} C_{n+1}^{n+1}\int_{-1}^{\alpha_i}\int_{-1}^{\alpha}\left[T_{n+1}(\beta) - T_{n-1}(\beta)\right] d\beta d\alpha \end{aligned}$$

It is possible to express this integral in closed form for each i but since we shall see that B_q^n is non-zero, it is not necessary to consider B_q^i for other values of i. For $n \geq 3$ we have

$$B_q^n = \frac{(n+3)(n+2)C_{n+1}^{n+1}}{4}\int_{-1}^{1}\left[\frac{T_{n+2}(\beta)}{n+2} - \frac{2T_n(\beta)}{n} + \frac{T_{n-2}(\beta)}{n-2}\right]_{-1}^{\alpha} d\alpha$$

Since the polynomials T_n and $T_{n\pm2}$ are odd functions, only the lower limit of the first integral contributes anything to B_q^n and we readily obtain

$$B_q^n = \frac{2(n+2)(n+3)C_{n+1}^{n+1}}{n(n^2-4)} \tag{3.42}$$

It is easy to show that this also holds when $n = 1$.

If n is even and $2q = n + 2$ then, by similar arguments,

$$B_q^i = \frac{(n+3)(n+4)}{4}\left[C_{n+1}^{n+2}(R_{i,n+1} - R_{i,n-1}) + C_{n+2}^{n+2}(R_{i,n+2} - R_{i,n-2})\right]$$

Once again we need only consider the special case $i = n$. By evaluating the integrals

$$R_{n,n+1} - R_{n,n-1} = \int_{-1}^{1}\int_{-1}^{\alpha}[T_{n+1}(\beta) - T_{n-1}(\beta)]\,d\beta d\alpha$$

and

$$R_{n,n+2} - R_{n,n-2} = \int_{-1}^{1}\int_{-1}^{\alpha}[T_{n+2}(\beta) - T_{n-2}(\beta)]\,d\beta d\alpha$$

we obtain

$$B_q^n = \frac{2n(n+3)(n+4)(2C_{n+2}^{n-2} - C_{n+1}^{n+2})}{(n^2-1)(n^2-9)} \tag{3.43}$$

It is trivial to show that the leading term of $T_r(x)$ is $2^{r-1}x^r$ for all $r \geq 0$, and hence

$$x^r = 2^{1-r}T_r(x) + \text{a polynomial of degree } (r-2)$$

so that

$$(\tfrac{1}{2}[1+x])^r = 2^{-r}\left[2^{1-r}T_r(x) + 2^{2-r}rT_{r-1}(x) + \text{a polynomial of degree } (r-2)\right]$$

Therefore,

$$C_r^r = \frac{1}{2^{2r-1}} \qquad \text{and} \qquad C_{r-1}^r = \frac{r}{2^{2r-2}}$$

Substituting these values into equations (3.42) and (3.43) and forming the error constants $(2B_p^n/(2p+2)!)$, we obtain the expressions given in the statement of the theorem. □

The leading term of the local truncation error at x_m is

$$\frac{h^{n+3}y^{(n+3)}(x_m)}{2^{2n-1}n(n^2-4)(n+1)!}, \qquad n \text{ odd}, \tag{3.44}$$

$$\frac{-h^{n+4}y^{(n+4)}(x_m)}{2^{2n}(n+2)(n^2-1)(n^2-9)(n-1)!}, \qquad n \text{ even}. \tag{3.45}$$

Panovsky & Richardson's [53] estimate for the modulus of the leading term is given by

$$\frac{h^{n+3}|y^{(n+3)}(x_m)|}{2^{2n-1}n^3(n+1)!} \qquad \text{for all } n.$$

Comparing this with our own expressions, we find that this estimate is quite accurate for n odd and not too small, but it fails to reveal the higher order when n is even.

3.4 Absolute stability and periodicity

In this section we will derive the stability function for Panovsky-Richardson methods of arbitrary degree n. We will further show that every such method has a non-empty interval of periodicity. Finally we will use our results to investigate the stability properties of the P-R methods of degrees 1 and 2.

We begin by writing equations (3.19) in matrix form. To do this we define the $(n+1)-$dimensional column vectors

$$\mathbf{Y}^{(\mathrm{m})} = \begin{pmatrix} y_m \\ y_{m+\xi_1} \\ \vdots \\ y_{m+1} \end{pmatrix}, \quad \bar{\mathbf{Y}}^{(\mathrm{m})} = \begin{pmatrix} y_m \\ y_{m-\xi_1} \\ \vdots \\ y_{m-1} \end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix} f_m \\ f_{m+\xi_1} \\ \vdots \\ f_{m+1} \end{pmatrix}, \quad \bar{\mathbf{F}} = \begin{pmatrix} f_m \\ f_{m-\xi_1} \\ \vdots \\ f_{m-1} \end{pmatrix},$$

$\mathbf{v_1} = (1,1,\ldots,1)^{\mathrm{T}}$ and an $(n+1)\times(n+1)$ matrix B with $B_{0j} = 0$, for $j = 0,1,\ldots,n$

and, for $i = 1, \ldots, n$,

$$B_{ij} = \begin{cases} \frac{1}{2n} A_{ij}, & \text{for } j = 1, 2, \ldots, n-1, \\ \frac{1}{4n} A_{ij}, & \text{for } j = 0, \\ \frac{1}{4n} A_{ij}, & \text{for } j = n. \end{cases}$$

Adding the identity $y_m = y_m$ to (3.19) we then have

$$\mathbf{Y^{(m)}} = 2y_m \mathbf{v_1} - \bar{\mathbf{Y}}^{(\mathbf{m})} + h^2 B(\mathbf{F} + \bar{\mathbf{F}}). \tag{3.46}$$

When applied to the test equation $y'' = -\omega^2 y$ we obtain the relation

$$P\mathbf{Y^{(m)}} = Q\bar{\mathbf{Y}}^{(\mathbf{m})}, \tag{3.47}$$

with $P = I_{n+1} + \nu^2 B$ and $Q = 2U_1 - P$, where I_{n+1} is the $(n+1)$-dimensional identity matrix, $\nu^2 = \omega^2 h^2$ and

$$U_1 = \begin{pmatrix} 1 & 0 & \ldots & 0 \\ 1 & 0 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & \ldots & 0 \end{pmatrix}$$

We seek a recurrence relation of the form

$$\mathbf{Y^{(m)}} = K\mathbf{Y^{(m-1)}} \qquad m = 1, 2, \ldots \tag{3.48}$$

linking the solution vectors $\{\mathbf{Y^{(m)}}\}$, where K is an $(n+1) \times (n+1)$ matrix depending only on the parameter ν and the coefficients of the method under consideration. To construct such a relation we use the fact that the extrema of the Chebyshev polynomials are symmetric on the interval $[-1, 1]$, and so

$$x_m - \xi_i h = x_{m-1} + \xi_{n-i} h, \quad \text{for } i = 0, 1, \ldots, n.$$

It follows that

$$P\mathbf{Y}^{(\mathbf{m})} = QT\mathbf{Y}^{(\mathbf{m-1})},$$

where T is the permutation matrix

$$T = \begin{pmatrix} 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & \dots & 1 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 1 & \dots & 0 & 0 \\ 1 & 0 & \dots & 0 & 0 \end{pmatrix}.$$

Thus we have our recurrence relation (3.48) with the matrix K given by

$$K = P^{-1}QT = (2P^{-1}U_1 - I_{n+1})T.$$

The stability properties of the method can now be investigated by analysing the eigenvalues of K. Suppose that P^{-1} has elements $\bar{p}_{ij}$ and let

$$\alpha_i = \sum_{j=0}^{n} \bar{p}_{ij}, \qquad \text{for } i = 0, 1, \dots, n.$$

Then

$$P^{-1}U_1 = \begin{pmatrix} \alpha_0 & 0 & \dots & 0 \\ \alpha_1 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_n & 0 & \dots & 0 \end{pmatrix}.$$

From the definition of P it can be shown that $\alpha_0 = 1$. The eigenvalues λ_i of K are

therefore the roots of the characteristic polynomial

$$\det\,(K-\lambda I_{n+1}) = (-1)^{n+1}\det\begin{pmatrix} \lambda & 0 & \dots & 0 & -1 \\ 0 & \lambda & \dots & 1 & -2\alpha_1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 1 & \dots & \lambda & -2\alpha_{n-1} \\ 1 & 0 & \dots & 0 & \lambda - 2\alpha_n \end{pmatrix}.$$

Observe that the structure of the above matrix will depend on whether it has an even or an odd number of rows, and may be determined by considering the sum $aI_r + bTI_r$, $a, b \in \mathbb{R}$, and using induction on r. The above polynomial can be greatly simplified by expanding the determinant about its bottom row to get

$$\det\,(K-\lambda I_{n+1}) = (-1)^{n+1}(\lambda^2 - 2\alpha_n\lambda + 1)d_{n-1}$$

where d_{n-1} is the $(n-1)\times(n-1)$ determinant

$$d_{n-1} = \det\begin{pmatrix} \lambda & 0 & \dots & 0 & 1 \\ 0 & \lambda & \dots & 1 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 1 & \dots & \lambda & 0 \\ 1 & 0 & \dots & 0 & \lambda \end{pmatrix}.$$

It is easy to show that $d_{n-1} = (\lambda^2 - 1)d_{n-3}$ and hence

$$\det\,(K-\lambda I_{n+1}) = \begin{cases} (\lambda^2 - 2\alpha_n\lambda + 1)(\lambda^2-1)^{(n-1)/2}, & n \text{ odd} \\ (\lambda^2 - 2\alpha_n\lambda + 1)(\lambda^2-1)^{(n-2)/2}(-\lambda - 1), & n \text{ even.} \end{cases}$$

Thus we have the remarkable result that the eigenvalues are ± 1 and the two roots of the quadratic equation

$$\lambda^2 - 2\alpha_n\lambda + 1 = 0.$$

Let the matrix P have elements p_{ij} and let π_{ij} be their corresponding cofactors in P. Then

$$\begin{aligned}
\alpha_n &= \sum_{j=0}^{n} \bar{p}_{nj} = \frac{1}{\det P} \sum_{j=0}^{n} \pi_{jn} \\
&= \frac{1}{\det P} \det \begin{pmatrix} p_{00} & \cdots & p_{0,n-1} & 1 \\ p_{10} & \cdots & p_{1,n-1} & 1 \\ \vdots & & \vdots & \vdots \\ p_{n0} & \cdots & p_{n,n-1} & 1 \end{pmatrix} \\
&= \frac{\det \begin{pmatrix} 1+\nu^2 B_{11} & \cdots & \nu^2 B_{1,n-1} & 1-\nu^2 B_{10} \\ \nu^2 B_{21} & \cdots & \nu^2 B_{2,n-1} & 1-\nu^2 B_{20} \\ \vdots & & \vdots & \vdots \\ \nu^2 B_{n1} & \cdots & \nu^2 B_{n,n-1} & 1-\nu^2 B_{n0} \end{pmatrix}}{\det \begin{pmatrix} 1+\nu^2 B_{11} & \cdots & \nu^2 B_{1,n-1} & \nu^2 B_{1n} \\ \nu^2 B_{21} & \cdots & \nu^2 B_{2,n-1} & \nu^2 B_{2n} \\ \vdots & & \vdots & \vdots \\ \nu^2 B_{n1} & \cdots & \nu^2 B_{n,n-1} & 1+\nu^2 B_{nn} \end{pmatrix}}
\end{aligned}$$

which is a quotient of polynomials of degree n in ν^2.

Finally we must verify that the multiple eigenvalues at ± 1 do not lead to unbounded solutions. To do this we must show that the matrix K is non-defective, i.e. possesses a full set of eigenvectors, when $\alpha_n \neq \pm 1$. This turns out to be a relatively simple task, for example with $\lambda = 1$ the matrix equation

$$(K - \lambda I_{n+1})\mathbf{r} = \mathbf{0}$$

has the components

$$\begin{aligned}
r_0 - r_n &= 0 \\
r_1 + r_{n-1} - 2\alpha_1 r_n &= 0
\end{aligned}$$

$$\vdots$$

$$r_0 + (1 - 2\alpha_n)r_n = 0.$$

Let $r_0 = 0 = r_n$. Then for $n = 2i$ these equations are satisfied if $r_i = 0$ and $r_{n-j} = -r_j$ for $j = 1, \ldots, i-1$. By choosing $r_1, \ldots, r_{i-1}$ in turn to be 1 while the other members of that set take the value 0 we obtain $(n-2)/2$ linearly independent eigenvectors corresponding to the eigenvalue $\lambda = 1$ which has multiplicity $(n-2)/2$. Similar arguments apply when n is odd, and for both odd and even n when $\lambda = -1$.

Our conclusions are summarised in the following theorem.

Theorem 3.2 *When the Panovsky-Richardson method of degree n is applied to the test equation $y'' = -\omega^2 y$ with a steplength h, the stability of the resulting solution is determined by the roots of the quadratic equation*

$$\lambda^2 - 2\alpha_n \lambda + 1 = 0$$

where α_n is a rational function of degree $[n/n]$ in $\nu^2 = \omega^2 h^2$. Intervals of periodicity are intervals of values of ν^2 for which $|\alpha_n| < 1$. For these methods intervals of periodicity and intervals of absolute stability coincide.

Proof NED. □

It follows from this theorem that, with regard to stability considerations, the methods of Panovsky and Richardson fall into the class of methods investigated by Coleman [21]. In the terminology of [21] the rational function α_n is the **stability function** of the method. For example, when the method of degree 2 is applied to the test equation, the matrix P defined above is given by

$$P = \begin{pmatrix} 1 & 0 & 0 \\ 7\nu^2/96 & 1 + \nu^2/16 & -\nu^2/96 \\ \nu^2/6 & \nu^2/3 & 1 \end{pmatrix}.$$

Then the stability function is

$$\alpha_n = \frac{288 - 126\nu^2 + 4\nu^4}{288 + 18\nu^2 + \nu^4}.$$

By Theorem 5 of [21] the method is not P-stable, by Theorem 7 its order of dispersion is 4, and the periodicity conditions (see p159 of [21]) are

$$\nu^2 < 48 \qquad \text{and} \qquad (\nu^2 - 12)(5\nu^2 - 48) > 0.$$

Therefore the primary interval of periodicity is (0,9.6) and there is a secondary interval of periodicity (12,48). The order of the method is 4 and its error constant, by Theorem 3.1 above, is 1/720. By contrast Numerov's method, which is based on the formula

$$y_{m+1} - 2y_m + y_{m-1} = \frac{1}{12}h^2(f_{m+1} + 10f_m + f_{m-1})$$

is also of order 4, but has only one implicit stage and requires less information to be carried forward to the next step. However the error constant for Numerov's method is three times that for the above Panovsky-Richardson method and it has a shorter interval of periodicity, (0,6).

Theorem 3.3 *Each Panovsky-Richardson method has a non-empty interval of periodicity, and is absolutely stable for ν^2 sufficiently small.*

Proof Two different methods of proof have been derived. The first proceeds by expanding the determinants in our expression for the stability function α_n, but is rather cumbersome and so is not given here. The second method is far more straightforward and uses the fact that α_n is an approximation for $\cos\nu$. The order of dispersion of the Panovsky-Richardson method of degree n is at least $n+1$, since it is the order of accuracy achieved when that method is applied to the test equation $y'' = -\omega^2 y$. Then from equation (2.8) of [21] we have, as $\nu \to 0$,

$$\alpha_n = \cos\nu + o(\nu^{n+1})$$

$$= 1 - \frac{\nu^2}{2} + o(\nu^2)$$

It follows that for $\nu^2 \in (0, \gamma)$, for some $\gamma > 0$, the modulus of α_n is less than 1. Consequently, $(0.\gamma)$ is an interval of periodicity and of absolute stability. □

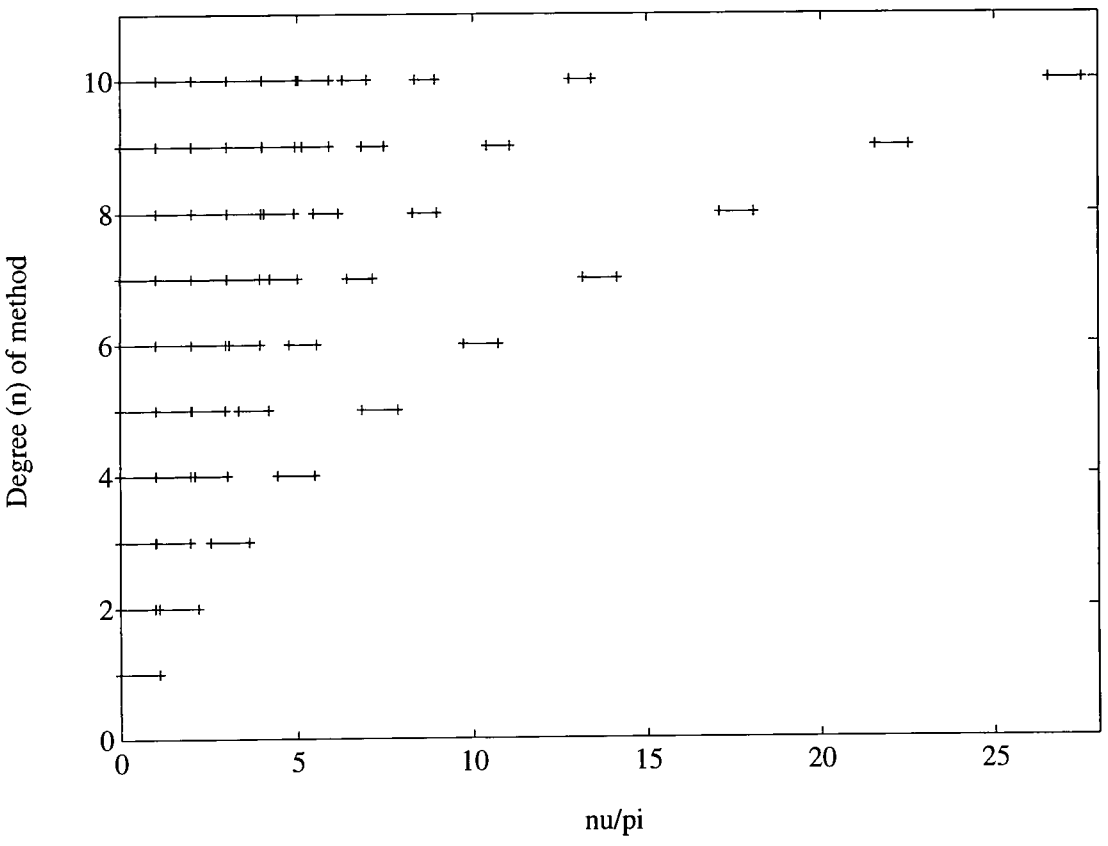

Figure 3.1: Intervals of periodicity for the Panovsky-Richardson methods of degrees 1 to 10.

We have computed the coefficients of the stability function α_n for $n \leq 10$ and then found the corresponding periodicity intervals. These periodicity intervals are shown in figure 3.1 and table 3.1. We have expressed the boundaries of these intervals in terms of ν/π in order to highlight a number of interesting trends in the data. The complexity of the calculations and consequently the time taken to produce the periodicity intervals increases quite sharply as n increases, so we have not pursued a detailed study beyond $n = 10$. However we have identified a number of periodicity

n	b_0	a_1	b_1	a_2	b_2	a_3	b_3	a_4	b_4
1	1.10266								
2	0.98625	1.10266	2.205						
3	0.99817	1.01187	1.972	2.546	3.3632				
4	0.99977	1.00110	1.982	2.103	3.017	4.435	5.488		
5	0.99998	1.00004	1.995	2.017	2.954	3.336	4.186	6.820	7.844
6	1.00000	1.00000	1.999	2.002	2.974	3.077	3.947	4.758	5.543
7	1.00000	1.00000	2.000	2.000	2.993	3.002	3.939	4.213	5.002
8	1.00000	1.00000	2.000	2.000	2.999	3.002	3.975	4.050	4.907
9	1.00000	1.00000	2.000	2.000	3.000	3.000	3.994	4.009	4.941
10	1.00000	1.00000	2.000	2.000	3.000	3.000	3.999	4.001	4.980

n	a_5	b_5	a_6	b_6	a_7	b_7	a_8	b_8	a_9	b_9
6	9.721	10.723								
7	6.400	7.130	13.145	14.131						
8	5.455	6.161	8.276	8.966	17.093	18.068				
9	5.133	5.904	6.824	7.495	10.395	11.056	21.566	22.533		
10	5.033	5.900	6.282	6.963	8.335	8.914	12.760	13.400	26.56	27.53

Table 3.1: Periodicity intervals for the P-R methods of degree n up to 10. The i^{th} periodicity interval takes the form $\nu^2 \in (a_i^2\pi^2, b_i^2\pi^2)$ with $a_0 = 0$.

intervals for n as high as 20.

Our results suggest the following conjectures for which at present we can offer no proof.

Conjectures

1. *The Panovsky-Richardson method of degree n has n disjoint periodicity intervals.*

2. *For fixed i, as $n \to \infty$,*

$$a_i \to i \qquad \text{and} \qquad b_i \to (i+1).$$

Consequently the length of the i^{th} periodicity interval tends to π^2 and the length of the interval of instability between the i^{th} and $(i+1)^{\text{th}}$ periodicity intervals tends to 0 as $n \to \infty$, for fixed i.

3. *For fixed n, the length $(a_{i+1}^2 - b_i^2)\pi^2$ of the i^{th} interval of instability increases with i. Furthermore, $(a_n - b_{n-1})$ increases without bound as $n \to \infty$, and it seems that so also does $(a_{n-i+1} - b_{n-i})$ for each fixed i. In particular, this means that the length of the gap between the penultimate and final intervals of periodicity increases without bound.*

We might wish to attempt to improve upon the performance of these methods by allowing the steplength h to vary. Before doing so however, we must investigate the possible effects of a step-changing routine choosing a steplength which lies in one of the intervals of instability mentioned above. As an example we will apply the Panovsky-Richardson method of degree 16 to an initial value problem used by Kramarz [44]

$$\begin{aligned} y'' &= 2498y + 4998z, \qquad y(0) = 2, \qquad y'(0) = 0 \\ z'' &= -2499y - 4999z, \qquad z(0) = -1, \qquad z'(0) = 0, \end{aligned}$$

for which the exact solution is

$$y(x) = 2\cos x, \qquad z(x) = -\cos x.$$

The initial conditions eliminate the higher-frequency component corresponding to $\omega = 50$. We carried out three calculations, with fixed steplengths $h_1 = 0.65\pi$, $h_2 = 3h_1/4$ and $h_3 = h_1/4$. With $\omega = 50$, the value of ν lies near the middle of the 15th periodicity interval when the steplength is h_1, between the 14th and 15th periodicity intervals when the steplength is h_2 and in the 8th periodicity interval when the steplength is h_3. The results of these calculations are given in Table 3.2. We see that reducing the steplength from h_1 to h_2 leads not to a reduction, but rather to a catastrophic blow-up of the global error. These results show that considerable care must be taken to ensure that the intervals of instability are excluded from the range of allowable steplengths in any variable-step implementation of these methods.

x	h_1	h_2	h_3
1.95π	$8.70\,E-13$	$3.42\,E-13$	$2.01\,E-15$
3.90π	$1.32\,E-12$	$1.31\,E-8$	$3.86\,E-15$
5.85π	$1.42\,E-12$	$5.31\,E-3$	$3.86\,E-15$
7.80π	$1.42\,E-12$	$2.16\,E+4$	$3.86\,E-15$
9.75π	$1.42\,E-12$	$8.79\,E+8$	$5.69\,E-15$

Table 3.2: The maximum absolute errors on intervals $[0, x]$ when the method $PR16$ is applied to a test problem of Kramarz with the steplengths h_1, h_2 and h_3.

3.5 Implementation

In this short section we consider the choice of method used to solve the non-linear equations (3.19) at each step. Panovsky & Richardson [53] used an iteration scheme which resembles the Gauss-Seidel scheme used for linear equations. They work with the methods in their original form (3.10) and iterate to form the a_k^+ quantities using starting values based on data from the previous step. An alternative approach, which

in our tests requires less computation per step, is to solve the equations (3.19) using the Gauss-Seidel-type iteration

$$\begin{aligned} y_{m+\xi_i}^{(r+1)} &= 2y_m - y_{m-1} + \frac{h^2}{2n}{\sum_{j=0}^{n}}'' A_{ij} f_{m-\xi_j} \\ &\quad + \frac{h^2}{2n}{\sum_{j=0}^{i-1}}' A_{ij} f_{m+\xi_j}^{(r+1)} + \frac{h^2}{2n}\sum_{j=i}^{n-1} A_{ij} f_{m+\xi_j}^{(r)} + \frac{h^2}{4n} A_{in} f_{m+1}^{(r)} \end{aligned} \tag{3.49}$$

where $f_{m+\xi_j}^{(r)} = f(x_{m+\xi_j}, y_{m+\xi_j}^{(r)})$ and $y_{m+\xi_j}^{(0)} = y_m$, for $j = 0, 1, \ldots, n$. The single prime on the second summation indicates that the first term in that sum is to be halved.

In the light of the remarks made by Lambert [45] (page 238) regarding the convergence of iterative schemes used in implicit methods for stiff first order systems, we would expect that, for a given problem, the rate of convergence of either of the iteration processes above will depend on the steplength h, and that for h sufficiently large the process will fail to converge. The following two examples show that care must be taken in choosing the iteration process if we are to make use of the relatively large stability intervals provided by these methods.

Example 1 When the degree 1 Panovsky-Richardson method is applied to the test equation $y'' = -\omega^2 y$ with steplength h our Gauss-Seidel-type iteration formula may be written

$$y_{m+1}^{(r+1)} = -\frac{\nu^2}{6} y_{m+1}^{(r)} + \eta,$$

where η contains information from the previous step and is a constant with respect to the iteration process. This method is periodic whenever $\nu^2 < 12$, but to ensure convergence of the iteration scheme we must impose the condition that $\nu^2 < 6$.

Example 2 Replacing the degree 1 Panovsky-Richardson method by the degree 2 method in the above example we obtain the following iteration formula

$$A\mathbf{y}_{\mathbf{m+1}}^{(\mathbf{r+1})} = B\mathbf{y}_{\mathbf{m+1}}^{(\mathbf{r})} + \mathbf{c},$$

where $\mathbf{c}$ is a constant with respect to the iteration process,

$$A = \begin{pmatrix} \frac{1}{96}(96 + 6\nu^2) & 0 \\ 0 & 1 \end{pmatrix}, \qquad B = \begin{pmatrix} 0 & \frac{1}{96}\nu^2 \\ -\frac{1}{3}\nu^2 & 0 \end{pmatrix}$$

and $\mathbf{y_{m+1}^{(r)}} = (y_{m+1/2}^{(r)}, y_{m+1}^{(r)})^T$, for $r = 0, 1, \ldots$. For the above iteration scheme to converge we require that the modulus of the largest eigenvalue of $A^{-1}B$ is bounded above by 1. We find that the eigenvalues of $A^{-1}B$ are of the form $\pm\lambda$, so we can take det $A^{-1}B < 1$ as our convergence condition. After some algebra our convergence condition becomes $\nu^2 < 9 + 3\sqrt{41} \simeq 28$, whereas the secondary periodicity interval in this case extends to 48.

For methods of higher degree also, the Gauss-Seidel scheme fails to converge in some steplength intervals for which the method is absolutely stable.

In most of our calculations we have used a Newton method instead of the Gauss-Seidel iteration. Equation (3.49), without the superscript denoting the mth step, may be written as

$$G(\mathbf{Y}) = \mathbf{Y} - h^2 B\mathbf{F} + \alpha = 0,$$

where α includes all terms which do not depend on the elements of $\mathbf{Y}$.. The Newton formula then gives

$$K(\mathbf{Y^{(r)}} - \mathbf{Y^{(r-1)}}) = -G(\mathbf{Y^{(r-1)}}),$$

where now the superscript denotes the iteration number and $K_{ij} = \delta_{ij} - h^2 B_{ij} J_j$ with

$$J_j = \left.\frac{\partial f}{\partial y}\right|_{m+\xi_j}.$$

The description given here applies to a single differential equation; for a system of equations J_j becomes a Jacobian matrix. This approach not only allows calculations at larger steplengths, but it also reduces, sometimes very substantially, the number of iterations needed to achieve convergence to a given accuracy. Of course an assessment of computational efficiency would involve not only the iteration count, but also the

cost of each iteration and of any overheads such as Jacobian evaluations for Newton's method.

3.6 Numerical results

In this section we present the results of a number of numerical experiments involving both linear and non-linear test problems. Unless otherwise stated, all these results were produced from FORTRAN programs running in double precision on a Sun 4 workstation. Our experiments have shown that, subject to the effects of rounding error, the first 20 Panovsky-Richardson methods exhibit roughly the same qualitative behaviour, consequently we have restricted our attention to the methods of orders 4, 6 and 8. Finally, in view of the oscillatory nature of the observed global errors of these methods, we take as our measure of accuracy the maximum absolute global error over a given interval.

Duffing's equation

Following Panovsky and Richardson [53] we take as our first test problem the conservative Duffing's equation

$$y'' + (1 - k^2)y = 2k^2y^3; \quad y(0) = 0, y'(0) = 1. \tag{3.50}$$

which has as its solution the Jacobi elliptic functions

$$y(x) = \mathrm{sn}(x; k),$$

(see e.g. Luke [48] p90).

Panovsky and Richardson give some results for this problem, but since they did not divulge the value of k they used, we conducted tests of our own using a number of different k values. Table 3.3 and figure 3.2 show the results of applying the eighth order Panovsky-Richardson methods PR6 and PR7, as well as an eighth order explicit

Runge-Kutta-Nyström method due to Hairer [32] to (3.50) with $k = 0.5$. We see from this table that for the fixed steplength $h = 0.5$, the PR7 method is the most accurate, and that the RKN8 method performs rather poorly. To compare the long-term behaviour of the global error we repeated our computations with the PR6 and RKN8 methods with stepsizes chosen so that the methods would have roughly the same maximum global error over the interval $[0, 200]$ as that of the PR7 method with $h = 0.5$. These results clearly demonstrate the linear dependence of the maximum global error on the length of integration interval for the two Panovsky-Richardson methods as noted by Panovsky and Richardson [53], and the near quadratic dependence in the case of the RKN8 method.

	$h = 0.5$			$h = 0.315$	$h = 0.145$
x	RKN8	PR6	PR7	PR6	RKN8
100	4.01 E-05	1.89 E-08	5.86 E-10	8.52 E-10	3.98 E-10
200	1.76 E-04	3.93 E-08	1.22 E-09	1.73 E-09	1.85 E-09
500	1.13 E-03	9.88 E-08	3.08 E-09	4.39 E-09	1.24 E-08
1000	4.54 E-03	1.98 E-07	6.15 E-09	8.78 E-09	5.06 E-08
2000	1.82 E-02	3.94 E-07	1.23 E-08	1.76 E-08	2.06 E-07
5000	1.14 E-01	9.88 E-07	3.08 E-08	4.40 E-08	1.29 E-06

Table 3.3: Maximum absolute errors on intervals $[0, x]$ when methods PR6, PR7 and RKN8 are applied to (3.50) with $k = 0.5$.

The Stiefel-Bettis problem

In testing an exponential-fitting method for second order equations, Stiefel and Bettis used the initial value problem

$$z'' + z = 0.001e^{ix}, \quad z(0) = 1, \quad z'(0) = 0.9995i, \tag{3.51}$$

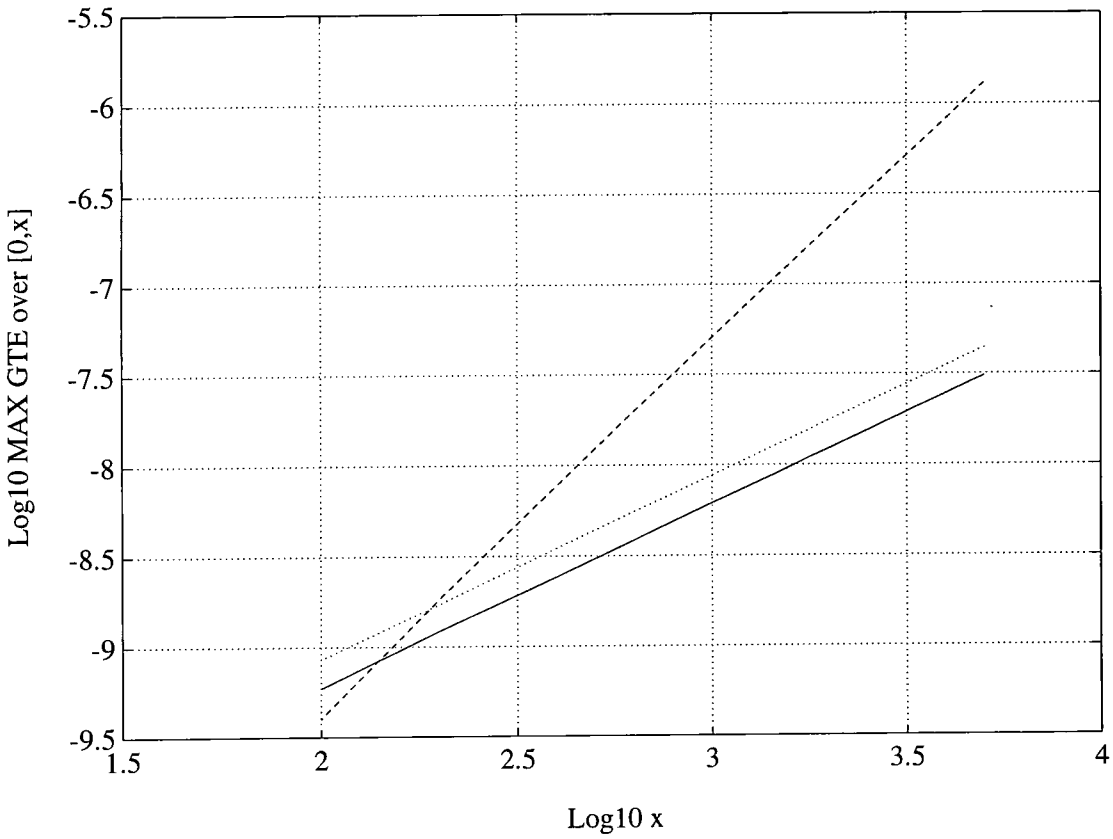

Figure 3.2: Long-term propagation of the maximum global errors in the methods PR6, PR7 and RKN8 when applied to Duffings equation with $k = 0.5$ and with steplengths chosen so that the maximum global errors on [0,200] were approximately in agreement with that of PR7 with $h = 0.5$. Solid line = PR7, dotted line = PR6, dashed line = RKN8

which represents a perturbed harmonic oscillator with a perturbation in resonance with the unperturbed oscillation. This problem has exact solution

$$z = (1 + 0.0005ix)e^{ix}.$$

This problem has subsequently been used by numerous authors to test and compare other methods, particularly those designed for problems with nearly periodic solutions. In order to solve this problem numerically we first split equation (3.51) into two coupled equations by setting $z = x + iy$.

h	RKN4	PR2	PR3	T4	PR4	PR5	T6
$\pi/2$	8.70E-01	-1.17E-02	-1.11E-03		-2.95E-05	3.57E-07	
$\pi/4$	5.89E-02	-7.53E-04	-6.58E-05	-7.15E-05	-4.71E-07	1.02E-08	-5.61E-06
$\pi/8$	1.75E-03	-4.81E-05	-4.06E-07	-7.94E-07	-7.40E-09	1.79E-10	-1.45E-08
$\pi/16$	4.54E-05	-3.03E-06	-2.53E-07	-1.35E-08	-1.16E-10	2.87E-12	7.60E-09

Table 3.4: Errors in the computed value of $|z(40\pi)|$, where z is the solution of the Stiefel-Bettis problem.

Table 3.4 shows the results obtained by applying several methods of orders 4 and 6 to this problem. The number tabulated in each case is the error in approximating $|z(40\pi)| = (1 + 0.0004\pi^2)^{1/2}$. The Panovsky-Richardson methods PR2 and PR3 have order 4, PR4 and PR5 have order 6; the columns headed T4 and T6 contain results produced by Thomas [60] using a fourth order method with a phase lag of order 6, and a sixth order method with a phase lag of order 8 respectively, and finally the column headed RKN4 contains results obtained from a popular explicit fourth order Runge-Kutta-Nyström method (see Hairer et al. [35], p262).

Thomas' fourth order method T4 is the most accurate of the four fourth order methods, which we would expect since it has the advantage of a sixth order phase lag. Since the RKN4 method is explicit and has no interval of periodicity, it is not surprising that this is the least accurate method, indeed we would expect a rather sharp increase in its global error if the integration interval were to be extended. By

contrast, the situation for the sixth order methods is not what we would have expected at all. Thomas' sixth order method T6 has the advantage of an eighth order phase lag and is the best of the methods considered by Thomas [60] for this problem, yet the Panovsky-Richardson method PR5, which lacks this advantage, is significantly more accurate. This is perhaps explained by the fact that the error constant for the PR5 method, which from equation (3.40) is approximately 2.6×10^{-8}, is very much smaller than the figures quoted by Thomas [60] for the methods studied in that paper.

We have also studied the propagation of the maximum global error over intervals $[0, x]$ for this problem and have found the same linear growth as was observed in the results for the previous problem.

The two body problem

Following Panovsky and Richardson [53] we adopted the two body problem as our final test problem. This problem is also used commonly in the literature for testing numerical methods. The problem as given by Panovsky and Richardson contains a misprint and should read

$$y'' + y/r^3 = 0; \quad y(0) = a(1-e), \quad y'(0) = 0, \tag{3.52}$$

$$z'' + z/r^3 = 0; \quad z(0) = 0, \quad z'(0) = a^{-1/2}\sqrt{(1+e)/(1-e)}, \tag{3.53}$$

with $r^2 = y^2 + z^2$. This has exact solution

$$y = a(\cos(E) - e), \qquad z = a\sqrt{1-e^2}\sin(E),$$

where e is the eccentricity of the orbit, and the eccentric anomaly E is defined implicitly by Kepler's equation

$$x = a^{3/2}(E - e\sin(E)).$$

To remove the confusion caused by the misprint in [53] and since the value of

a used to produce the numerical results was not given in that paper, most of our calculations were carried out with a set to 1. Some time after these calculations were performed we learned that the authors had in fact used $a = (10/(2\pi))^{2/3}$. Using this

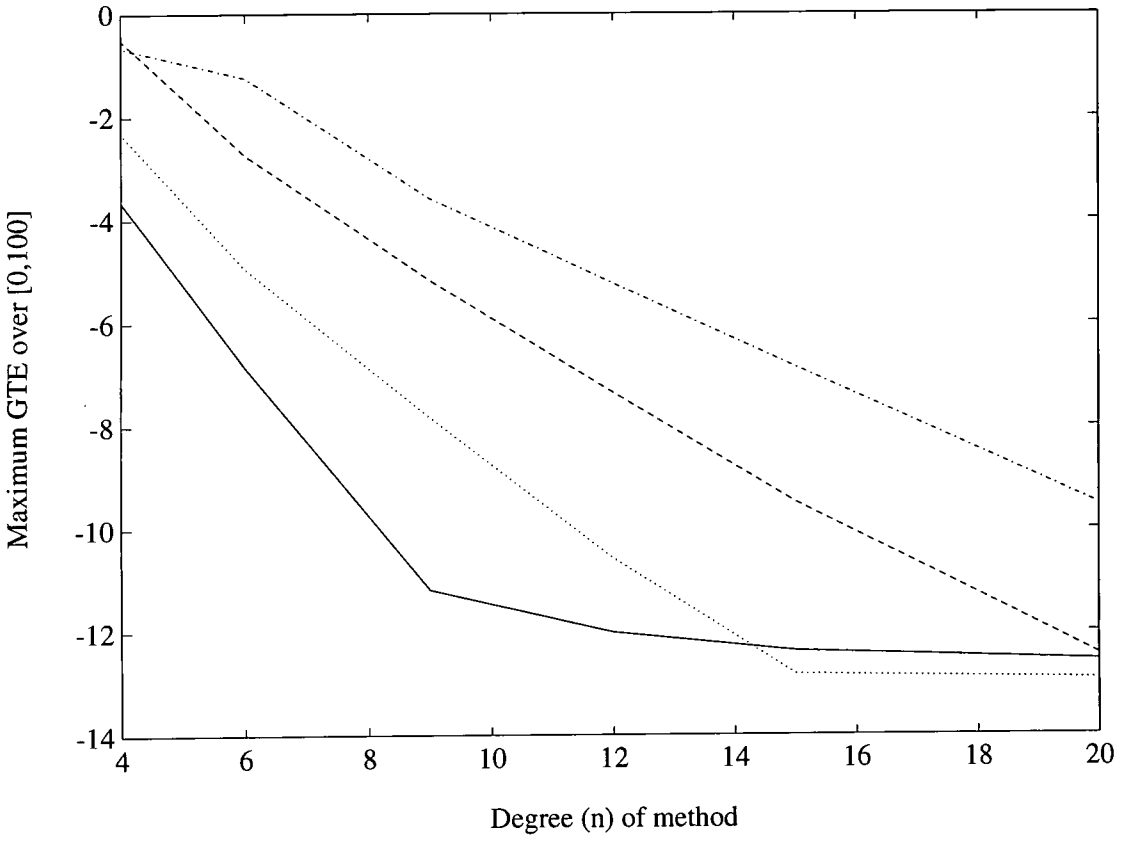

Figure 3.3: Maximum global errors over the interval $[0, 100]$ for methods PR4, PR6, PR9, PR12, PR15 and PR20 with four different stepsizes. Solid line: $h = 0.5$, dotted line: $h = 1.0$, dashed line: $h = 2.0$ and dash-dotted line: $h = 3.0$.

value of a we have produced figure 3.3, which is an attempt to reproduce figure 2 of [53]. Our results are very close to those of Panovsky and Richardson, except for those at around 10^{-12}. By repeating our calculations using FORTRAN quadruple precision (32 digits) we confirmed our suspicion that both our results and those of Panovsky and Richardson were severely affected by rounding errors, and that these differences were most likely due to the different floating point representations used by our respective computers. This rather severe build up of rounding error has been

evident in our results for all three test problems where small stepsizes were used, and could cause difficulties if these methods were ever used in a variable stepsize code. Later in this chapter we will show that by supplying alternative starting values to the Panovsky-Richardson methods, they can be reformulated in such a way as to significantly reduce the effect of rounding errors.

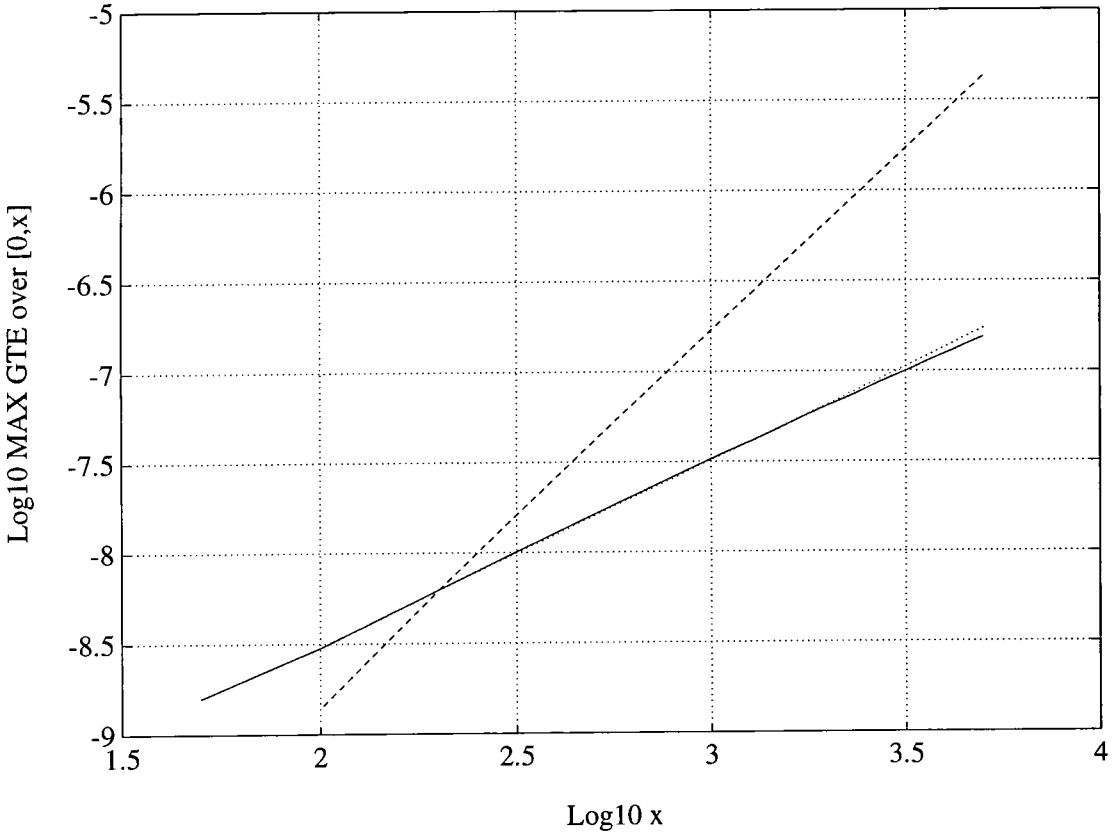

Figure 3.4: Long-term propagation of the maximum global errors in the methods PR6, PR7 and RKN8 when applied to the two body problem with $a = 1$ and $e = 0.1$ and with steplengths chosen so that the maximum global errors on [0,200] were approximately in agreement with that of PR7 with $h = 0.5$. Solid line = PR7, dotted line = PR6, dashed line = RKN8

Table 3.5 and figure 3.4 show the results of applying the three eighth order methods PR6, PR7 and RKN8 to the two body problem with $a = 1$ and $e = 0.1$. For the fixed stepsize $h = 0.5$ we see that the PR7 is the most accurate and that once again the RKN8 method performs rather poorly. To investigate the long-term behaviour of the

	$h = 0.5$			$h = 0.309$	$h = 0.125$
x	RKN8	PR6	PR7	PR6	RKN8
100	3.19 E-04	1.04 E-07	2.99 E-09	2.98 E-09	1.39 E-09
200	1.40 E-03	2.16 E-07	6.24 E-09	6.22 E-09	6.22 E-09
500	9.38 E-03	5.63 E-07	1.62 E-08	1.59 E-08	4.14 E-08
1000	3.86 E-02	1.14 E-06	3.27 E-08	3.23 E-08	1.69 E-08
2000	1.54 E-01	2.28 E-06	6.44 E-08	6.54 E-08	6.78 E-07
5000	9.19 E-01	5.66 E-06	1.54 E-07	1.72 E-07	4.26 E-06

Table 3.5: Maximum absolute errors on intervals $[0, x]$ when methods PR6, PR7 and RKN8 are applied to the two body problem with $a = 1$ and $e = 0.1$

maximum global error of these methods for this problem we repeated our calculations with the PR6 and RKN8 method with stepsizes chosen so that their maximum global errors over the interval $[0, 200]$ were approximately equal to that of the PR7 method with $h = 0.5$; the results of these calculations are shown in figure 3.4 and in the final two columns of table 3.5. Once again we see a near linear dependence on x of the maximum global error for the Panovsky-Richardson methods, while for the RKN8 method this dependence is approximately quadratic. It is also interesting to note that the ratio of the maximum global errors of the two Panovsky-Richardson methods remains approximately constant over the interval $[0, 5000]$.

Calvo & Sanz-Serna [5] has shown that if a symplectic Runge-Kutta-Nyström method (see section 2.2.3) is applied to Kepler's two-body problem with a constant stepsize, then the maximum global error will exhibit a linear dependence on the length of the integration interval. Since the Panovsky-Richardson methods of degrees 1 to 20 exhibit this same linear dependence when applied to this problem, we began to wonder if these methods were in fact symplectic. Later in this chapter we will see that this is not the case. We have as yet been unable to determine why the maximum global error should grow linearly in the case of the Panovsky-Richardson methods, and quadratically in the case of certain explicit Runge-Kutta-Nyström methods

3.7 Generalised Panovsky-Richardson methods

In this section we extend the methods of Panovsky and Richardson to allow arbitrary interpolation nodes. These methods, which we call "Generalised Panovsky-Richardson methods", or GPR methods, have been introduced in order to both extend the applicability of the main result of the next section, and to greatly simplify the proof of that result.

We begin, as in Section 3.1, with the identity

$$y(x+sh) - 2y(x) + y(x-sh) = \int_x^{x+sh} (x+sh-z)[f(z) + f(2x-z)]dz \qquad (3.54)$$

where, as before, the second argument of the function f has been temporarily suppressed. Once again we let $x_m = x_0 + mh$ for $m = 0, 1, 2, \ldots$ and h fixed. Taking $x = x_m$ and $z = x_m + \tau h$ we can write (3.54) as

$$y(x_m+sh) - 2y(x_m) + y(x_m-sh) = h^2 \int_0^s (s-\tau)[f^+(\tau) + f^-(\tau)]d\tau \qquad (3.55)$$

where

$$f^{\pm}(\tau) = f(x_m \pm \tau h)$$

Let $f^{\pm}(\tau)$ be approximated by interpolating polynomials of degree n based on a set of $n+1$ distinct nodes $\{c_i\}_{i=0}^n$, i.e.,

$$f^{\pm}(\tau) = \sum_{j=0}^{n} l_j(\tau) f^{\pm}(c_j)$$

with

$$l_j(\tau) = \prod_{\substack{i=0 \\ i \neq j}}^{n} \frac{\tau - c_i}{c_j - c_i} = \frac{M(\tau)}{(\tau - c_j)M'(c_j)} \qquad (3.56)$$

and

$$M(\tau) = \prod_{i=0}^{n} (\tau - c_i).$$

Let y_m and $y_{m\pm c_i}$ be approximations for $y(x_m)$ and $y(x_{m\pm c_i})$ respectively, and let

$$f_{m\pm c_i} = f(x_{m\pm c_i}, y_{m\pm c_i}),$$

then from equation (3.55) we obtain the formulae

$$y_{m+c_i} = 2y_m - y_{m-c_i} + h^2 \sum_{j=0}^{n} B_{ij}(f_{m+c_j} + f_{m-c_j}) \tag{3.57}$$

where

$$B_{ij} = \int_0^{c_i} (c_i - \tau) l_j(\tau) d\tau, \qquad i, j = 0, 1, \ldots, n. \tag{3.58}$$

If the nodes $\{c_i\}_{i=0}^n$ are restricted to the interval $[0, 1]$ with

$$0 = c_0 < c_1 < \ldots < c_{n-1} < c_n = 1 \tag{3.59}$$

then (3.57) gives a set of n equations from which y_{m+1} and the off-step values y_{m+c_i}, for $i = 1, 2, \ldots, n-1$, may be calculated. As with the methods of Panovsky and Richardson, in any implementation of these 2-step hybrid methods we must provide the $n+1$ starting values $y_m, y_{m-c_1}, \ldots, y_{m-c_{n-1}}, y_{m-1}$. If these methods were to be included in a variable stepsize code, then a similar problem would arise at each change of the steplength h.

The Panovsky-Richardson method of degree n is based on the nodes

$$c_j = \tfrac{1}{2}(1 + \alpha_j), \qquad \text{with} \qquad \alpha_j = \cos[(n-j)\pi/n], \tag{3.60}$$

for $j = 0, 1, \ldots, n$. With this choice of nodes it can be shown that, for $j = 1, 2, \ldots, n-1$,

$$l_j(\tau) = \frac{(-1)^{n-j+1}(1-\alpha^2)T_n'(\alpha)}{n^2(\alpha - \alpha_j)} \tag{3.61}$$

where $\alpha = 2\tau - 1$. The corresponding expressions for the cases $j = 0, n$ are found by halving the right-hand side of the above equation and substituting the appropriate value of j. It can then be shown that (3.57) gives (3.19) with the coefficients as given

in equation (3.28).

The Panovsky-Richardson interpolation nodes display the symmetry property

$$c_{n-j} = 1 - c_j, \qquad \text{for} \qquad j = 0, 1, \ldots, \lceil (n-1)/2 \rceil. \tag{3.62}$$

This symmetry property, which is a feature of a number of node choices based on the zeros or extrema of orthogonal polynomials, plays a crucial role in the equivalence to be discussed in the next section, and also in the following preparatory lemma.

Lemma 3.4 *If the set of real numbers* $\{c_i\}_{i=0}^n$ *satisfies conditions (3.59) and (3.62) then, for* $j = 0, 1, \ldots, n$,

$$B_{nj} + B_{nn-j} = \int_0^1 l_j(\tau) d\tau. \tag{3.63}$$

Proof From (3.56) we can write

$$l_{n-j}(\tau) = \prod_{\substack{i=0 \\ i \neq j}}^{n} \frac{\tau - c_{n-i}}{c_{n-j} - c_{n-i}} = \prod_{\substack{i=0 \\ i \neq j}}^{n} \frac{(1-\tau) - c_i}{c_j - c_i} = l_j(1-\tau). \tag{3.64}$$

Hence

$$B_{nn-j} = \int_0^1 (1-\tau) l_j(1-\tau) d\tau = \int_0^1 \sigma l_j(\sigma) d\sigma, \tag{3.65}$$

with $\sigma = 1 - \tau$. The required result follows immediately. □

3.8 The equivalence of GPR and collocation methods

In this section we will show how the Generalised Panovsky-Richardson methods are equivalent to one-step collocation methods providing that the starting values for the GPR methods are chosen in a particular way.

Let $\{c_i\}_{i=0}^n$ be distinct real numbers satisfying condition (3.59). Let h, x_m and y_m be as previously defined, and let z_m be an approximation for $y'(x_m)$. Recall from

section 2.2.4 that a one-step collocation method for the differential equation (3.1) based on the nodes $\{c_i\}_{i=0}^n$ may be written as the following Runge-Kutta-Nyström method:

$$y_{m+c_i} = y_m + c_i h z_m + h^2 \sum_{j=0}^{n} B_{ij} f_{m+c_j}, \qquad i = 0, 1, \ldots, n \tag{3.66}$$

$$y_{m+1} = y_m + h z_m + h^2 \sum_{j=0}^{n} b_j f_{m+c_j} \tag{3.67}$$

$$z_{m+1} = z_m + h \sum_{j=0}^{n} d_j f_{m+c_j} \tag{3.68}$$

where

$$B_{ij} = \int_0^{c_i} (c_i - \tau) l_j(\tau) d\tau \tag{3.69}$$

$$b_j = \int_0^1 (1 - \tau) l_j(\tau) d\tau \tag{3.70}$$

$$d_j = \int_0^1 l_j(\tau) d\tau. \tag{3.71}$$

For brevity, we shall refer to these collocation-based Runge-Kutta-Nyström methods as CRKN methods. A symmetric CRKN method is one whose collocation nodes satisfy the symmetry conditions (3.62).

The following lemma will be used in the proof of the main result of this section.

Lemma 3.5 *The approximations determined by a symmetric CRKN method satisfy the equations*

$$c_i h z_{m+1} = y_{m+1} - y_{m+c_{n-i}} + h^2 \sum_{j=0}^{n} B_{ij} f_{m+c_{n-j}}$$

for $i = 1, \ldots, n$ *and* $m = 0, 1, \ldots$.

Proof Let $u \in \mathcal{P}_{n+2}$ be the polynomial satisfying the collocation conditions defining the symmetric CRKN method, then we have

$$u''(x_m + sh) = \sum_{j=0}^{n} l_j(s) f_{m+c_j}$$

Integrating this twice over the range $(s,1)$ and using $u(x_{m+1}) = y_{m+1}$ and $u'(x_{m+1}) = z_{m+1}$, we obtain

$$(1-s)hz_{m+1} = y_{m+1} - u(x_m + sh) + h^2 \sum_{j=0}^{n} \int_s^1 (\tau - s) l_j(\tau) d\tau \; f_{m+c_j}$$

In particular, if $s = c_{n-i} = 1 - c_i$ then

$$\int_{1-c_i}^{1} (\tau - 1 + c_i) l_j(\tau) d\tau = \int_0^{c_i} (c_i - \sigma) l_j(1-\sigma) d\sigma = B_{in-j}$$

from (3.64). The required results follows. □

Define the quantities $w_m^{(i)}$, for $i = 1, \ldots, n$ and $m = 1, 2, \ldots$, by the relations

$$c_i h w_m^{(i)} = y_m - y_{m-c_i} + h^2 \sum_{j=0}^{n} B_{ij} f_{m-c_j}. \tag{3.72}$$

Using these definitions, the forward stepping stage of our GPR method (3.57) may be written as

$$y_{m+1} = y_m + h w_m^{(n)} + h^2 \sum_{j=0}^{n} B_{nj} f_{m+c_j} \tag{3.73}$$

Substituting $m+1$ for m and setting $i = n$ in (3.72), and using (3.73) we obtain

$$h w_{m+1}^{(n)} = h w_m^{(n)} + h^2 \sum_{j=0}^{n} B_{nj} (f_{m+1-c_j} + f_{m+c_j}) \tag{3.74}$$

Making use of the symmetry condition (3.62), we may write this as

$$w_{m+1}^{(n)} = w_m^{(n)} + h \sum_{j=0}^{n} (B_{nj} + B_{nn-j}) f_{m+c_j}$$

Using Lemma 3.4 and equation (3.71) to simplify this further, we obtain

$$w_{m+1}^{(n)} = w_m^{(n)} + h \sum_{j=0}^{n} d_j f_{m+c_j}. \tag{3.75}$$

Equations (3.73) and (3.75) are of the same form as equations (3.67) and (3.68) of

the corresponding CRKN method, but the off-step values f_{m+c_i} appearing in the two sets of equations may be different.

More generally, the GPR method (3.57) can be re-expressed as

$$y_{m+c_i} = y_m + c_i h w_m^{(i)} + h^2 \sum_{j=0}^{n} B_{ij} f_{m+c_j} \tag{3.76}$$

with $w_m^{(i)}$ as defined in (3.72). This differs from the CRKN method (3.66)-(3.68) in that this method appears to use a different derivative approximation, $w_m^{(i)}$, in calculating each of the off-step values y_{m+c_i}.

In theorem 3.6 we show that if the corresponding CRKN method is used to start the GPR method, then the derivative approximations $w_m^{(i)}$ are independent of i, and the two methods are equivalent.

Theorem 3.6 *Let $\{c_i\}_{i=0}^n$ be a set of distinct nodes in $[0,1]$ such that $c_0 = 0 < c_1 < \ldots < c_{n-1} < 1 = c_n$ and $c_{n-i} = 1 - c_i$, for $i = 0, 1, \ldots, \lceil n/2 \rceil$. Two numerical methods are based on these nodes, the GPR method (3.57) and the CRKN method (3.66)-(3.68). If the starting values provided for the former method are the approximations generated by the latter on $[x_0, x_1]$, then the two methods would give identical results at all subsequent steps if the arithmetic could be done exactly.*

Proof Suppose that the CRKN method is used to provide the starting values required by the GPR method on $[x_0, x_1]$. Now consider the first step of the GPR method. From Lemma 3.5 we have

$$w_1^{(i)} = z_1 \qquad \text{for } i = 1, \ldots, n$$

so that, for this step, the two methods give identical results. In the second step, lemma 3.5 once again gives us that $w_2^{(i)} = z_2$ and so the two methods produce identical results in this step also. The required result follows by induction on the number of steps. □

It can be shown that if the GPR method is started by an alternative method, then it

is still the case that the derivative approximations $w_m^{(i)}$ are independent of i, however the equivalence between the CRKN and GPR methods is lost.

3.9 P-stability and symplecticness

In section 3.4 we derived the stability function for the Panovsky-Richardson methods and tabulated the periodicity intervals of the methods of degree up to 10. Based on these results we conjectured that none of the Panovsky-Richardson methods would be P-stable. With the equivalence established in the previous section, we are now in a position to be able to prove the more general result that none of the Generalised Panovsky-Richardson methods are P-stable. This equivalence has also greatly simplified the analysis of the symplecticness of the Panovsky-Richardson methods, and has led to a proof of the second result of this section: that none of the Panovsky-Richardson methods are symplectic.

We begin with the question of P-stability.

Theorem 3.7 *Generalised Panovsky-Richardson methods are not P-stable for any choice of interpolation nodes.*

Proof The stability analysis of section 3.4 was devised for the Panovsky-Richardson methods, but it does not rely on a particular choice of interpolation nodes. With the appropriate interpretation of the matrix B, the analysis applies to all GPR methods. Furthermore, this analysis makes no reference to the choice of starting values, so it applies to the CRKN methods, and to any other implementations of the GPR formulae. Since Coleman [22] has proved that there are no P-stable symmetric one-step collocation methods (i.e. CRKN methods), the result follows. □

In view of the equivalence established in the previous section, we have at our disposal two quite different methods of analysing the stability properties of the GPR methods: our method from section 3.4, and that of Kramarz [44]. Whilst we express the stability function α_n as a ratio of determinants of $n \times n$ matrices, Kramarz'

expression is a ratio of determinants of 2×2 matrices. Clearly the matrices involved in these expressions must be related in some way, but this relation has so far eluded us.

Conditions under which a Runge-Kutta-Nyström method with no redundant stages is symplectic have been derived and are attributed to Suris. In the notation of the previous section, these conditions are

$$b_i = (1 - c_i)d_i \qquad 0 \leq i \leq n \tag{3.77}$$

and

$$d_j(b_i - B_{ji}) = d_i(b_j - B_{ij}) \qquad 0 \leq i, j \leq n \tag{3.78}$$

For a brief discussion of symplecticness and symplectic methods, the reader is referred to section 2.2.3.

Theorem 3.8 *The Panovsky-Richardson methods are not symplectic.*

Proof *(i) The conditions (3.77).*

From equations (3.70), (3.71) and (3.56).

$$\begin{aligned} b_i - (1 - c_i)d_i &= \int_0^1 (c_i - \tau) l_i(\tau) d\tau \\ &= \frac{1}{M'(c_i)} \int_0^1 M(\tau) d\tau. \end{aligned}$$

For symmetric nodes,

$$M(1 - s) = (-1)^{n+1} M(s)$$

and consequently conditions (3.77) are satisfied when n is even, and in fact for all choices of the interpolation nodes $\{c_i\}_{i=0}^n$. In other words every symmetric CRKN method with an odd number of stages satisfies the first set of the Suris conditions.

Such a general result does not exist for methods with an even number of stages, so we restrict our attention to the Panovsky-Richardson methods. In this case, letting

$\tau = \frac{1}{2}(1+\alpha)$ and with $c_i = \frac{1}{2}(1+\alpha_i)$ where α_i is as previously defined, we have

$$\begin{aligned}\int_0^1 M(\tau)d\tau &= \frac{-1}{n2^{2n+1}}\int_{-1}^1 (1-\alpha^2)T_n'(\alpha)d\alpha \\ &= \frac{1}{n(n^2-4)2^{2n-1}}\end{aligned}$$

from our derivation of the coefficients A_{ii} in section 3.2. It follows that the Panovsky-Richardson methods of odd degree are not symplectic.

(ii) The conditions (3.78).

In what follows it will be assumed that n is even, so that conditions (3.77) are satisfied. If $c_n = 1$ then the method is an FSAL method, i.e.

$$b_i = B_{ni} \qquad 0 \leq i \leq n$$

and condition (3.77) with $i = n$ gives

$$b_n = 0.$$

Then the conditions (3.78) corresponding to the choice $j = n$ reduce to

$$d_i B_{in} = 0 \qquad 0 \leq i \leq n \tag{3.79}$$

We will now prove that both d_1 and B_{1n} are non-zero for the Panovsky-Richardson methods.

Equation (3.69) gives

$$B_{1n} = \int_0^{c_1} (c_1 - \tau) l_1(\tau) d\tau \neq 0$$

since the integrand is of constant sign on the interval $(0, c_1)$.

Two methods of proof have been found to show that $d_1 \neq 0$. The first proceeds by deriving an alternative expression for d_1, but this is rather long and is not given

here, for further details see Coleman & Booth [23]. For the second method we notice that the numbers d_i are, apart from a factor of 2, the weights of a Clenshaw-Curtis quadrature formula, so that the conclusion $d_1 > 0$ is a special case of the result, proved by Imhof [39], that the Clenshaw-Curtis weights are all positive. □

The two body problem revisited

In section 3.6 we noted that for the two body problem, and indeed for all the problems considered, the maximum global error of the Panovsky-Richardson methods appears to exhibit a linear dependence on the length of integration interval. The errors quoted in that section for the two body problem were the maximum modulus of the global errors in the approximation of $y(x)$ and $z(x)$. It turns out that the error in the approximation for $z(x)$ is, at least on the integration intervals considered, very much larger than the corresponding error in the $y(x)$ approximation, and it is this error which appears to grow linearly with the length of the integration interval. The error in the approximation for $y(x)$, on the other hand, displays a quadratic dependence on the length of the integration interval and will, if this interval is extended sufficiently, eventually exceed the error in the approximation for $z(x)$. Figure 3.5 shows the results of applying the sixth order PR5 method to the two body problem with $a = 1$, $e = 0.1$ and h set to $\pi/5$, so that the method performs ten steps per orbit. Similar results were obtained for other steplengths and degrees of method.

3.10 Propagation of rounding errors

In carrying out the calculations in section 3.6 we found that the effects of rounding error can build up rapidly in the Panovsky-Richardson methods. These effects are illustrated by the changes in the shape of the curves at around 10^{-12} in the graphs contained in that section. We have found that, in addition to its other benefits, the CRKN formulation of these methods is far more stable with respect to the propagation of rounding errors.

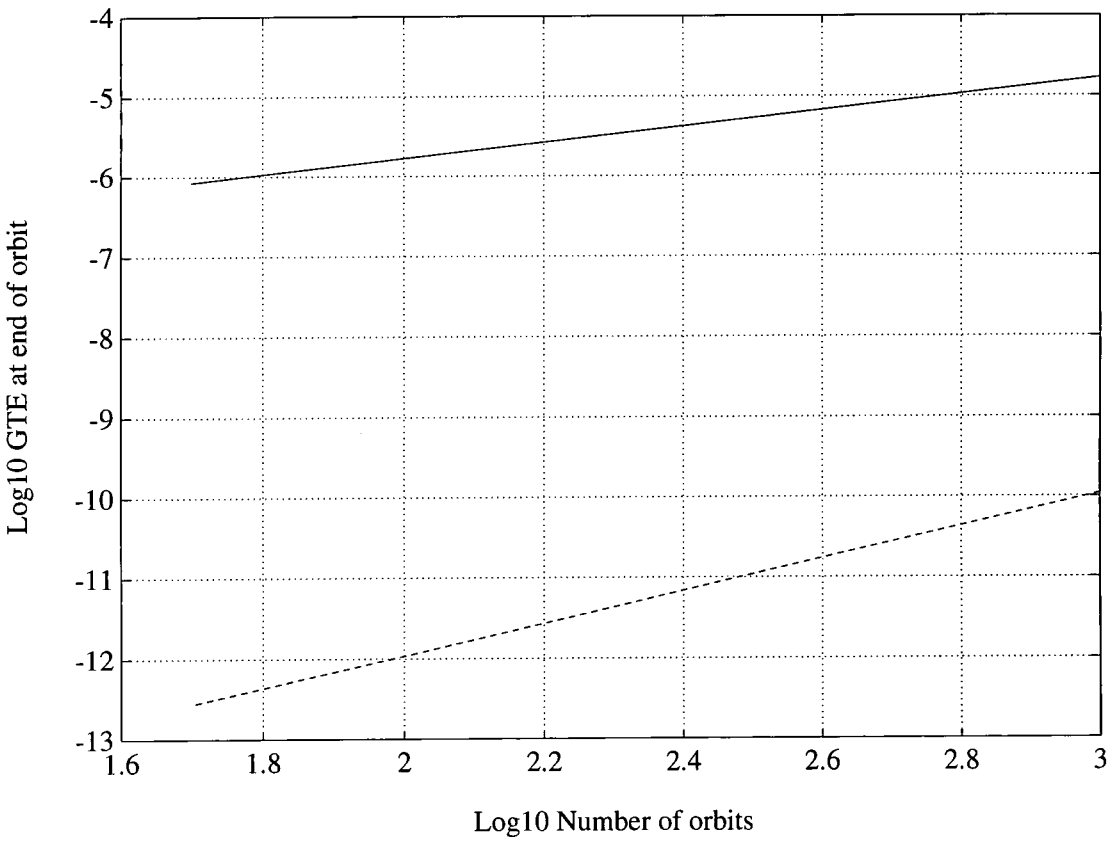

Figure 3.5: Maximum global errors in the approximations for $y(x)$ (dotted line) and $z(x)$ (solid line) at the end of each orbit when the PR5 method is applied to the two body problem with $a = 1$, $e = 0.1$ and $h = \pi/5$.

There are many instances of mathematically equivalent formulations of a numerical method producing very different results. Hairer et al. [35] applied the Störmer formula

$$y_{n+1} - 2y_n + y_{n-1} = \frac{h^2}{12}(13f_n - 2f_{n-1} + f_{n-2})$$

in this form, and in an equivalent one-step formulation to $y'' = -y$. The effects of rounding error were found to be far more severe in the original version. Also Henrici [38] pointed out the superiority of the "summed form" of the Störmer-Cowell methods in this respect. Note that, unlike our CRKN formulation of the GPR methods, while the reformulated methods of Hairer et al. [35] and Henrici [38] may be interpreted as one-step methods, they still require the same number of starting values as the original methods. In view of the structural similarity of the Störmer-Cowell methods and our GPR methods, it is reasonable to expect our one-step formulation to be the more stable with respect to the propagation of rounding errors, and indeed this turns out to be the case.

The Panovsky-Richardson methods may be formulated as in equation (20) of [53], as the two-step hybrid form of equation (3.19) of section 3.2 and as the CRKN method (3.66)-(3.68) of section 3.8 with the nodes $\{c_i\}$ given by (3.60). In exact arithmetic these three formulations would yield identical results, however our computers are not capable of exact floating point arithmetic and so rounding errors are inevitable. To show the differences in the build-up of rounding errors in these formulations we have applied them to a linear, a non-linear and a stiff test problem. Since we have observed no significant differences in the results given by the first two formulations, we concentrate on comparisons of the two-step hybrid form and the equivalent CRKN method. For all the calculations reported in this section, the steplengths were chosen so that the magnitude of the global truncation error on the interval considered was less than the unit round-off in the arithmetic used. We have also confirmed that our conclusions are not affected by reasonable changes in the tolerance parameter for the iterations necessary to solve the implicit equations at each step.

The Harmonic Oscillator

The sixth order Panovsky-Richardson method PR4 and the equivalent Runge-Kutta-Nyström method, denoted by RKN6, were used to solve the linear initial value problem

$$y'' = -y, \qquad y(0) = 1, \qquad y'(0) = 0. \tag{3.80}$$

For the fixed steplength $h = 0.01$, the magnitude of the global truncation error is less

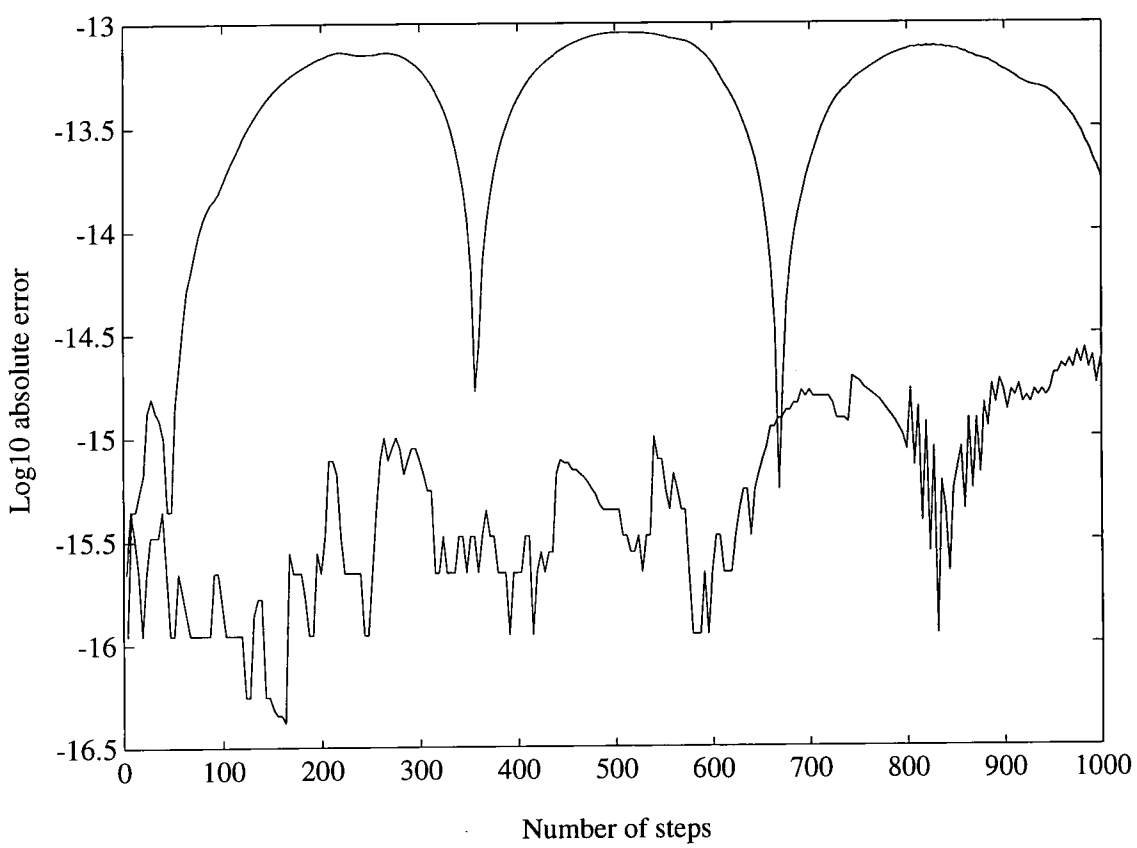

Figure 3.6: Global errors of the sixth order methods PR4 and RKN6 when applied to (3.80) over the interval $[0, 100]$ with steplength $h = 0.01$. Smooth line = PR4, jagged line = RKN6.

than 5×10^{-18} on $[0, 10]$ and less than 6×10^{-17} on $[0, 100]$. Figure 3.6 shows the observed global errors in the two methods over the range $[0, 10]$. These results were generated by a double precision FORTRAN program run on a SUN workstation.

Table 3.6 compares the results obtained from the PR4 and RKN6 methods over

the interval $[0, 100]$ in a variety of computing environments. The MATLAB program employed a Gauss-Seidel-type iteration scheme to solve the system of implicit equations arising at each step, whereas the FORTRAN programs run on both the mainframe and SUN workstation used a Newton scheme (see section 3.5). The entries in Table 3.6 are due solely to the propagation of rounding errors, and clearly demonstrate the greater stability of the one-step CRKN formulation for this problem. Unlike the Microcomputer and the SUN, the mainframe stores floating point numbers as hexadecimal digits and operates a chopping, rather than a rounding, algorithm. This accounts for the increased rate of error growth observed in the mainframe simulations.

	MATLAB		FORTRAN Double Precision			
	SUN Workstation		SUN Workstation		Mainframe	
x	PR4	RKN6	PR4	RKN6	PR4	RKN6
1	3.4 E-14	5.6 E-16	1.7 E-14	4.4 E-16	4.9 E-13	1.2 E-15
2	5.2 E-14	9.4 E-16	6.8 E-14	4.4 E-16	1.1 E-12	1.6 E-15
5	1.1 E-13	1.1 E-15	9.0 E-14	1.1 E-15	3.0 E-12	5.8 E-15
10	1.1 E-13	2.7 E-15	9.1 E-14	2.8 E-15	5.0 E-12	1.7 E-14
20	2.4 E-13	4.4 E-15	1.0 E-13	2.9 E-15	1.2 E-11	3.3 E-14
50	4.6 E-13	7.9 E-15	2.2 E-13	1.2 E-14	3.1 E-11	8.7 E-14
100	4.6 E-13	1.2 E-14	5.0 E-13	1.3 E-14	6.3 E-11	1.7 E-13

Table 3.6: Maximum absolute errors on intervals $[0, x]$ when methods PR4 and RKN6 are applied to (3.80) with steplength $h = 0.01$.

Two-body Problem

For our non-linear test problem we once again take the two body problem

$$y'' + y/r^3 = 0, \qquad y(0) = 1 - e, \qquad y'(0) = 0 \tag{3.81}$$

$$z'' + z/r^3 = 0, \qquad z(0) = 0, \qquad z'(0) = \sqrt{(1+e)/(1-e)} \tag{3.82}$$

with $r^2 = y^2 + z^2$. The two equivalent methods PR4 and RKN6 were applied to this problem with the fixed steplength $h = 0.01$, which guaranteed that the modulus of

x	PR4	RKN6
1	1.2 E-14	1.0 E-15
2	2.2 E-14	4.2 E-15
5	2.1 E-13	2.8 E-14
10	6.9 E-13	5.1 E-14
20	1.4 E-12	1.2 E-13
50	1.4 E-11	2.3 E-13
100	2.5 E-11	1.1 E-12

Table 3.7: Maximum absolute errors on intervals $[0, x]$ when methods PR4 and RKN6 are applied to problem (3.81)-(3.82) with steplength $h = 0.01$.

the maximum global error was less than 3×10^{-16} on $[0, 10]$, and less than 5×10^{-15} on $[0, 100]$. The results shown in table 3.7 were obtained using the SUN double-precision FORTRAN implementation of these methods.

A 'stiff' problem

The results from the two non-stiff problems above clearly demonstrate the superiority of the Runge-Kutta-Nyström formulation of these methods. The question we now ask is whether this remains the case if these methods are applied to a stiff problem. To answer this we applied the two sixth order methods PR4 and RKN6 with the fixed steplength $h = 0.01$ to Kramarz' ([44]) test problem

$$y'' = 2498y + 4998z; \qquad y(0) = 2,\ y'(0) = 0, \tag{3.83}$$

$$z'' = -2499y - 4999z; \qquad z(0) = -1,\ z'(0) = 0. \tag{3.84}$$

For this steplength, the modulus of the maximum global errorin these methods is less than 9×10^{-17} on $[0, 10]$ and less than 9×10^{-16} on $[0, 80]$. The results shown in table 3.8 were generated using a MATLAB program run on a microcomputer.

x	PR4	RKN6
1	6.8 E-14	1.1 E-15
2	1.0 E-13	1.9 E-15
5	2.2 E-13	2.2 E-15
10	2.2 E-13	5.8 E-15
20	4.6 E-13	1.4 E-14
40	6.4 E-13	2.3 E-14
80	9.0 E-13	4.3 E-14

Table 3.8: Maximum absolute errors on intervals $[0, x]$ when methods PR4 and RKN6 are applied to problem (3.83)-(3.84) with steplength $h = 0.01$.

3.11 Conclusion

Remarks in the introduction to Panovsky & Richardson's paper [53] imply that the methods they propose are designed for problems "whose solutions have a quasi-periodic character". While it seems that the authors' main interest lay in solving such problems, their methods take no account of the possible oscillatory behaviour of the solution, unlike the exponential fitting methods mentioned in chapter 2. The fact that $T_n(x) = \cos(n \cos^{-1}(x))$, and that $T_n(x)$ oscillates on $[-1, 1]$, does not imply any connection with trigonometric interpolation or with any other device designed to mimic the behaviour of periodic solutions.

The work of Panovsky & Richardson has given us an interesting family of methods for initial value problems of the form (3.1). For each positive integer r there are two methods of order $2r$, one corresponding to polynomial interpolation of degree $2r - 1$ and the other to interpolation of degree $2r - 2$. We have shown that the information required to analyse the stability properties of the method of degree n is contained in the rational function $\alpha_n(\nu^2)$, and that every method from this family possesses a non-vanishing interval of periodicity.

The total length of the union of the periodicity intervals increases with n, but the fact that these intervals remain disjoint is an undesirable feature. The example at the end of section 3.4 shows what may happen when a steplength reduction results

in moving from an interval of periodicity to an interval of instability. The gaps between periodicity intervals shrink as n increases, but the methods remain unstable for $\nu^2 = k\pi^2$ for sufficiently small non-negative integers k, for example, with $n = 9$ this is true for $k = 0, 1, \ldots, 6$.

The Gauss-Seidel-type iterations suggested by Panovsky & Richardson, or our version given by (3.49), to solve the implicit system of non-linear equations arising at each step are economical when convergence is rapid. However, as demonstrated in section 3.5, these schemes can place severe restrictions on the range of possible stepsizes in order to guarantee convergence.

Numerical results in [53] and section 3.6 show that these methods can produce solutions of high accuracy. Comparisons show them to be more accurate than some established methods of the same order. Of particular interest is the fact that the global errors of these methods appears to exhibit a near-linear dependence on the length of the integration interval, whereas for some RKN methods this dependence is quadratic. We still have no explanation as to why this is the case.

In section 3.8 we showed that the methods of Panovsky & Richardson are equivalent to certain collocation-based Runge-Kutta-Nyström methods. In any implementation of these methods, the RKN formulation is to be preferred since it is both easier to start and is more stable with respect to the build-up of rounding errors, as demonstrated in section 3.10.

In section 3.9 we showed that these methods are neither P-stable nor symplectic. By looking at the individual components of the global error of some of these methods when applied to Kepler's two-body problem, we found that only one component grows approximately linearly with the length of the integration interval, the other component, though very much smaller, grows approximately quadratically.

Chapter 4

Multistep collocation methods I: The multistep Runge-Kutta-Nyström methods

Aspects of one-step collocation methods for initial value problems of the form

$$y'' = f(x, y); \quad y(x_0) = y_0, \quad y'(x_0) = z_0, \tag{4.1}$$

involving second order ordinary differential equations in which the first derivative does not appear explicitly have recently been investigated by Coleman [22], Coleman & Booth [23] and Van der Houwen et al. [67], [68]. In particular, Coleman [22] has shown that there are no P-stable collocation-based Runge-Kutta-Nyström methods. Nørsett and Lie [50], [47], have derived and investigated properties of multistep collocation methods for first order differential equations.

In this and the following chapter we derive and investigate two classes of multistep collocation methods for (4.1). The methods presented in this chapter incorporate both y and y' values from previous step-points. These methods are natural extensions of the one-step collocation-based Runge-Kutta-Nyström methods, and so we refer to then as MCRKN (Multistep Collocation-based RKN) methods. In chapter 5 we look

at methods for which derivative data is not required.

Before attempting to construct an MCRKN method we must first ensure that the interpolation problem defining that method is uniquely solvable. In section 4.1.1 we show that this requirement places few restrictions on the range of possible collocation nodes. MCRKN methods with arbitrary stepnumber k and number of collocation points m are constructed in section 4.1.2 and are shown to be natural extensions of the one-step collocation methods.

Since our interest lies in solving problems of the form (4.1) whose solutions are oscillatory in nature, we seek methods which possess non-vanishing intervals of periodicity. In an attempt to derive such methods we restrict our attention to the two-step symmetric MCRKN methods whose off-step points, $\{x_{n+c_i}\}_{i=1}^{m}$, are symmetrically distributed in the interval $[x_{n-1}, x_{n+1}]$. Order conditions for these methods are considered in section 4.2, and their stability properties are investigated using the results of section 4.3.

Some specific examples of two-step symmetric MCRKN methods are analysed in section 4.4. For the methods considered in this section we find that the requirement of periodicity drastically reduces the range of available collocation nodes. The results of numerical experiments comparing some of these methods with the Panovsky-Richardson methods requiring comparable computational effort are given in section 4.5.

4.1 Construction

In this section we consider the construction of the MCRKN methods and give expressions for the coefficients for arbitrary stepnumber k and number of collocation points m. These expressions will be seen to be natural generalisations of the coefficients for the one-step case.

First however, we consider the existence of a unique solution to the collocation problem, and give examples of cases where a unique solution is not defined. In order

to do this we associate each MCRKN method with a corresponding interpolation problem which is independent of our differential equation. The uniqueness conditions are derived in the normal way by considering the generalised Gram determinant for this problem. For the cases looked at so far, the conditions imposed by the uniqueness criterion do not unduly restrict the range of possible interpolation nodes.

4.1.1 Unique solvability of the interpolation problem

In this section we define the interpolation problem associated with each MCRKN and give conditions which ensure that the problem is uniquely solvable. These conditions are then simplified, and examples are given for a number of specific methods.

Let $x_r = x_0 + rh$ for all $r \in \mathbb{R}$, and let $\{c_i\}_{i=1}^m$ $(m \geq 1)$ be distinct real numbers. A k-step, m-point MCRKN method is defined as follows

Find $u \in \mathcal{P}_{m+2k-1}$ such that

$$\begin{aligned} u(x_n - jh) &= y_{n-j} && j = 0 \ldots k-1 \\ u'(x_n - jh) &= z_{n-j} && j = 0 \ldots k-1 \\ u''(x_n + c_i h) &= f(x_{n+c_i}, u(x_{n+c_i})) && i = 1 \ldots m \end{aligned}$$

then take

$$y_{n+1} = u(x_{n+1}) \quad \text{and} \quad z_{n+1} = u'(x_{n+1})$$

where y_{n+r} and z_{n+r} are approximations to $y(x_{n+r})$ and $y'(x_{n+r})$ respectively, for $r \in \mathbb{R}$.

The solution to this problem will be discussed in the next section. With this method we associate the following interpolation problem:

Find $p \in \mathcal{P}_{m+2k-1}$ such that

$$p(x - jh) = g(x - jh) \qquad j = 0 \ldots k-1 \tag{4.2}$$

$$p'(x - jh) = g'(x - jh) \qquad j = 0 \ldots k-1 \tag{4.3}$$

$$p''(x + c_i h) = g''(x + c_i h) \qquad i = 1 \ldots m \tag{4.4}$$

where the function g is assumed to be as differentiable as we please.

It is easy to show that the problem defining the MCRKN method is uniquely solvable if and only if there exists a unique solution to the above interpolation problem. Let $p(x) = \sum_{n=0}^{m+2k-1} a_n x^n$, and define $\boldsymbol{a} = (a_0, \ldots, a_{m+2k-1})^{\mathrm{T}}$. We may now replace the interpolation problem by the system of linear equations

$$A\boldsymbol{a} = \boldsymbol{b} \tag{4.5}$$

where A is the $(m + 2k) \times (m + 2k)$ matrix

$$A = \begin{pmatrix} 1 & 0 & 0 & 0 & \ldots & 0 \\ 1 & -1 & 1 & -1 & \ldots & (-1)^r \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ 1 & (1-k) & (1-k)^2 & (1-k)^3 & \ldots & (1-k)^r \\ 0 & 1 & 0 & 0 & \ldots & 0 \\ 0 & 1 & -2 & 3 & \ldots & r(-1)^{r-1} \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ 0 & 1 & 2(1-k) & 3(1-k)^2 & \ldots & r(1-k)^{r-1} \\ 0 & 0 & 2 & 6c_1 & \ldots & r(r-1)c_1^{r-2} \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 2 & 6c_m & \ldots & r(r-1)c_m^{r-2} \end{pmatrix}$$

and $\boldsymbol{b} \in \mathbb{R}^r$ is given by:

$$\boldsymbol{b} = (g(0), \ldots, g(1-k), g'(0), \ldots, g'(1-k), g''(c_1), \ldots, g''(c_m))^{\mathrm{T}}$$

where for notational convenience we have taken $x = 0$ and $r = m + 2k - 1$. From Davis [27], the above interpolation problem will have a unique solution if and only if

A is non-singular.

We now show how the determinant of A may be reduced to the determinant of an $m \times m$ matrix. The matrix A may be partitioned as:

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$$

where $A_{11} \in \mathbb{R}^{2k} \times \mathbb{R}^{2k}$, $A_{12} \in \mathbb{R}^{2k} \times \mathbb{R}^{m}$, $A_{21} \in \mathbb{R}^{m} \times \mathbb{R}^{2k}$ and $A_{22} \in \mathbb{R}^{m} \times \mathbb{R}^{m}$. We can view A_{11} as the coefficient matrix arising from a Hermite interpolation problem where the values $g(x)$ and $g'(x)$ are fitted at the nodes $x = 0, \ldots, k-1$. It is easy to verify that since these interpolation nodes are distinct, the Hermite interpolation problem is uniquely solvable, and A_{11} is non-singular. Let $B \in \mathbb{R}^{m+2k} \times \mathbb{R}^{m+2k}$ be given by

$$B = \begin{pmatrix} A_{11}^{-1} & 0 \\ 0 & I_m \end{pmatrix}$$

where the zero blocks have the same dimensions as the corresponding blocks of A, and I_m is the $m \times m$ identity matrix. Premultiplying A by B gives:

$$BA = \begin{pmatrix} I_{2k} & A_{11}^{-1}A_{12} \\ A_{21} & A_{22} \end{pmatrix} \tag{4.6}$$

where I_{2k} is the $2k \times 2k$ identity matrix. Note that since B is independent of the collocation nodes $\{c_i\}_{i=1}^{m}$, $\det(BA)$ is just a constant multiple of $\det(A)$. By premultiplying BA by the matrix

$$C = \begin{pmatrix} I_{2k} & 0 \\ -A_{21} & I_m \end{pmatrix}$$

we obtain:

$$CBA = \begin{pmatrix} I_{2k} & A_{11}^{-1}A_{12} \\ 0 & A_{22} - A_{21}A_{11}^{-1}A_{12} \end{pmatrix} \tag{4.7}$$

and:

$$\begin{aligned} \det A &= \alpha \det CBA \\ &= \alpha \det \bar{A} \end{aligned} \tag{4.8}$$

where $\bar{A} = (A_{22} - A_{21}A_{11}^{-1}A_{12})$, and α is some real number. Further simplification is possible by imposing constraints (e.g., symmetry) on the nodes $\{c_i\}_{i=1}^{m}$.

Below are three examples of two-step MCRKN methods. These examples show that one cannot just assume that the interpolation problem is uniquely solvable. Although no further results are known at this time, it seems logical to anticipate similar problems in methods with higher values of m and k, and to take the necessary precautions.

Example 1 $k = 2, m = 1$.

In this case the matrices A and $\bar{A}$ are as follows:

$$A = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & -1 & 1 & -1 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & -2 & 3 & -4 \\ 0 & 0 & 2 & 6c_1 & 12c_1^2 \end{pmatrix}$$

$$\bar{A} = \begin{pmatrix} 2(6c_1^2 + 6c_1 + 1) \end{pmatrix}$$

and

$$\det \bar{A} = -2(6c_1^2 + 6c_1 + 1)$$

Thus the interpolation problem is uniquely solvable provided $c_1 \neq \frac{1}{2}(-1 \pm \frac{1}{\sqrt{3}})$.

Example 2 $k = 2, m = 2$.

The matrices A and $\bar{A}$ are as follows:

$$A = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -1 & 1 & -1 & 1 & -1 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 3 & -4 & 5 \\ 0 & 0 & 2 & 6c_1 & 12c_1^2 & 20c_1^3 \\ 0 & 0 & 2 & 6c_2 & 12c_2^2 & 20c_2^3 \end{pmatrix}$$

$$\bar{A} = \begin{pmatrix} 2(6c_1^2 + 6c_1 + 1) & 2(10c_1^3 - 9c_1 - 2) \\ 2(6c_2^2 + 6c_2 + 1) & 2(10c_2^3 - 9c_2 - 2) \end{pmatrix}$$

and

$$\begin{aligned} \det \bar{A} &= 4(c_1 - c_2)(60c_1^2c_2^2 + 60c_1c_2(c_1 + c_2) + 10(c_1^2 + c_2^2) + \\ &\quad 12(c_1 + c_2) + 64c_1c_2 + 3) \end{aligned}$$

Here the interpolation problem is uniquely solvable provided the nodes $\{c_1, c_2\}$ are distinct and satisfy

$$c_1 \neq \frac{-30c_2^2 - 32c_2 - 6 \pm \sqrt{300c_2^4 + 600c_2^3 + 384c_2^2 + 84c_2 + 6}}{10(6c_2^2 + 6c_2 + 1)} \tag{4.9}$$

Later in this chapter we will restrict our attention to those methods whose nodes satisfy the symmetry condition

$$c_i + c_{m+1-i} = 2 - k \qquad i = 1, \ldots, \lfloor \tfrac{m}{2} \rfloor \tag{4.10}$$

or more specifically for the case k=2, those methods whose nodes are symmetric about zero. If we impose this condition now, our uniqueness criterion becomes:

$$c_1(60c_1^4 - 44c_1^2 + 3) \neq 0 \tag{4.11}$$

i.e.

$$c_1 \neq 0 \qquad \text{and} \qquad c_1^2 \neq \frac{11 \pm 2\sqrt{19}}{30} \tag{4.12}$$

Example 3 $k = 2$, $m = 3$, symmetric nodes.

To save ourselves some unnecessarily complex algebra, we once again impose our symmetry constraints: $c_3 = -c_1$ and $c_2 = 0$, and look only at the matrix $\bar{A}$. In this case

$$\bar{A} = \begin{pmatrix} 2(6c_1^2 + 6c_1 + 1) & 2(10c_1^3 - 9c_1 - 2) & 6(5c_1^4 + 4c_1 + 1) \\ 2 & -4 & 6 \\ 2(6c_2^2 - 6c_2 + 1) & 2(-10c_2^3 + 9c_2 - 2) & 6(5c_1^4 - 4c_1 + 1) \end{pmatrix}$$

and

$$\det \bar{A} = -48(50c_1^4 - 45c_1^2 + 6)c_1^3$$

The interpolation problem is thus uniquely solvable provided

$$c_1 \neq 0 \qquad \text{and} \qquad c_1^2 \neq \frac{9 \pm \sqrt{36}}{20}$$

Much of this section is an extension of a paper by Lie & Nørsett [47], in which multistep collocation methods for general first order differential equation $y' = f(x, y)$, $y(x_0) = y_0$ are studied. In that paper they state without proof that their collocation problem is uniquely solvable. We show here that this is not always the case, and give examples of where uniqueness fails. Once again we consider the approximation of an arbitrary function g, assumed to be as differentiable as we please. Lie & Nørsett's interpolation problem is as follows:

Find $u \in \mathcal{P}_{m+k-1}$ such that

$$u(x - jh) = g(x - jh) \qquad j = 0 \ldots, k-1 \tag{4.13}$$

$$u'(x + c_i h) = g'(x + c_i h) \qquad i = 1, \ldots, m \tag{4.14}$$

In the same way as before, we form the corresponding matrix A given by

$$A = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ 1 & -1 & 1 & \dots & (-1)^r \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & (1-k) & (1-k)^2 & \dots & (1-k)^r \\ 0 & 1 & 2c_1 & \dots & rc_1^{r-1} \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 1 & 2c_m & \dots & rc_m^{r-1} \end{pmatrix}$$

where for notational convenience we have taken $x = 0$ and $r = m + k - 1$. Since our aim is to find an example where uniqueness fails, we will not attempt to simplify the matrix A. As before, we seek nodes $\{c_i\}_{i=1}^m$ such that det $A = 0$. We know that when $k = 1$ a unique solution always exists, so we try $k = 2$:

Example 1, k=2, m=1

In this case the matrix A is given by:

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 1 & -1 & 1 \\ 0 & 1 & 2c_1 \end{pmatrix}$$

and

$$\det A = -(2c_1 + 1)$$

so that the interpolation problem has a unique solution provided $c_1 \neq -\frac{1}{2}$.

Example 2, k=2, m=2

The matrix A in this case is given by:

$$A = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & -1 & 1 & -1 \\ 0 & 1 & 2c_1 & 3c_1^2 \\ 0 & 1 & 2c_2 & 3c_2^2 \end{pmatrix}$$

and

$$\det A = (c_1 - c_2)(6c_1c_2 + 3(c_1 + c_2) + 2)$$

so that the interpolation problem has a unique solution provided

$$c_1 \neq c_2 \qquad \text{and} \qquad c_1 \neq -\frac{3c_2 + 2}{3(2c_2 + 1)}$$

If we were to impose the symmetry constraint $c_1 = -c_2$, then the uniqueness criterion becomes $c_1 \neq \frac{1}{\sqrt{3}}$.

Example 3, k=2, m=3

In this case the matrix A is given by:

$$A = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & -1 & 1 & -1 & 1 \\ 0 & 1 & 2c_1 & 3c_1^2 & 4c_1^3 \\ 0 & 1 & 2c_2 & 3c_2^2 & 4c_2^3 \\ 0 & 1 & 2c_3 & 3c_3^2 & 4c_3^3 \end{pmatrix}$$

and

$$\begin{aligned} \det A \;=\; & 2(c_1 - c_2)(c_1 - c_3)(c_2 - c_3)(12c_1c_2c_3 + 6(c_1c_2 + c_2c_3 + c_3c_1) \\ & +4(c_1 + c_2) + c_3 + 3) \end{aligned}$$

so that the interpolation problem is uniquely solvable provided the nodes $\{c_1, c_2, c_3\}$

are distinct and satisfy

$$c_1 \neq -\frac{6c_3c_2 + 4(c_2 + c_3) + 3}{2(6c_2c_3 + 3(c_2 + c_3) + 2)}$$

If we were to impose the symmetry constraint $c_3 = -c_1$, $c_2 = 0$ then the uniqueness criterion would become $c_1 \neq 0$ and $c_1 \neq \frac{1}{\sqrt{2}}$.

It is interesting to note that in all three of the above examples the determinant of A is given by:

$$\det A = \alpha \int_0^{-1} \prod_{i=1}^{m} (\tau - c_i)\, d\tau \tag{4.15}$$

for some real number α. We shall come back to this point at the end of the next subsection.

After completing this work we found that the existence of a unique solution to Lie & Nørsett's interpolation problem had also been investigated by Hairer & Wanner in their book [37]. In this work they show that uniqueness may be guaranteed by requiring that all the nodes $\{c_i\}_{i=1}^m$ be positive.

4.1.2 Construction of the collocation solution.

In this section we return to the task of solving the differential equation (4.1). We show how to construct a k-step, m-point multistep collocation method (MCRKN) and show that these methods form a subclass of the multistep Runge-Kutta-Nyström methods. We begin with some definitions.

Let $\{y_n, z_n\}_{n=0}^{k-1}$ be given approximations for $\{y(x_n), y'(x_n)\}_{n=0}^{k-1}$. For notational convenience we change variable to

$$s = \frac{x - x_n}{h} \qquad \text{(i.e. } x = x_n + sh\text{)}$$

for the rest of this section. Define

$$U(s) \;=\; u(x_n + sh) \tag{4.16}$$

$$F(s,U(s)) \;=\; f(x_n + sh, u(x_n + sh)) \tag{4.17}$$

and let a prime denote differentiation with respect to s (observe that $d/ds = h\,d/dx$).

A k-step m-point collocation method for (4.1) is constructed as follows:

Find $U \in \mathcal{P}_{m+2k-1}$ such that

$$U(-j) \;=\; y_{n-j} \qquad j = 0,\ldots,k-1 \tag{4.18}$$

$$U'(-j) \;=\; hz_{n-j} \qquad j = 0,\ldots,k-1 \tag{4.19}$$

$$U''(c_i) \;=\; h^2 F(c_i, U(c_i)) \qquad i = 1,\ldots,m \tag{4.20}$$

then as approximations to $y(x_{n+1})$ and $hy'(x_{n+1})$ we take:

$$y_{n+1} = U(1), \qquad hz_{n+1} = U'(1) \tag{4.21}$$

The following lemma shows that the multistep collocation methods form a subclass of the multistep Runge-Kutta-Nyström methods.

Lemma 4.1 *The multistep collocation method defined by (4.18)-(4.21) may be written as the multistep Runge-Kutta-Nyström method:*

$$\begin{aligned} Y_i \;=\; & \sum_{j=0}^{k-1} \lambda_j(c_i) y_{n-j} + h \sum_{j=0}^{k-1} \mu_j(c_i) z_{n-j} + \\ & h^2 \sum_{l=1}^{m} \nu_l(c_i) F(c_l, Y_l) \qquad i = 1,\ldots,m \end{aligned} \tag{4.22}$$

$$\begin{aligned} y_{n+1} \;=\; & \sum_{j=0}^{k-1} \lambda_j(1) y_{n-j} + h \sum_{j=0}^{k-1} \mu_j(1) z_{n-j} + \\ & h^2 \sum_{l=1}^{m} \nu_l(1) F(c_l, Y_l) \end{aligned} \tag{4.23}$$

$$\begin{aligned} hz_{n+1} \;=\; & \sum_{j=0}^{k-1} \lambda'_j(1) y_{n-j} + h \sum_{j=0}^{k-1} \mu'_j(1) z_{n-j} + \\ & h^2 \sum_{l=1}^{m} \nu'_l(1) F(c_l, Y_l) \end{aligned} \tag{4.24}$$

where $\lambda_j,\ \mu_j,\ \nu_l \in \mathcal{P}_{m+2k-1}$.

Proof Let $Y_i = U(c_i), \quad i = 1, \ldots, m$. Then for some $\lambda_j,\ \mu_j,\ \nu_l \in \mathcal{P}_{m+2k-1}$ we have from (4.18)–(4.20) that

$$\begin{aligned} U(s) &= \sum_{j=0}^{k-1} \lambda_j(s) y_{n-j} + h \sum_{j=0}^{k-1} \mu_j(s) z_{n-j} + \\ & \quad h^2 \sum_{l=1}^{m} \nu_l(s) F(c_l, Y_l) \end{aligned} \tag{4.25}$$

Expressions (4.22)–(4.24) follow immediately. □

We now show how to construct the polynomials $\lambda_j,\ \mu_j,\ \nu_l$. Without loss of generality we take $x_n = 0$ and $h = 1$ for the remainder of this section.

The polynomials $\nu_i \quad (i = 1, \ldots, m)$

From the collocation conditions (4.18)-(4.20) we see that the following conditions are imposed on ν_i:

$$\nu_i(-r) = 0 \qquad r = 0, \ldots, k-1 \tag{4.26}$$

$$\nu_i'(-r) = 0 \qquad r = 0, \ldots, k-1 \tag{4.27}$$

$$\nu_i''(c_j) = \delta_{ij} \qquad j = 1, \ldots, m \tag{4.28}$$

Condition (4.28) can be satisfied by a polynomial of the form

$$\nu_i''(s) = l_i(s) \left(1 + \sum_{p=0}^{2k-3} \alpha_{ip} (s - c_i) s^p \right) \tag{4.29}$$

$$= l_i(s) + M(s) \sum_{p=0}^{2k-3} a_{ip} s^p \tag{4.30}$$

where $l_i(s)$ is the i^{th} fundamental Lagrange basis function based on the nodes $\{c_i\}_{i=1}^m$,

$$M(s) = \prod_{i=1}^{m} (s - c_i)$$

and $a_{ip} = \alpha_{ip}/M'(c_i)$. Integrating (4.30) and using (4.27) we obtain:

$$\nu_i'(s) = \int_0^s l_i(\tau)d\tau + \sum_{p=0}^{2k-3} a_{ip} \int_0^s \tau^p M(\tau)d\tau. \tag{4.31}$$

A further integration gives

$$\begin{aligned} \nu_i(s) &= \int_0^s d\sigma \int_0^\sigma l_i(\tau)d\tau + \sum_{p=0}^{2k-3} a_{ip} \int_0^s d\sigma \int_0^\sigma \tau^p M(\tau)d\tau & (4.32) \\ &= \int_0^s (s-\tau) l_i(\tau)d\tau + \sum_{p=0}^{2k-3} a_{ip} \int_0^s (s-\tau)\tau^p M(\tau)d\tau & (4.33) \end{aligned}$$

The remaining collocation conditions (4.26) and (4.27) may now be re-expressed as:

$$\begin{aligned} \sum_{p=0}^{2k-3} a_{ip} \int_{-r}^0 \tau^p M(\tau)d\tau &= -\int_{-r}^0 l_i(\tau)d\tau & (4.34) \\ \sum_{p=0}^{2k-3} a_{ip} \int_{-r}^0 (-r-\tau)\tau^p M(\tau)d\tau &= -\int_{-r}^0 (-r-\tau) l_i(\tau)d\tau & (4.35) \end{aligned}$$

for $r = 1, \ldots, k-1$. Using equation (4.34) it is possible to simplify (4.35) to get:

$$\sum_{p=0}^{2k-3} a_{ip} \int_{-r}^0 \tau^{p+1} M(\tau)d\tau = -\int_{-r}^0 \tau l_i(\tau)d\tau \tag{4.36}$$

Equations (4.34) and (4.36) form a linear system of $2k-2$ equations for the $2k-2$ unknowns $\{a_{ip}\}_{p=0}^{2k-3}$. Using Cramer's Rule we readily obtain

$$\nu_i(s) = \frac{1}{D_{2k-2}} \left(D_{2k-2} \int_0^s l_i(\tau)d\tau + \sum_{p=0}^{2k-3} D_{ip}^{(\nu)} \int_0^s (s-\tau)\tau^p M(\tau)d\tau \right) \tag{4.37}$$

where, for $k > 1$,

$$D_{2k-2} = \det \begin{pmatrix} \int_{-1}^{0} M(\tau)d\tau & \dots & \int_{-1}^{0} \tau^{2k-3} M(\tau)d\tau \\ \vdots & & \vdots \\ \int_{1-k}^{0} M(\tau)d\tau & \dots & \int_{1-k}^{0} \tau^{2k-3} M(\tau)d\tau \\ \int_{-1}^{0} \tau M(\tau)d\tau & \dots & \int_{-1}^{0} \tau^{2k-2} M(\tau)d\tau \\ \vdots & & \vdots \\ \int_{1-k}^{0} \tau M(\tau)d\tau & \dots & \int_{1-k}^{0} \tau^{2k-2} M(\tau)d\tau \end{pmatrix} \tag{4.38}$$

and $D_{ip}^{(\nu)}$ is the determinant obtained when the p^{th} column of D_{2k-2} is replaced by the vector

$$\boldsymbol{v}_i^{(\nu)} = \left(\int_{-1}^{0} -l_i(\tau)d\tau, \dots, \int_{1-k}^{0} -l_i(\tau)d\tau, \int_{-1}^{0} -\tau l_i(\tau)d\tau, \dots, \int_{1-k}^{0} -\tau l_i(\tau)d\tau \right)^T \tag{4.39}$$

The polynomials μ_j $(j = 1, \dots, k-1)$

From the collocation conditions (4.18)-(4.20) we see that the following conditions are imposed on μ_j:

$$\mu_j(-r) = 0 \qquad r = 0, \dots, k-1 \tag{4.40}$$

$$\mu_j'(-r) = \delta_{jr} \qquad r = 0, \dots, k-1 \tag{4.41}$$

$$\mu_j''(c_i) = 0 \qquad i = 1, \dots, m \tag{4.42}$$

The last condition can be satisfied by a polynomial of the form

$$\mu_j''(s) = M(s) \sum_{p=0}^{2k-3} \beta_{jp} s^p$$

Integrate this with respect to s:

$$\mu_j'(s) = \sum_{p=0}^{2k-3} \beta_{jp} \int_0^s \tau^p M(\tau)d\tau + \mu_j'(0). \tag{4.43}$$

Integrating once more we obtain:

$$\mu_j(s) = \sum_{p=0}^{2k-3} \beta_{jp} \int_0^s (s-\tau)\tau^p M(\tau)d\tau + s\mu_j'(0) + \mu_j(0). \tag{4.44}$$

From (4.40) and (4.41) we have that $\mu_j(0) = 0$ and $\mu_j'(0) = \delta_{j0}$, Using these, and equations (4.43) and (4.44) we can rewrite condition (4.40) as:

$$\sum_{p=0}^{2k-3} \beta_{jp} \int_{-r}^0 \tau^p M(\tau)d\tau = \delta_{j0} - \delta_{jr} \qquad r = 1, \ldots, k-1 \tag{4.45}$$

and condition (4.41) as:

$$\sum_{p=0}^{2k-3} \beta_{jp} \int_{-r}^0 \tau^{p+1} M(\tau)d\tau = r\delta_{jr} \qquad r = 1, \ldots, k-1 \tag{4.46}$$

Let $\boldsymbol{e}_j \in \mathbb{R}^{k-1}$ be a column vector which has 1 as the j^{th} entry and all other entries zero. Let $D_{jp}^{(\mu)}$ be the determinant obtained when the p^{th} column of D_{2k-2} is replaced by the vector

$$\boldsymbol{v}_j^{(\mu)} = \begin{cases} (1, \ldots, 1 | 0, \ldots, 0)^T & j = 0 \\ (\ -\boldsymbol{e}_j^{\mathrm{T}} \ | \ j\boldsymbol{e}_j^{\mathrm{T}} \ )^T & j > 0 \end{cases} \tag{4.47}$$

Using Cramer's Rule once again to solve the system (4.45), (4.46) we obtain

$$\mu_j(s) = s\delta_{j0} + \sum_{p=0}^{2k-3} \frac{D_{jp}^{(\mu)}}{D_{2k-2}} \int_0^s (s-\tau)\tau^p M(\tau)d\tau \tag{4.48}$$

The polynomials λ_j $(j = 1, \ldots, k-1)$

From the collocation conditions (4.18)-(4.20) we see that the following conditions are imposed on λ_j:

$$\lambda_j(-r) = \delta_{jr} \qquad r = 0, \ldots, k-1 \tag{4.49}$$

$$\lambda_j'(-r) = 0 \qquad r = 0, \ldots, k-1 \tag{4.50}$$

$$\lambda_j''(c_i) = 0 \qquad i = 1, \ldots, m \tag{4.51}$$

The last condition can be satisfied by a polynomial of the form

$$\lambda_j''(s) = M(s) \sum_{p=0}^{2k-3} \gamma_{jp} s^p$$

Integrate this with respect to s:

$$\lambda_j'(s) = \sum_{p=0}^{2k-3} \gamma_{jp} \int_0^s \tau^p M(\tau) d\tau + \lambda_j'(0) \tag{4.52}$$

A further integration gives

$$\lambda_j(s) = \sum_{p=0}^{2k-3} \gamma_{jp} \int_0^s (s-\tau)\tau^p M(\tau) d\tau + s\lambda_j'(0) + \lambda_j(0) \tag{4.53}$$

From (4.49) and (4.50) with $r = 0$ we have that $\lambda_j'(0) = 0$ and $\lambda_j(0) = \delta_{j0}$. We may now rewrite the conditions (4.49) and (4.50) as the following system of linear equations:

$$\sum_{p=0}^{2k-3} \gamma_{jp} \int_{-r}^{0} \tau^p M(\tau) d\tau = 0 \qquad r = 1, \ldots, k-1 \tag{4.54}$$

$$\sum_{p=0}^{2k-3} \gamma_{jp} \int_{-r}^{0} \tau^{p+1} M(\tau) d\tau = \delta_{jr} - \delta_{j0} \qquad r = 1, \ldots, k-1 \tag{4.55}$$

Let $D_{jp}^{(\lambda)}$ be the determinant obtained by replacing the p^{th} column of D_{2k-2} with the vector

$$\boldsymbol{v}_j{}^{(\lambda)} = \begin{cases} (0, \ldots, 0 | -1, \ldots, -1)^T & j = 0 \\ (0, \ldots, 0 | \quad \boldsymbol{e}_j^{\mathrm{T}} \quad)^T & j > 0 \end{cases} \tag{4.56}$$

Using Cramer's Rule we can readily solve the system (4.54),(4.54) giving:

$$\lambda_j(s) = \delta_{j0} + \sum_{p=0}^{2k-3} \frac{D_{jp}^{(\lambda)}}{D_{2k-2}} \int_0^s (s-\tau)\tau^p M(\tau) d\tau \tag{4.57}$$

The above results are summarised in the following lemma.

Lemma 4.2 *The polynomials λ_j, μ_j and ν_i defined in Lemma 4.1 are given by*

$$\lambda_j(s) = \frac{D_j^{(\lambda)}}{D_{2k-2}} \qquad \mu_j(s) = \frac{D_j^{(\mu)}}{D_{2k-2}} \qquad \nu_j(s) = \frac{D_j^{(\nu)}}{D_{2k-2}} \tag{4.58}$$

where

$$D_j^{(\lambda)} = \det \begin{pmatrix} \delta_{j0} & \boldsymbol{w}^{\mathrm{T}} \\ \boldsymbol{v}_j^{(\lambda)} & A_{2k-2} \end{pmatrix} \tag{4.59}$$

$$D_j^{(\mu)} = \det \begin{pmatrix} s\delta_{j0} & \boldsymbol{w}^{\mathrm{T}} \\ \boldsymbol{v}_j^{(\mu)} & A_{2k-2} \end{pmatrix} \tag{4.60}$$

$$D_j^{(\nu)} = \det \begin{pmatrix} \int_0^s (s-\tau) l_j(\tau) d\tau & \boldsymbol{w}^{\mathrm{T}} \\ \boldsymbol{v}_j^{(\nu)} & A_{2k-2} \end{pmatrix} \tag{4.61}$$

$$A_{2k-2} = \begin{pmatrix} \int_{-1}^0 M(\tau)d\tau & \dots & \int_{-1}^0 \tau^{2k-3} M(\tau)d\tau \\ \vdots & & \vdots \\ \int_{1-k}^0 M(\tau)d\tau & \dots & \int_{1-k}^0 \tau^{2k-3} M(\tau)d\tau \\ \int_{-1}^0 \tau M(\tau)d\tau & \dots & \int_{-1}^0 \tau^{2k-2} M(\tau)d\tau \\ \vdots & & \vdots \\ \int_{1-k}^0 \tau M(\tau)d\tau & \dots & \int_{1-k}^0 \tau^{2k-2} M(\tau)d\tau \end{pmatrix} \tag{4.62}$$

$$\boldsymbol{w} = \left(\int_0^s (s-\tau) M(\tau)d\tau, \dots, \int_0^s (s-\tau)\tau^{2k-3} M(\tau)d\tau\right)^{\mathrm{T}} \tag{4.63}$$

$$\boldsymbol{v}_i^{(\nu)} = \left(\int_{-1}^0 -l_i(\tau)d\tau, \dots, \int_{1-k}^0 -l_i(\tau)d\tau, \int_{-1}^0 -\tau l_i(\tau)d\tau, \dots, \int_{1-k}^0 -\tau l_i(\tau)d\tau\right)^T$$

$$\boldsymbol{v}_j{}^{(\mu)} = \begin{cases} (1, \dots, 1 | 0, \dots, 0)^T & j = 0 \\ (\ -\boldsymbol{e}_j^{\mathrm{T}} \ | \ j\boldsymbol{e}_j^{\mathrm{T}}\ )^T & j > 0 \end{cases}$$

$$\boldsymbol{v}_j{}^{(\lambda)} = \begin{cases} (0, \dots, 0 | -1, \dots, -1)^T & j = 0 \\ (0, \dots, 0 |\ \ \boldsymbol{e}_j^{\mathrm{T}}\ \ )^T & j > 0 \end{cases}$$

and $D_{2k-2} = \det A_{2k-2}$.

Proof NED. □

Before looking at an example of MCRKN methods, we briefly return to the question of the unique solvability of the associated interpolation problem. In the previous section we were able to derive a necessary and sufficient condition for unique solvability involving the determinant of an $m \times m$ matrix. From the proof of Lemma 4.2 we see that this condition can be re-expressed in terms of the determinant of the $(2k-2) \times (2k-2)$ matrix A_{2k-2}, whose entries are considerably more complicated. In practice, since the determinant D_{2k-2} must be constructed in order to find the polynomials λ_j, μ_j and ν_i, there seems little point in constructing the determinant used in the previous section. It is however interesting to note that, as in the case of the stability analysis for the Panovsky-Richardson methods, we have two very different ways of expressing the same condition, and as yet we have not established a link between them. In the case of the Lie & Nørsett multistep collocation methods, the uniqueness condition may be re-expressed in terms of the determinant of the following $(k-1) \times (k-1)$ matrix:

$$\begin{pmatrix} \int_{-1}^{0} M(\tau)d\tau & \dots & \int_{-1}^{0} \tau^{k-2} M(\tau)d\tau \\ \vdots & & \vdots \\ \int_{1-k}^{0} M(\tau)d\tau & \dots & \int_{1-k}^{0} \tau^{k-2} M(\tau)d\tau \end{pmatrix}$$

In particular, when $k = 2$ we readily obtain the uniqueness condition

$$\int_{-1}^{0} M(\tau)d\tau = 0$$

which we saw at the end of the previous section. As an example we now consider the simplest two-step MCRKN method:

Example $k = 2,\ m = 1$

In this case $M(s) = s - c_1$, and so the matrix A_{2k-2} and vector $\boldsymbol{w}$ are given by

$$A_{2k-2} = \begin{pmatrix} -\dfrac{1+2c_1}{2} & \dfrac{2+3c_1}{6} \\ \dfrac{2+3c_1}{6} & -\dfrac{3+4c_1}{12} \end{pmatrix}$$

$$\boldsymbol{w} = \left(\frac{s^2(s-3c_1)}{6}, \frac{s^3(s-2c_1)}{12} \right)^T$$

After constructing the polynomial $U(s)$ in the way described above, we obtain the following MCRKN method:

$$\begin{aligned} 2(6c_1^2+6c_1+1)y_{n+c_1} &= -2(6c_1^5+15c_1^4+8c_1^3-6c_1^2-6c_1-1)y_n \\ &\quad +2c_1^3(6c_1^2+15c_1+8)y_{n-1} \\ &\quad +2c_1(3c_1^4+10c_1^3+12c_1^2+6c_1+1)hz_n \\ &\quad +2c_1^3(3c_1^2+5c_1+2)hz_{n-1} \\ &\quad +c_1^2(c_1+1)^2h^2f_{n+c_1} \end{aligned} \tag{4.64}$$

$$\begin{aligned} (6c_1^2+6c_1+1)y_{n+1} &= 8(1-3c_1^2)y_n+(30c_1^2+6c_1-7)y_{n-1} \\ &\quad +4(6c_1^2+3c_1-1)hz_n+2(6c_1^2-1)hz_{n-1} \\ &\quad +2h^2f_{n+c_1} \end{aligned} \tag{4.65}$$

$$\begin{aligned} (6c_1^2+6c_1+1)hz_{n+1} &= 24(1-3c_1^2)(y_n-y_{n-1}) \\ &\quad +4(12c_1^2+3c_1-4)hz_n \\ &\quad +(30c_1^2-6c_1-7)hz_{n-1} \\ &\quad +6h^2f_{n+c_1} \end{aligned} \tag{4.66}$$

with $f_{n+c_1} = f(x_{n+c_1}, x_{n+c_1})$. By looking at the coefficients of the left hand sides of these equations we see immediately that the method will collapse unless $(6c_1^2+6c_1+$

$1) \neq 0$. Recall from Example 1 of the previous section that this is the criterion for the unique solvability of the interpolation problem.

Since we are more interested in methods which possess intervals of periodicity rather than just absolute stability, following Lambert & Watson [46] we try imposing the symmetry constraint $c_1 = 0$. In this case the interpolation problem is uniquely solvable and leads to the method:

$$\begin{aligned} y_{n+1} &= 8y_n - 7y_{n-1} - 4hz_n - 2hz_{n-1} + 2h^2 f_n \\ hz_{n+1} &= 24(y_n - y_{n-1}) - 16hz_n - 7hz_{n-1} + 6h^2 f_n \end{aligned}$$

Unfortunately, as we shall show in section 4.4, this method has no interval of periodicity, and is therefore useless. However it is possible to obtain methods from this family with a non-empty interval of absolute stability by choosing c_1 appropriately.

4.2 Order conditions

In the case of one-step collocation methods for first order equations Nørsett & Wanner [51] have shown that by using the Gröbner-Alekseev Theorem, the order conditions may be derived using a simple quadrature approach. This analysis has been extended to cover multistep collocation methods for first order equations by Lie & Nørsett [47] and one-step collocation methods for second order equations by Nørsett [50] and van der Houwen et al. [68].

In this section we modify the Gröbner-Alekseev Theorem so that it can be used directly on second order equations. Then, following the work of Lie & Nørsett [47] and van der Houwen et al. [68] we go on to derive order conditions for the two-step m-point symmetric MCRKN methods.

Theorem 4.3 *(Gröbner (1960), Alekseev (1961)) Let u, y be the solutions of the*

following initial value problems

$$\begin{aligned} y'(x) &= f(x,y), & y(0) &= y_0 \\ u'(x) &= f(x,u) + g(x,u), & u(0) &= y_0 \end{aligned}$$

where a prime denotes differentiation with respect to x, and suppose that $\partial f/\partial y$ exists and is continuous. Then y and u are connected by

$$y(x) - u(x) = \int_0^x \Phi(x,\tau,u(\tau))g(\tau,u(\tau))d\tau$$

where

$$\Phi(x,\tau,u(\tau)) = -\frac{\partial y}{\partial u}(x,\tau,u(\tau))$$

Proof See Hairer et al. [35]. □

Corollary 4.4 *Let u, y be the solutions of the following initial value problems*

$$\begin{aligned} y''(x) &= f(x,y); & y(0) &= y_0,\ y'(0) = z_0 \\ u''(x) &= f(x,u) + g(x,u) & u(0) &= y_0,\ u'(0) = z_0 \end{aligned}$$

where a prime denotes differentiation with respect to x, and suppose that $\partial f/\partial y$ exists and is continuous. Then

$$y'(x) - u'(x) = \int_0^x \Phi(x,\tau,u(\tau),u'(\tau))g(\tau,u(\tau))d\tau \tag{4.67}$$

$$y(x) - u(x) = \int_0^x (x-\tau)\Gamma(x,\tau,u(\tau),u'(\tau))g(\tau,u(\tau))d\tau \tag{4.68}$$

for some functions Φ and Γ.

Proof Equation (4.67) follows immediately from the above theorem for first order equations. Integrating this with respect to x gives:

$$y(x) - u(x) = \int_0^x \int_0^\tau \Phi(\tau, \sigma, u(\sigma), u'(\sigma)) g(\sigma, u(\sigma)) d\sigma d\tau$$

Changing the order of integration gives:

$$\begin{aligned} y(x) - u(x) &= \int_0^x d\sigma \int_\sigma^x \Phi(\tau, \sigma, u(\sigma), u'(\sigma)) g(\sigma, u(\sigma)) d\tau \\ &= \int_0^x g(\sigma, u(\sigma)) \int_\sigma^x \Phi(\tau, \sigma, u(\sigma), u'(\sigma)) d\tau d\sigma \end{aligned}$$

Observe that the inner integral vanishes when $\sigma = x$, so that for some function Γ we have

$$y(x) - u(x) = \int_0^x g(\sigma, u(\sigma))(x - \sigma)\Gamma(x, \sigma, u(\sigma), u'(\sigma)) d\sigma$$

□

For notational convenience we will change variable for the rest of this section from x to the s-variable used in the previous section. Without loss of generality we also take $x_n = 0$ and $h = 1$.

In order to find the local truncation error of a k-step, m-point MCRKN method defined by (4.18)-(4.21) we consider the slightly different interpolation problem:

Find $V \in \mathcal{P}_{m+2k-1}$ such that

$$V(-r) = y(-r) \qquad r = 0, \ldots, k-1 \tag{4.69}$$

$$V'(-r) = y'(-r) \qquad r = 0, \ldots, k-1 \tag{4.70}$$

$$V''(c_i) = F(c_i, V(c_i)) \qquad i = 1, \ldots, m. \tag{4.71}$$

This is just another way of imposing the usual localising assumptions that all back-step approximations have zero error.

Define the local truncation error vector $\boldsymbol{L}$ to be:

$$\boldsymbol{L} = (y(1) - V(1),\ y'(1) - V'(1))^T$$

Now V satisfies the following initial value problem

$$V''(s) = F(s, V(s)) + \delta(s); \qquad V(0) = y(0),\ V'(0) = y'(0)$$

where δ has the property that it vanishes at the collocation nodes $\{c_i\}_{i=1}^m$. Applying our corollary to the Gröbner-Alekseev theorem we obtain the following expressions connecting V and y:

$$y'(s) - V'(s) = \int_0^s \Phi\delta(\tau)d\tau \tag{4.72}$$

$$y(s) - V(s) = \int_0^s (s-\tau)\Gamma\delta(\tau)d\tau \tag{4.73}$$

where the arguments of Φ and Γ have been suppressed for brevity. We may now re-express our localising assumptions as follows:

$$\int_0^{-\tau} \Phi\delta(\tau)d\tau = 0 \qquad r = 1, \ldots, k-1 \tag{4.74}$$

$$\int_0^{-\tau} (-r-\tau)\Gamma\delta(\tau)d\tau = 0 \qquad r = 1, \ldots, k-1 \tag{4.75}$$

and the local truncation error vector as:

$$\boldsymbol{L} = \left(\int_0^1 (1-\tau)\Gamma\delta(\tau)d\tau,\ \int_0^1 \Phi\delta(\tau)d\tau\right)^T \tag{4.76}$$

Following Lie & Nørsett's ([47]) approach we define a linear vector space $\mathcal{S}$ as follows:

$$\mathcal{S} = \left\{\rho \mid \int_0^{-\tau} \rho(\tau)d\tau = 0, \quad \int_0^{-\tau}\int_0^{\tau} \rho(\sigma)d\sigma d\tau = 0; \quad r = 1, \ldots, k-1.\right\} \tag{4.77}$$

We construct an interpolatory quadrature rule for the integral

$$\int_0^1 G(\tau)d\tau, \qquad G \in \mathcal{S}$$

which replaces G by a polynomial $P \in \mathcal{S}$ interpolating to G at the collocation nodes

$\{c_i\}_{i=1}^m$. The quadrature error is then

$$\int_0^1 (G(\tau) - P(\tau))d\tau = \int_0^1 R(\tau)M(\tau)d\tau \tag{4.78}$$

where $RM \in \mathcal{S}$ and M is as defined in the previous section.

We now consider the application of this quadrature rule to the y' component of $\boldsymbol{L}$. Since the integrand vanishes at the collocation nodes $\{c_i\}_{i=1}^m$, we have immediately that

$$\int_0^1 \Phi\delta(\tau)d\tau = \int_0^1 R(\tau)M(\tau)d\tau \tag{4.79}$$

We would like this quadrature error to vanish for R a polynomial of as high a degree as possible. Let

$$R_i(s) = \sum_{j=0}^{2k-2} a_{ij}s^{i+j} \qquad i = 0, 1, \ldots$$

and $\boldsymbol{a}_i = (a_{i0}, \ldots, a_{i\,2k-2})^{\mathrm{T}}$. Then the condition $R_iM \in \mathcal{S}$ becomes

$$B_i\boldsymbol{a}_i = \boldsymbol{0} \tag{4.80}$$

and the condition that the quadrature error is zero becomes:

$$\boldsymbol{b}_i^{\mathrm{T}}\boldsymbol{a}_i = 0 \tag{4.81}$$

where, for $i = 0, 1, \ldots$

$$B_i = \begin{pmatrix} \int_0^{-1} \tau^i M(\tau)d\tau & \cdots & \int_0^{-1} \tau^{2k-2+i} M(\tau)d\tau \\ \vdots & & \vdots \\ \int_0^{1-k} \tau^i M(\tau)d\tau & \cdots & \int_0^{1-k} \tau^{2k-2+i} M(\tau)d\tau \\ \int_0^{-1}(-1-\tau)\tau^i M(\tau)d\tau & \cdots & \int_0^{-1}(-1-\tau)\tau^{2k-2+i} M(\tau)d\tau \\ \vdots & & \vdots \\ \int_0^{1-k}(1-k-\tau)\tau^i M(\tau)d\tau & \cdots & \int_0^{1-k}(1-k-\tau)\tau^{2k-2+i} M(\tau)d\tau \end{pmatrix}$$

and

$$\boldsymbol{b}_i = \left(\int_0^1 \tau^i M(\tau) d\tau, \ldots, \int_0^1 \tau^{2k-2+i} M(\tau) d\tau \right)^T.$$

Let

$$P_i = \begin{pmatrix} B_i \\ \boldsymbol{b}_i{}^T \end{pmatrix} \tag{4.82}$$

and $Q_i = \det P_i$, for $i = 0, 1, \ldots$, then the system $P_i \boldsymbol{a}_i = \mathbf{0}$ has a non-trivial solution if and only if $Q_i = 0$.

In order to make any further progress with our derivation we must at this point restrict our attention to the two-step m-point MCRKN methods whose collocation nodes are distributed symmetrically in the interval $[-1, 1]$. Using this symmetry property we may simplify the matrix P for these methods to get

$$P_i = \begin{pmatrix} I(i) & -I(i+1) & I(i+2) \\ I(i+1) & -I(i+2) & I(i+3) \\ I(i) & I(i+1) & I(i+2) \end{pmatrix},$$

where, for $j = 0, 1, \ldots$,

$$I(j) = \int_0^1 \tau^j M(\tau) d\tau.$$

After some simple algebra we find that Q_i factorizes to give

$$Q_i = I(i+1) \det \begin{pmatrix} I(i) & I(i+2) \\ I(i+1) & I(i+3) \end{pmatrix}.$$

Suppose first that $I(i+1) \neq 0$, then for $P\boldsymbol{a}_i = \mathbf{0}$ to have a non-trivial solution, we require that the second term in our expression for Q_i vanishes.

Next suppose that $I(i+1) = 0$. In this case the quadrature condition becomes

$$I(i) a_{i0} + I(i+2) a_{i2} = 0, \tag{4.83}$$

and R_iM lies in $\mathcal{S}$ if

$$-I(i+2)a_{i1} + I(i+3)a_{i2} = 0. \tag{4.84}$$

For the interpolation problem to remain uniquely solvable we must have that $I(i) \times I(i+2) \neq 0$. The system (4.83)-(4.84) has solutions

$$\begin{aligned} R_i &= -\tfrac{I(i)}{I(i+2)}a_{i2} + a_{i2}s^2, && \text{if } I(i+3) = 0, \\ R_i &= -\tfrac{I(i)}{I(i+2)}a_{i2} + \tfrac{I(i+2)}{I(i+3)}a_{i1}s + a_2 s^2, && \text{if } I(i+3) \neq 0. \end{aligned}$$

with $a_2 \neq 0$. Observe that the corresponding integral arising from the y component of the local truncation error vector is evaluated exactly by our quadrature formula if $I(i+3) = 0$. Hence the following theorem is seen to hold:

Theorem 4.5 *If the nodes of a two-step m-point MCRKN method are chosen so that for each $i \in \{0, \ldots, p_0\}$, the interpolation problem (4.18)-(4.20) remains uniquely solvable and either*

$$I(i+1) \neq 0 \qquad \textit{and} \qquad I(i)I(i+3) - I(i+1)(I(i+2) = 0,$$

or

$$I(i+1) = 0 \qquad \textit{and} \qquad I(i+3) = 0,$$

then the resulting method will have order at least $m + 2 + (p_0 + 1)$.

Proof NED □

We close this subsection with an example.

Example $k = 2$, $m = 2$ and $c_2 = -c_1$.

The minimum order of a method from this family is four. Set $i = 0$, then

$$\begin{aligned} I(i) &= (1 - 3c_1^2)/2 \\ I(i+1) &= (1 - 2c_1^2)/4 \\ I(i+2) &= (3 - 5c_1^2)/15 \end{aligned}$$

$$I(i+3) \;=\; (2-3c_1^2)/12.$$

If $c_1^2 = 1/2$, then $I(i+1) = 0$, but $I(i+3) \neq 0$, so we cannot increase the order of the method this way. However with $c_1^2 = (6 \pm \sqrt{(21)})/15$, $I(i)I(i+2) - I(i+1)I(i+3) = 0$, hence the method has order at least five. Further investigation shows that five is the maximum order of a method from this class. We will see from the example at the end of section 4.4 that the methods from this class which have order five are unstable, and so are useless. In that section we will also verify the order conditions derived here using Taylor analysis.

4.3 Stability analysis

In this section we derive an explicit expression for the stability polynomial $\pi(\lambda)$ for a general k-step, m-point multistep collocation method. Our method of construction follows closely that of Kramarz [44], who analysed the stability of one-step collocation methods.

In order to study the stability properties of these methods we apply them to the standard scalar test problem:

$$\frac{d^2y}{dx^2} = -\omega^2 y, \qquad y(x_0) = y_0, \; \frac{dy}{dx}(x_0) = z_0 \tag{4.85}$$

When a k-step MCRKN method is applied to (4.85) with constant stepsize h we obtain a numerical solution of the form

$$\boldsymbol{u}_n = A^{n-(k-1)}\boldsymbol{y}_{k-1} \qquad n = k-1, k, \ldots \tag{4.86}$$

where A, the so-called *iteration matrix*, is a $2k \times 2k$ matrix whose entries are independent of n, and whose eigenvalues are functions of $\nu^2 = \omega^2 h^2$,

$$\boldsymbol{u}_n \;=\; \left(u(x_n), \ldots, u(x_{n-k+1}), \frac{du}{dx}(x_n), \ldots, \frac{du}{dx}(x_{n-k+1})\right)^T,$$

$$\boldsymbol{y}_n = (y_n, z_n, \ldots, y_{n-k+1}, z_{n-k+1})^T, \quad n = k-1, k, \ldots$$

and $\{y_j, z_j\}_{j=0}^{k-1}$ are approximations to $\{y(x_j), dy(x_j)/dx\}_{j=0}^{k-1}$ obtained from a suitable starting procedure.

The stability polynomial for these methods is given by

$$\pi(\lambda) = \det\,(A - \lambda I_{2k})$$

where I_{2k} is the $2k \times 2k$ identity matrix. Let $\lambda_1(\nu^2), \ldots, \lambda_{2k}(\nu^2) \in \mathbb{C}$ be the roots of $\pi(\lambda)$, i.e. the eigenvalues of A, ordered so that $|\lambda_1(\nu^2)| \geq |\lambda_2(\nu^2)| \geq \ldots \geq |\lambda_{2k}(\nu^2)|$. Recall from chapter 2 that for the method to be absolutely stable we require that the roots of $\pi(\lambda)$ lie in the unit disc $\{z \in \mathbb{C} : |z| \leq 1\}$ and that all roots of modulus one have multiplicity at most two. Recall also that the method will be periodic if $\lambda_1(\nu^2)$ and $\lambda_2(\nu^2)$ are complex conjugates lying on the unit circle $\{z \in \mathbb{C} : |z| = 1\}$, and if the remaining roots lie in the unit disc.

We begin by constructing the iteration matrix A. Instead of attempting to express A in terms of the coefficients of the method, we follow the ideas of Kramarz [44] and Wright [69] and try to express it solely in terms of the collocation nodes $\{c_i\}_{i=1}^m$.

When a k-step m-point MCRKN method is applied to the scalar test problem (4.85) the collocation problem (4.18)-(4.20) becomes:

Find $u \in \mathcal{P}_{m+2k-1}$ such that

$$\begin{aligned} u(x_{n-j}) &= y_{n-j} && j = 0, \ldots, k-1 \\ \frac{du}{dx}(x_{n-j}) &= z_{n-j} && j = 0, \ldots, k-1 \\ \frac{d^2u}{dx^2}(x_{n+c_i}) &= -\omega^2 u(x_{n+c_i}) && i = 1, \ldots, m \end{aligned} \tag{4.87}$$

The function $d^2u(x)/dx^2 + \omega^2 u(x)$ is a polynomial of degree $m + 2k - 1$ with roots at $x = x_{n+c_i}$, $i = 1, \ldots, m$. Using this, and the collocation conditions (4.87), we see

that u is a solution of the following initial value problem:

$$\begin{aligned} \frac{d^2u}{dx^2}(x) + \omega^2 u(x) &= R(x) \sum_{p=0}^{2k-1} \alpha_p x^p, \\ u(x_{n-k+1}) &= y_{n-k+1} \\ \frac{du}{dx}(x_{n-k+1}) &= z_{n-k+1} \end{aligned} \tag{4.88}$$

where

$$R(x) = \prod_{i=1}^{m} (x - x_{n+c_i})$$

and $\alpha_p \in \mathbb{R}$, $p = 0, \ldots, 2k-1$. For notational convenience we will use the scaled variable

$$s = \frac{x - x_{n-k+1}}{h}$$

and let a prime denote differentiation with respect to s for the rest of this section. Take $n = k-1$ so that we are considering the first step in which the MCRKN method is applied. Using the method of variation of constants it is possible to solve the initial value problem (4.88) to get:

$$\begin{aligned} u(sh) &= y_0 \cos(\nu s) + \frac{z_0}{\omega} \sin(\nu s) + \\ &\quad \frac{1}{\omega} \int_0^s \sin[(s-\tau)\nu] \tilde{M}(\tau) \sum_{p=0}^{2k-1} a_p \tau^p d\tau \end{aligned} \tag{4.89}$$

$$\begin{aligned} \frac{du}{dx}(sh) &= -\omega y_0 \sin(\nu s) + z_0 \cos(\nu s) + \\ &\quad \int_0^s \cos[(s-\tau)\nu] \tilde{M}(\tau) \sum_{p=0}^{2k-1} a_p \tau^p d\tau \end{aligned} \tag{4.90}$$

where

$$\tilde{M}(\tau) = M(\tau - k + 1)$$

with $M(\tau)$ as previously defined, and $a_p = \alpha_p h^{m+1+p}$, for $p = 0, \ldots, 2k-1$. Since u is a polynomial, we can immediately obtain two equations relating y_0 and z_0 to the $\{a_p\}_{p=0}^{2k-1}$ by equating the coefficients of $\cos(\nu s)$ and $\sin(\nu s)$ in (4.89) and (4.90) to

zero. First however, we must evaluate the integrals contained in (4.89) and (4.90), to do this we will need the following lemma.

Lemma 4.6 *Let $g \in \mathcal{P}_n$, $n \geq 0$, and let $q = \lfloor n/2 \rfloor$, then*

$$\begin{aligned}
\int_0^s \sin[(s-\tau)\nu] g(\tau) d\tau &= \sum_{j=0}^{q} \frac{(-1)^j g^{(2j)}(s)}{\nu^{2j+1}} \\
&\quad - \sum_{j=0}^{q} \frac{(-1)^j g^{(2j)}(0)\cos(\nu s)}{\nu^{2j+1}} \\
&\quad - \sum_{j=0}^{q} \frac{(-1)^j g^{(2j+1)}(0)\sin(\nu s)}{\nu^{2j+2}} \qquad (4.91) \\
\int_0^s \cos[(s-\tau)\nu] g(\tau) d\tau &= \sum_{j=0}^{q} \frac{(-1)^j g^{(2j+1)}(s)}{\nu^{2j+2}} \\
&\quad - \sum_{j=0}^{q} \frac{(-1)^j g^{(2j+1)}(0)\cos(\nu s)}{\nu^{2j+2}} \\
&\quad - \sum_{j=0}^{q} \frac{(-1)^j g^{(2j)}(0)\sin(\nu s)}{\nu^{2j+1}} \qquad (4.92)
\end{aligned}$$

Proof Use induction on n, and integration by parts. □

Let

$$\Phi_p^{(r)}(\tau) = \frac{d^r}{d\tau^r}\left[\tilde{M}(\tau)\tau^p\right] \qquad (4.93)$$

then by Leibniz' rule:

$$\Phi_p^{(r)}(\tau) = \sum_{i=0}^{\min(r,p)} \binom{r}{i} \tilde{M}^{(r-i)}(\tau) \frac{p!}{(p-i)!} \tau^{(p-i)} \qquad (4.94)$$

Let

$$I_p(s) = \int_0^s \sin[(s-\tau)\nu] \tilde{M}(\tau)\tau^p d\tau$$

and

$$J_p(s) = \int_0^s \cos[(s-\tau)\nu] \tilde{M}(\tau)\tau^p d\tau$$

then, using the above Lemma, we have that

$$\begin{aligned} I_p(s) &= \sum_{j=0}^{N_p} \left(\frac{-1}{\nu^2}\right)^j \left(\frac{1}{\nu}\Phi_p^{(2j)}(s) - \frac{1}{\nu}\cos(\nu s)\Phi_p^{(2j)}(0) \right. \\ &\quad \left. -\frac{1}{\nu^2}\sin(\nu s)\Phi_p^{(2j+1)}(0)\right) \end{aligned} \tag{4.95}$$

$$\begin{aligned} J_p(s) &= \sum_{j=0}^{N_p} \left(\frac{-1}{\nu^2}\right)^j \left(\frac{1}{\nu^2}\Phi_p^{(2j+1)}(s) - \frac{1}{\nu^2}\cos(\nu s)\Phi_p^{(2j+1)}(0) \right. \\ &\quad \left. -\frac{1}{\nu}\sin(\nu s)\Phi_p^{(2j)}(0)\right) \end{aligned} \tag{4.96}$$

where $N_p = \lfloor \frac{1}{2}(m+p) \rfloor$. Equating coefficients of $\cos(\nu s)$ and $\sin(\nu s)$ in $u(sh)$ to zero, we obtain the following equations expressing $\boldsymbol{a} = (a_0, \ldots, a_{2k-1})^{\mathrm{T}}$ in terms of y_0 and z_0:

$$\begin{pmatrix} 1 & 0 \\ 0 & \omega^{-1} \end{pmatrix} = \frac{1}{\omega} \begin{pmatrix} C_0 & \ldots & C_{2k-1} \\ S_0 & \ldots & S_{2k-1} \end{pmatrix} \boldsymbol{a} \tag{4.97}$$

where C_p and S_p are the coefficients of $\cos(\nu s)$ and $\sin(\nu s)$ in $I_p(s)$ respectively. Using these conditions to simplify $u(sh)$ and $u'(sh)$ we obtain:

$$u(sh) = h \sum_{p=0}^{2k-1} a_p \Psi_p(s) \tag{4.98}$$

$$\frac{du}{dx}(sh) = \sum_{p=0}^{2k-1} a_p \Psi_p'(s) \tag{4.99}$$

where

$$\Psi_p(s) = \frac{1}{\nu^2} \sum_{j=0}^{N_p} \left(\frac{-1}{\nu^2}\right)^j \Phi_p^{(2j)}(s) \tag{4.100}$$

With u in this form we can easily enforce the collocation conditions

$$u(jh) = y_j, \qquad \frac{du}{dx}(jh) = z_j, \qquad j = 0, \ldots, k-1$$

to get the following equations expressing $\boldsymbol{a}$ in terms of $\boldsymbol{y}_{k-1}$:

$$\boldsymbol{y}_{k-1} = P\boldsymbol{a} \tag{4.101}$$

where P is given by

$$P = \begin{pmatrix} h\Psi_0(k-1) & \dots & h\Psi_{2k-1}(k-1) \\ \Psi_0'(k-1) & \dots & \Psi_{2k-1}'(k-1) \\ \vdots & \vdots & \vdots \\ h\Psi_0(0) & \dots & h\Psi_{2k-1}(0) \\ \Psi_0'(0) & \dots & \Psi_{2k-1}'(0) \end{pmatrix}$$

Evaluating $u(sh)$ and $du(sh)/dx$ at $s = k$ (i.e. $x = x_{n+1}$), and using (4.101) gives:

$$\begin{aligned} \left(u(kh), \frac{du}{dx}(kh)\right)^T &= Q\boldsymbol{a} \\ &= QP^{-1}\boldsymbol{y}_{k-1} \end{aligned} \tag{4.102}$$

where Q is a $2 \times 2k$ matrix given by

$$Q = \begin{pmatrix} h\Psi_0(k) & \dots & h\Psi_{2k-1}(k) \\ \Psi_0'(k) & \dots & \Psi_{2k-1}'(k) \end{pmatrix}$$

We note in passing that the factor h appearing in the odd rows of P and Q may be removed by replacing $\boldsymbol{y}_n$ by the vector:

$$\bar{\boldsymbol{y}_n} = (y_n, hz_n, \dots, y_{n-k+1}, hz_{n-k+1})^T.$$

The MCRKN method defines y_k and z_k to be $u(kh)$ and $du(kh)/dx$ respectively, so we now have an explicit expression for our y and y' approximations at step 1 in terms of the information carried forward from step 0. Using the same idea we can write the approximations at step 2 in terms of the information carried forward from step 1, and

so on. The iteration matrix A such that $\boldsymbol{y}_{n+1} = A\boldsymbol{y}_n = A^{n-k+2}\boldsymbol{y}_{k-1}$ is now trivial to form, and is given by

$$A = \begin{pmatrix} & QP^{-1} & \\ I_{2k-2} & & \mathbf{0}_{2k-2,2} \end{pmatrix} \tag{4.103}$$

where I_{2k-2} is the $(2k-2)\times(2k-2)$ identity matrix and $\mathbf{0}_{2k-2,2}$ is a $(2k-2)\times 2$ matrix of zeroes. In the following section we consider the two-step MCRKN methods with 1,2,3 and 4 collocation nodes, and use this matrix to derive their stability properties.

In order to analyse the stability properties of a particular MCRKN method or class of MCRKN methods we need to re-express the functions Ψ_p as functions of the collocation nodes $\{c_i\}_{i=1}^m$. Substituting back for $\Phi_p^{(2j)}$ gives:

$$\Psi_p(s) = \frac{h}{\nu^2}\sum_{i=0}^{p}\binom{p}{i}s^{p-i}\sum_{j=0}^{N_p}\left(\frac{-1}{\nu^2}\right)^j\frac{(2j)!}{(2j-i)!}\tilde{M}^{(2j-i)}(s)$$

with the convention that $\tilde{M}^{(r)}(s) \equiv 0$ if $r < 0$. Letting

$$\Gamma_i(s) = \sum_{j=0}^{N_p}\left(\frac{-1}{\nu^2}\right)^j\frac{(2j)!}{(2j-i)!}\tilde{M}^{(2j-i)}(s)$$

it is immediately obvious that the range of the summation index in the above sum is in fact $\{\lceil\frac{1}{2}i\rceil,\ldots,\lfloor\frac{1}{2}(m+i)\rfloor\}$. After some algebra we obtain the following expressions for $\Gamma_i(s)$ and $\Gamma_i'(s)$:

$$\Gamma_i(s) = \begin{cases} \left(\frac{-1}{\nu^2}\right)^{\frac{1}{2}i}\sum_{j=0}^{N}\left(\frac{-1}{\nu^2}\right)^j\frac{(2j+i)!}{(2j)!}\tilde{M}^{(2j)}(s) & i \text{ even}, \\ \left(\frac{-1}{\nu^2}\right)^{\frac{1}{2}(i+1)}\sum_{j=0}^{N}\left(\frac{-1}{\nu^2}\right)^j\frac{(2j+i+1)!}{(2j+1)!}\tilde{M}^{(2j+1)}(s) & i \text{ odd}, \end{cases}$$

$$\Gamma_i'(s) = \begin{cases} \left(\frac{-1}{\nu^2}\right)^{\frac{1}{2}i}\sum_{j=0}^{N}\left(\frac{-1}{\nu^2}\right)^j\frac{(2j+1+i)!}{(2j+1)!}\tilde{M}^{(2j+1)}(s) & i \text{ even}, \\ \left(\frac{-1}{\nu^2}\right)^{\frac{1}{2}(i-1)}\sum_{j=0}^{N}\left(\frac{-1}{\nu^2}\right)^j\frac{(2j+i)!}{(2j)!}\tilde{M}^{(2j)}(s) & i \text{ odd}. \end{cases}$$

These expressions are natural generalisations of the corresponding expressions given

by Kramarz [44] for the case of one-step collocation methods.

In view of the work done for one-step methods, it seems a lot to ask to draw useful conclusions regarding the stability properties of an MCRKN method with arbitrary stepnumber and number of collocation nodes. In an attempt to make at least some progress we will restrict our attention to the case $k = 2$. Since these methods are designed to approximate the solutions of periodic initial value problems (4.1), we would prefer them to be periodic rather than just absolutely stable. Following Lambert and Watson [46] we impose the following symmetry constraint on the collocation nodes $\{c_i\}_{i=1}^m$:

$$c_i + c_{m+1-i} = 0, \qquad i = 1, \ldots, \lceil \tfrac{1}{2}m \rceil \tag{4.104}$$

In order to show more clearly any possible symmetry properties in the stability polynomial we will use the shifted variable $t = s - 1$, along with the following definitions for the rest of this section:

$$\phi_p^{(r)}(t) = \Phi_p^{(r)}(s), \quad \psi_p(t) = \Psi_p(s) \quad \text{and} \quad \gamma_i(t) = \Gamma_i(s).$$

Under the constraint (4.104), the polynomial $M(t)$ satisfies

$$M^{(r)}(t) = (-1)^{m-r} M^{(r)}(-t) \quad r = 0, 1, \ldots$$

from which the following identities involving the functions $\gamma_i(t)$ may easily be derived:

$$\gamma_i(t) = (-1)^{m+i} \gamma_i(-t), \tag{4.105}$$

$$\gamma_i'(t) = (-1)^{m+i+1} \gamma_i'(-t), \tag{4.106}$$

$$\gamma_i(0) = 0, \qquad m + i \text{ even}, \tag{4.107}$$

$$\gamma_i'(0) = 0, \qquad m + i \text{ odd}. \tag{4.108}$$

Using these identities the matrix P may be written as:

$$P = \begin{pmatrix} \gamma_0(0) & \gamma_0(0) & \gamma_0(0)+\gamma_2(0) & \gamma_0(0)+3\gamma_2(0) \\ 0 & \gamma_1'(0) & 2\gamma_1'(0) & 3\gamma_1'(0)+\gamma_3'(0) \\ \gamma_0(1) & -\gamma_1(1) & \gamma_2(1) & -\gamma_3(1) \\ -\gamma_0'(1) & \gamma_1'(1) & -\gamma_2'(1) & \gamma_3'(1) \end{pmatrix}$$

when m is even, and

$$P = \begin{pmatrix} 0 & \gamma_1(0) & 2\gamma_1(0) & 3\gamma_1(0)+\gamma_3(0) \\ \gamma_0'(0) & \gamma_0'(0) & \gamma_0'(0)+\gamma_2'(0) & \gamma_0'(0)+3\gamma_2'(0) \\ -\gamma_0(1) & \gamma_1(1) & -\gamma_2(1) & \gamma_3(1) \\ \gamma_0'(1) & -\gamma_1'(1) & \gamma_2'(1) & -\gamma_3'(1) \end{pmatrix}$$

when m is odd. The matrix Q is given by

$$Q^T = \begin{pmatrix} \boldsymbol{q} & \boldsymbol{q}' \end{pmatrix}$$

where

$$\boldsymbol{q} = \begin{pmatrix} \gamma_0(1) \\ 2\gamma_0(1) + \gamma_1(1) \\ 4\gamma_0(1) + 4\gamma_1(1) + \gamma_2(1) \\ 8\gamma_0(1) + 12\gamma_1(1) + 6\gamma_2(1) + \gamma_3(1) \end{pmatrix}$$

and

$$\boldsymbol{q}' = \begin{pmatrix} \gamma_0'(1) \\ 2\gamma_0'(1) + \gamma_1'(1) \\ 4\gamma_0'(1) + 4\gamma_1'(1) + \gamma_2'(1) \\ 8\gamma_0'(1) + 12\gamma_1'(1) + 6\gamma_2'(1) + \gamma_3'(1) \end{pmatrix}.$$

Theorem 4.7 *Let the collocation nodes $\{c_i\}_{i=1}^m$ of a 2-step MCRKN method satisfy the symmetry constraint (4.104), then the determinant of the iteration matrix A is 1 for all values of m.*

Proof We will only prove the theorem for MCRKN methods with an even number of collocation nodes, since the proof for methods where m is odd is almost identical. Let $\boldsymbol{p}_i^{\mathrm{T}}$ be the i^{th} row of P, for $i = 1, \ldots, 4$, and let $\bar{Q} = (\boldsymbol{q}, \boldsymbol{q}', \boldsymbol{p}_1, \boldsymbol{p}_2)^{\mathrm{T}}$. We may now rewrite the iteration matrix A as $A = \bar{Q}P^{-1}$. From our expression for P above, we have that

$$\begin{pmatrix} \boldsymbol{q}^T \\ \boldsymbol{q}'^T \end{pmatrix} = \begin{pmatrix} \boldsymbol{p}_3^T \\ -\boldsymbol{p}_4^T \end{pmatrix} B$$

where

$$B = \begin{pmatrix} 1 & 2 & 4 & 8 \\ 0 & -1 & -4 & -12 \\ 0 & 0 & 1 & 6 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

By inspection we see that

$$\begin{pmatrix} \boldsymbol{p}_1^T \\ \boldsymbol{p}_2^T \end{pmatrix} = \begin{pmatrix} \boldsymbol{p}_1^T \\ -\boldsymbol{p}_2^T \end{pmatrix} B$$

so that $\bar{Q}$ may be written as:

$$\bar{Q} = JPB$$

where J is given by

$$J = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}.$$

Finally we have that

$$\begin{aligned} \det A &= \det (JPBP^{-1}) \\ &= \det P \det P^{-1} \end{aligned}$$

since B and J both have determinant 1. The result follows immediately. □

Theorem 4.8 *Under the conditions of the above theorem, the characteristic polynomial of A is symmetric.*

Proof Write A as

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

then it can be shown that

$$\begin{aligned} \pi(\lambda) &= \det\,(A - \lambda I_4) \\ &= \lambda^4 - \mathrm{tr}(A)\lambda^3 + (a_{11}a_{22} - a_{21}a_{12} - a_{13} - a_{24})\lambda^2 \\ &\quad -\mathrm{tr}(A^{-1})\lambda + 1 \end{aligned}$$

From the above theorem we have that

$$\begin{aligned} A^{-1} &= (JPBP^{-1})^{-1} \\ &= PB^{-1}P^{-1}J^{-1} \\ &= J^{-1}AJ \end{aligned}$$

since $J^2 = B^2 = I_4$. It is easy to show that $\mathrm{tr}(JW) = \mathrm{tr}(WJ)$ for all matrices W, and thus $\mathrm{tr}(A) = \mathrm{tr}(A^{-1})$. Hence the required result:

$$\begin{aligned} \pi(\lambda) &= \lambda^4 - (a_{11} + a_{22})\lambda^3 + (a_{11}a_{22} - a_{21}a_{12} - a_{13} - a_{24})\lambda^2 \\ &\quad -(a_{11} + a_{22})\lambda + 1 \end{aligned}$$

□

In order to determine the stability properties of an MCRKN method we make use

of the well-known Routh-Hurwitz transformation described in chapter 2. Let

$$R(\zeta) = (1-\zeta)^4 \pi(\lambda) \qquad \text{with} \qquad \lambda = \frac{1+\zeta}{1-\zeta}$$

In view of the above two theorems, we see that the Routh-Hurwitz polynomial will be of the form

$$R(\zeta) = \alpha_4 \zeta^4 + \alpha_2 \zeta^2 + \alpha_0,$$

with $\alpha_0, \alpha_2, \alpha_4 \in \mathbb{R}$, which is a quadratic in ζ^2. Thus for all roots of $R(\zeta)$ to lie in the left half plane $\{z \in \mathbb{C} : \mathrm{Re} z \leq 0\}$, they must lie on the imaginary axis. From this we can deduce that if our method has an interval of absolute stability, then it is also an interval of periodicity. The conditions under which $R(\zeta)$ has purely imaginary roots are as follows:

$$\mathrm{sign}(\alpha_0) = \mathrm{sign}(\alpha_2) = \mathrm{sign}(\alpha_4) \tag{4.109}$$

and

$$\alpha_2^2 - 4\alpha_4\alpha_0 > 0 \tag{4.110}$$

The first condition is just the well-known Routh-Hurwitz criterion for quadratics which ensures that the squares of the roots of $R(\zeta)$ have negative real parts, and the second condition ensures that they have no imaginary parts.

Using these conditions we have been able to determine the stability properties of a number of specific 2-step MCRKN methods. Unfortunately, apart from noting that the constraints imposed by the two stability conditions above are rather severe, no general trends have so far emerged from our results. We have also encountered numerous problems on the analytical front, and so the question of existence of periodicity intervals for 2-step MCRKN methods with an arbitrary number of collocation nodes remains unanswered.

4.4 Some symmetric two-step MCRKN methods

In this section we analyse the order and stability properties of two-step MCRKN methods with 1,2,3 and 4 collocation nodes. Since we are interested in methods which may possess intervals of periodicity, we consider only those methods whose collocation nodes are symmetrically distributed in $[-1, 1]$.

The 2-step 1-point symmetric MCRKN method

There is only one 2-step 1-point symmetric MCRKN method:

$$\begin{aligned} y_{n+1} &= 8y_n - 7y_{n-1} - 4hz_n - 2hz_{n-1} + h^2 f_n \\ hz_{n+1} &= 24(y_n - y_{n-1}) - 16hz_n - 7hz_{n-1} + 6h^2 f_n. \end{aligned}$$

By construction, this method has order at least three. To see if the method has order greater than three we check to see if the conditions of theorem 4.5 hold with $i = 0$. $I(i+1) = 1/3$, so for order greater than three we must have that $I(i)I(i+2) - I(i+1)I(i+3) = 0$, which is not the case here.

The Routh-Hurwitz polynomial for this method is given by

$$R(\zeta) = a_4\zeta^4 + a_2\zeta^2 + a_0$$

with

$$a_4 = 3\nu^2, \qquad a_2 = 12 - 4\nu^2 \qquad \text{and} \qquad a_0 = \nu^2 - 8.$$

For $\nu^2 \in (0, 8)$, a_0 is negative while the other coefficients are positive, and for $\nu^2 > 8$, a_2 is negative. Hence this method is unstable for all values of ν^2 and so is useless.

The 2-step 2-point MCRKN methods

The symmetry constraint for these methods is $c_2 = -c_1$. In view of the complexity of the expressions involved we will not give the general method from this family, or from

the families with $m = 3, 4$. By construction, methods from this family have order not less than four. In section 4.2 we saw that with the choices $c_1^2 = (6 \pm \sqrt{(21)})/15$ we obtain methods of order five. We can verify this by expanding the y and y' components of the local truncation error vector as Taylor series. The leading terms in the two expansions are

$$\frac{(3 - 10c_1^2)(15c_1^4 - 12c_1^2 + 1)h^6 y^{(6)}(x_n)}{180(60c_1^4 - 44c_1^2 + 3)}$$

and

$$\frac{(1 - 2c_1^2)(15c_1^4 - 12c_1^2 + 1)h^5 y^{(6)}(x_n)}{12(60c_1^4 - 44c_1^2 + 3)}$$

respectively. With $c_1^2 = 1/2$, we increase the order of the y' approximation, but not the y approximation, and so this does not lead to an increase in the order of the method. If c_1^2 takes either of the above values, then the orders of both the y and y' approximations are increased by one, hence the resulting method will have order five.

The Routh-Hurwitz polynomial for methods from this family is

$$R(\zeta) = a_4\zeta^4 + a_2\zeta^2 + a_0$$

where the coefficients a_0, a_2 and a_4, and the discriminant D are given by:

$$\begin{aligned}
a_4 &= 8\nu^2((13c_1^4 - 5c_1^2 + 2)\nu^2 + 30(2c_1^2 - 1)) \\
a_2 &= 16((3c_1^6 - 9c_1^4 + 8c_1^2 - 2)\nu^4 + 2(33c_1^4 - 52c_1^2 + 16)\nu^2 + 60(2c_1^2 - 1) \\
a_0 &= 8((2c_1^8 - 10c_1^6 + 17c_1^4 - 11c_1^2 + 2)\nu^4 + 2(32c_1^6 - 98c_1^4 + 82c_1^2 - 17)\nu^2 \\
&\quad +16(30c_1^4 - 37c_1^2 + 9)) \\
D &= 256c_1^4\nu^8(3c_1^8 - 14c_1^6 + 24c_1^4 - 18c_1^2 + 5) \\
&\quad +1024c_1^2\nu^6(21c_1^8 - 61c_1^6 + 50c_1^4 - 5c_1^2 - 5) \\
&\quad -1024\nu^4(51c_1^8 - 402c_1^6 + 508c_1^4 - 192c_1^2 + 11) \\
&\quad -61440\nu^2(54c_1^6 - 71c_1^4 + 26c_1^2 - 2)
\end{aligned}$$

$$+921600(4c_1^4 - 4c_1^2 + 1)$$

In an attempt to reduce the range of allowable values for c_1 we look at our stability conditions in the case where ν is small enough for us to be able to neglect terms of order ν^2. In this case the coefficients and discriminant of the Routh-Hurwitz polynomial are given by

$$\begin{aligned} a_4 &= \alpha_4(2c_1^2 - 1) \\ a_2 &= \alpha_2(2c_1^2 - 1) \\ a_0 &= \alpha_0(10c_1^2 - 9)(3c_1^2 - 1) \\ D &= \alpha_5(2c_1 - 1)^2 \end{aligned}$$

where the α's are positive constants independent of c_1. On applying the stability conditions we find that the MCRKN method is periodic for small values of ν if and only if $c_1^2 \in (1/3, 1/2) \cup (9/10, 1)$. Notice that already the range of allowable values for c_1 has decreased by a factor of 5. Our interest lies in determining the boundary of the first interval of periodicity in terms of c_1, for, if these methods were to be used in a variable stepsize code, then it is this boundary that would impose an upper bound on the range of allowable stepsizes. The boundaries of the periodicity intervals may be determined as functions of c_1 by finding the roots of the coefficients and discriminant of our Routh-Hurwitz polynomial. These functions were plotted over the range of allowable values of c_1, (i.e. $c_1^2 \in (1/2, 1/3) \cup (9/10, 1)$), and the results are shown in figures 4.1 and 4.2. So far we have not succeeded in finding a closed form expression for the roots of the discriminant D, though we have been able to approximately determine where it changes sign by producing contour plots as shown in figures 4.1 and 4.2. In figure 4.3 we have super-imposed all the plots for each range of c_1. The primary interval of periodicity is now given by the vertical distance from the c_1^2 axis to the nearest curve. By examining these plots we see that the largest possible interval of periodicity has length approximately 7, and is achieved when $c_1^2 \approx 0.46$. After

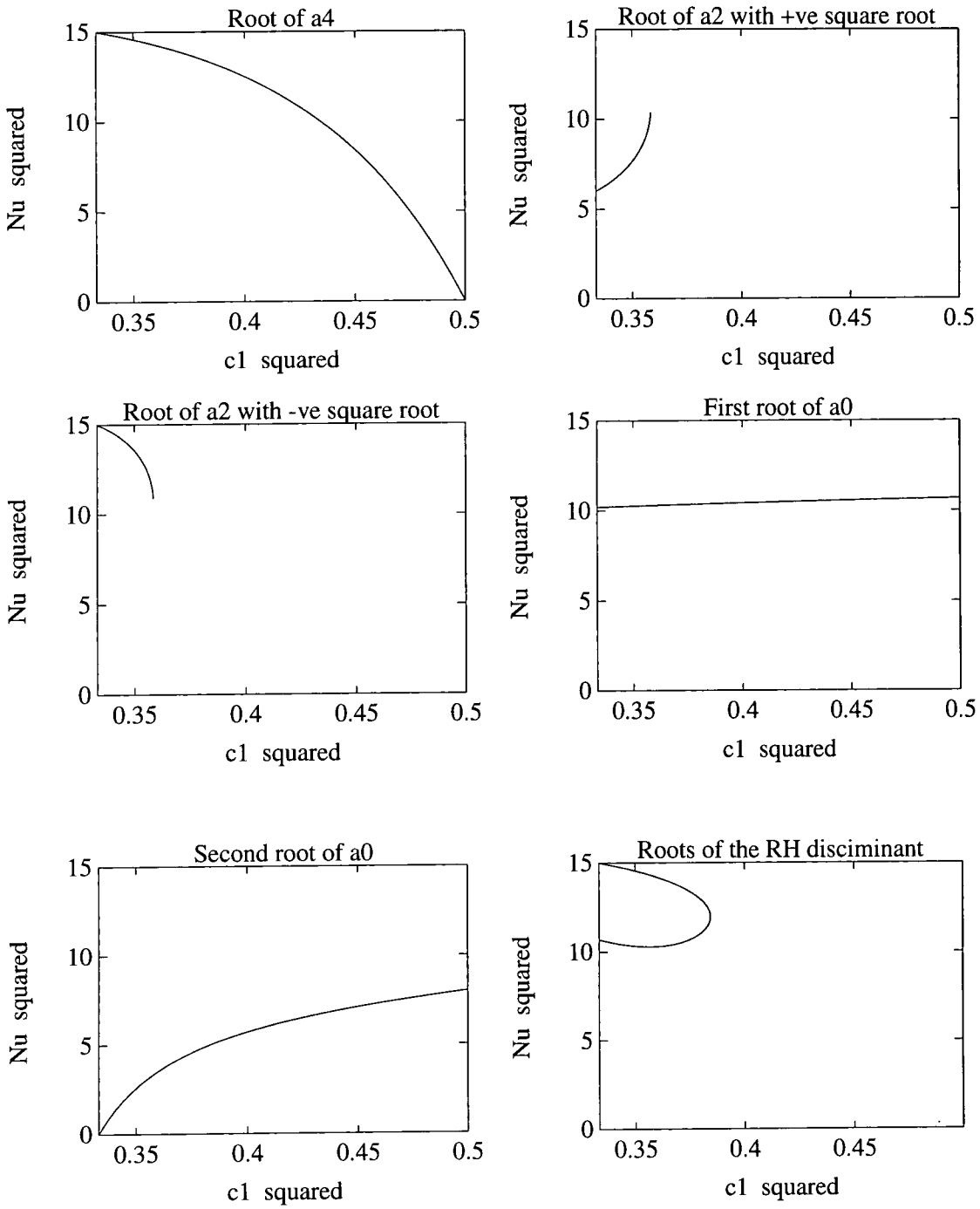

Figure 4.1: Graphs of the roots of the Routh-Hurwitz coefficients and discriminant for 2-step 2-point symmetric MCRKN methods as functions of c_1, with $c_1^2 \in (1/2, 1/3)$.

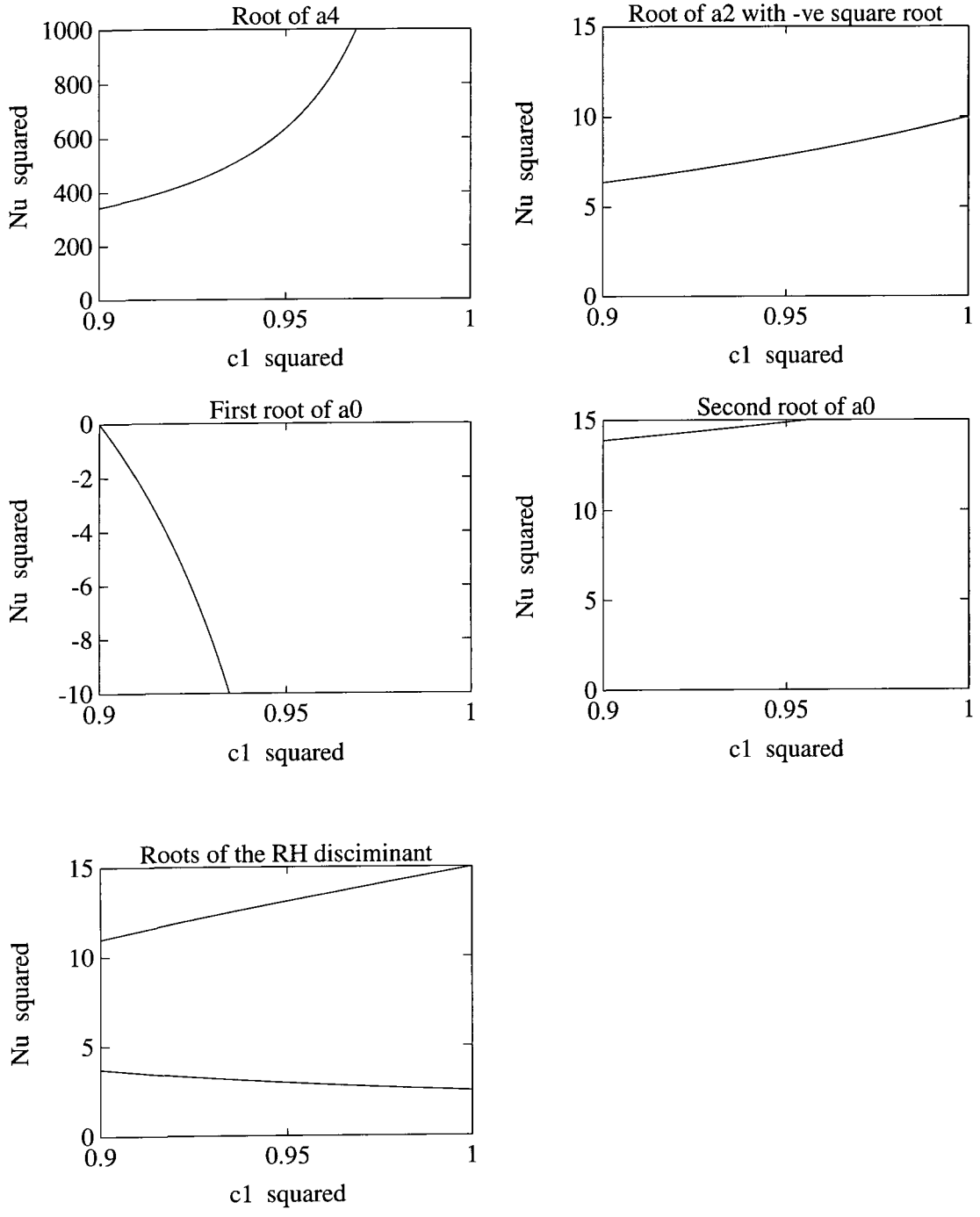

Figure 4.2: Graphs of the roots of the Routh-Hurwitz coefficients and discriminant for 2-step 2-point symmetric MCRKN methods as functions of c_1, with $c_1^2 \in (9/10, 1)$.

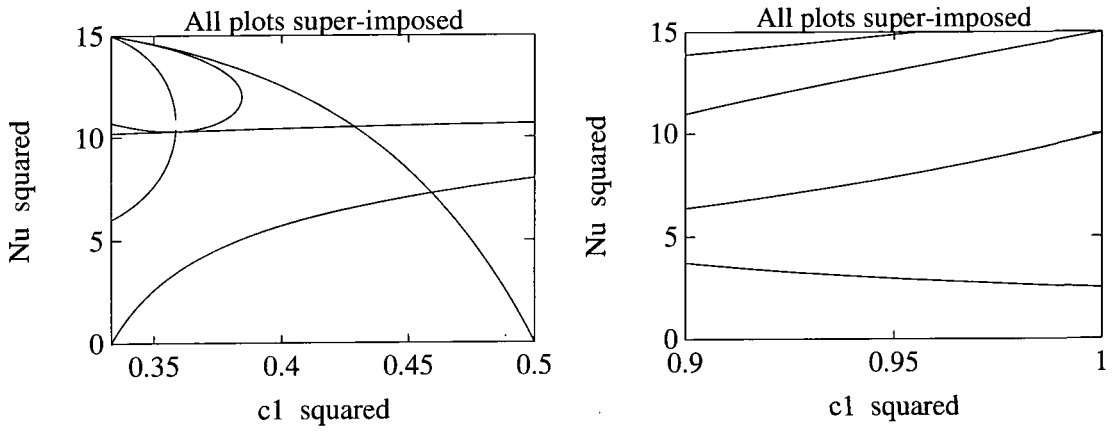

Figure 4.3: Superpositions of the graphs contained within figures 4.1 (left) and 4.2 (right).

some analysis we find that the maximum attainable interval of periodicity is in fact (0,7.2771) (4 d.p.), and is achieved when $c_1^2 = 0.4592$ (4 d.p.).

From our investigations of the order of these methods we know that any method from this family which has a non-empty interval of periodicity must have order 4, and two fully implicit stages. From chapter 3, the degree 2 Panovsky-Richardson method also has order 4 and 2 fully implicit stages, but it is an FSAL method and has a primary periodicity interval of (0,9.6). The 2-step 2-point MCRKN method does have one advantage over the Panovsky-Richardson method however, the polynomial $u(x)$ can be used to generate an order 4 approximation to $y(x)$ for any $x \in (x_{n-1}, x_{n+1})$, which might be useful in a variable stepsize implementation.

The 2-step 3-point symmetric MCRKN methods

The collocation nodes for these methods are required to satisfy the symmetry constraints $c_2 = 0$ and $c_3 = -c_1$. By construction, the minimum order of methods from this family is five. To see if we can raise the order beyond five we check to see if the conditions of theorem 4.5 can be satisfied with $i = 0$. Set $i = 0$, then $I(i+1) = (3 - 5c_1^2)/15$. With $I(i+1) = 0$, $I(i+3) \neq 0$, so we cannot increase the order of the method this way. If $I(i+1) \neq 0$, then $I(i)I(i+2) - I(i+1)I(i+3) = 0$,

and the resulting method will have order six, provided $c_1^2 = (10 \pm \sqrt{37})/21$. It is a simple matter to verify that the conditions of theorem 4.5 do not hold when $i = 1$, and so the maximum order of a method from this family is six.

The Routh-Hurwitz polynomial for methods from this family is

$$R(\zeta) = a_4\zeta^4 + a_2\zeta^2 + a_0$$

where the coefficients a_4, a_2 and a_0, and the discriminant D are given by

$$\begin{aligned}
a_4 &= 4\nu^2[\nu^4(3c_1^8 - 11c_1^6 + 15c_1^4 - 9c_1^2 + 2) + 6\nu^2(25c_1^6 - 62c_1^4 + 50c_1^2 - 13) \\
&\quad +180(10c_1^4 - 13c_1^2 + 4)] \\
a_2 &= 16\nu^6(-c_1^8 + 4c_1^6 - 6c_1^4 + 4c_1^2 - 1) + 16\nu^4(3c_1^8 - 61c_1^6 + 150c_1^4 - 128c_1^2 + 36) \\
&\quad +96\nu^2(25c_1^6 - 162c_1^4 + 190c_1^2 - 60) + 2880(10c_1^4 - 13c_1^2 + 4) \\
a_0 &= 4\nu^6(c_1^8 - 5c_1^6 + 9c_1^4 - 7c_1^2 + 2) + 8\nu^4(-4c_1^8 + 43c_1^6 - 112c_1^4 + 106c_1^2 - 33) \\
&\quad +16\nu^2(-100c_1^6 + 462c_1^4 - 537c_1^2 + 180) + 384(-50c_1^4 + 75c_1^2 - 27) \\
D &= 64[\nu^{12}c_1^4(c_1^{12} - 6c_1^{10} + 15c_1^8 - 20c_1^6 + 15c_1^4 - 6c_1^2 + 1) \\
&\quad +4\nu^{10}c_1^2(22c_1^{12} - 109c_1^{10} + 219c_1^8 - 226c_1^6 + 124c_1^4 - 33c_1^2 + 3) \\
&\quad +4\nu^8(9c_1^{16} - 66c_1^{14} + 860c_1^{12} - 2898c_1^{10} + 4216c_1^8 - 3052c_1^6 + 1090c_1^4 \\
&\qquad -168c_1^2 + 9) \\
&\quad +48\nu^6(75c_1^{14} - 461c_1^{12} + 1752c_1^{10} - 3191c_1^8 + 2815c_1^6 - 1194c_1^4 + 216c_1^2 - 12) \\
&\quad +144\nu^4(925c_1^{12} - 4590c_1^{10} + 9294c_1^8 - 9210c_1^6 + 4339c_1^4 - 860c_1^2 + 36) \\
&\quad +8640\nu^2(250c_1^{10} - 945c_1^8 + 1306c_1^6 - 828c_1^4 + 238c_1^2 - 24) \\
&\quad +129600(100c_1^8 - 260c_1^6 + 249c_1^4 - 104c_1^2 + 16)]
\end{aligned}$$

In view of the complexity of these expressions we shall once again begin by restricting our attention to those values of ν which are sufficiently low to allow us to neglect terms

of order ν^2. In this case the coefficients and discriminant become

$$\begin{aligned} a_4 &= 0 \\ a_2 &= \alpha_2(2c_1^2-1)(5c_1^2-4) \\ a_0 &= \alpha_0(3-5c_1^2)(10c_1^2-9) \\ D &= \alpha_5(2c_1^2-1)^2(5c_1^2-4)^2 \end{aligned}$$

where the α's are positive constants independent of c_1^2. Applying our stability conditions we find that a method from this family will possess a non-empty interval of periodicity provided $c_1^2 \in (1/2, 3/5) \cup (4/5, 9/10)$. Comparing these ranges with the values obtained from considerations of the order of these methods, we find that there are no sixth order methods from this family which possess non-vanishing intervals of periodicity. In the same way as for the 2-point methods discussed earlier, we have

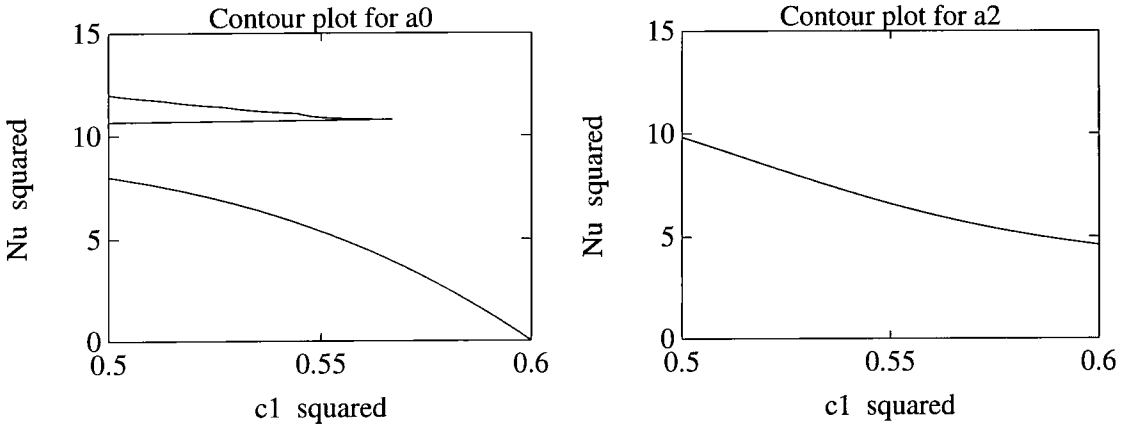

Figure 4.4: Contour plots of the Routh-Hurwitz coefficients and discriminant for the 2-step 3-point symmetric MCRKN method with $c_1^2 \in (1/2, 3/5)$.

produced contour plots to determine where the coefficients and discriminant change sign for c_1^2 in the ranges $(1/2, 3/5)$ and $(4/5, 9/10)$. The relevant plots are shown in figures 4.4 and 4.5. Figure 4.6 shows the results of super-imposing each of the sets of contour plots. Once again, the length of the first interval of periodicity, if it exists, is given by the vertical distance from the c_1^2-axis to the nearest curve. These graphs

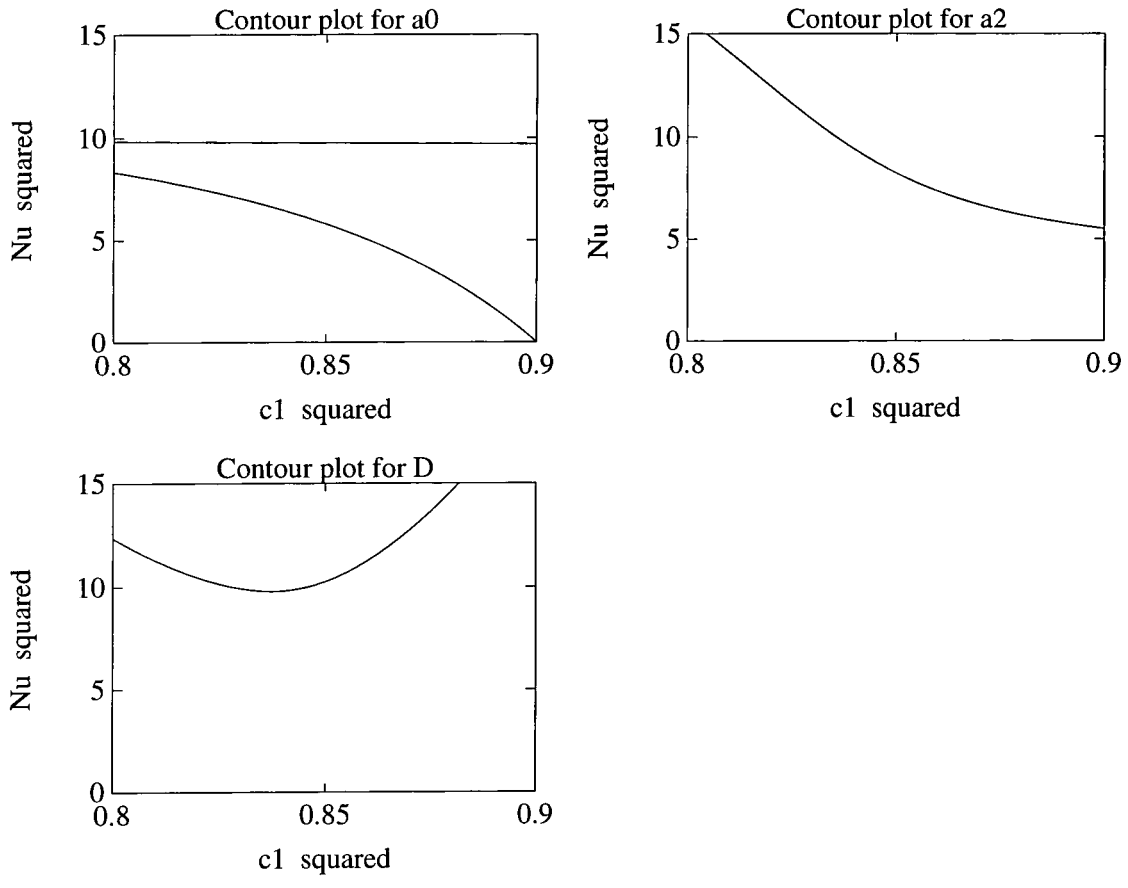

Figure 4.5: Contour plots of the Routh-Hurwitz coefficients and discriminant for the 2-step 3-point symmetric MCRKN method with $c_1^2 \in (4/5, 9/10)$.

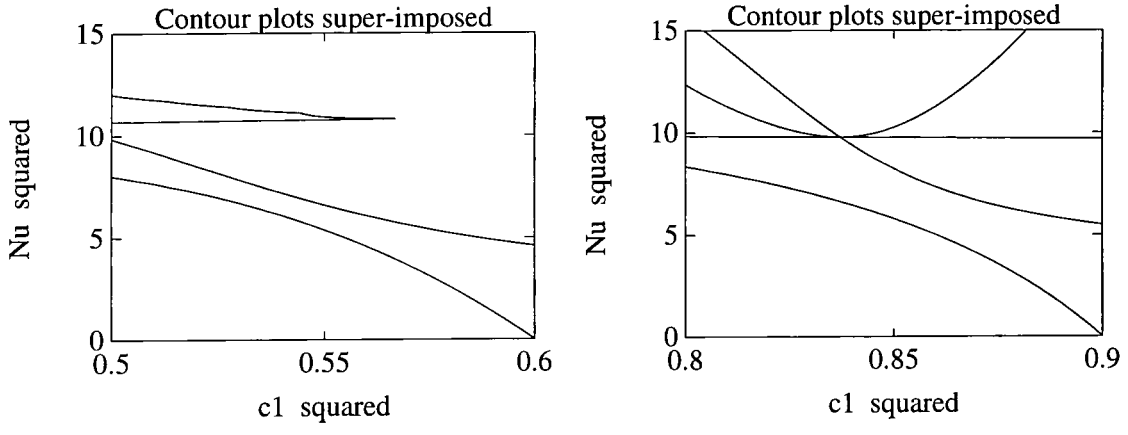

Figure 4.6: Superpositions of the graphs contained within figures 4.4 (left) and 4.5 (right).

show that the largest interval of periodicity is obtained when $c_1^2 = 4/5$ and is of length 25/3 (8.3333 to 4d.p.). Here again we find that the order and periodicity conditions are incompatible, i.e. there are no methods from this class of order six which possess non-empty intervals of periodicity.

The 2-step 4-point MCRKN methods

The symmetry constraints for these methods are $c_4 = -c_1$ and $c_3 = -c_2$. By construction, methods from this family have order at least six. To see if any methods from this family with order greater than six exist, we look at the conditions of theorem 4.5 with $i = 0$. Set $i = 0$, then $I(i+1) = 0$ if the nodes are chosen so that

$$c_2^2 = (3c_1^2 - 2)/(6c_1^2 - 3).$$

Due to the limitations of the algebraic manipulation package used to generate the results in this section, and the complexity of the expressions involved, we have been able to continue our analysis only in the case $I(i+1) = 0$. In this case, $I(i+3)$ vanishes if

$$c_1^2 = \frac{1 + 1/\sqrt{3}}{2} \qquad \text{and} \qquad c_2^2 = \frac{1 - 1/\sqrt{3}}{2}.$$

It is easy to verify that with this choice of nodes, the conditions of theorem 4.5 are satisfied for $i = 1$, and so the resulting method will be of order eight.

Our attempts at analysing the stability properties of these methods have also been hampered by the limitations of our algebra package and the complexity of the expressions involved. Consequently we have not been able to produce contour plots similar to those for the 2- and 3-point methods. We have, however, succeeded in showing that the eighth order method mentioned above, unlike the superconvergent methods discussed previously, does possess a non-vanishing interval of periodicity, and that this interval is $(0, 9)$.

4.5 Numerical results

In view of the concluding remarks we will make at the end of this chapter, we feel that there is little to be gained in exhaustively testing the two-step symmetric MCRKN methods. Instead, as an illustration of the unremarkable performance of these methods, we give here the results of applying the 2-point fourth order method with the largest possible interval of periodicity and the 4-point superconvergent method of order eight to both a linear and a non-linear test problem. For comparison purposes we also give the results obtained by applying the RKN formulation of the Panovsky-Richardson methods RKN4 and RKN6, of degrees 2 and 4 respectively, to these problems.

The harmonic oscillator

For our linear test problem we take the scalar equation

$$y'' = -y; \quad y(0) = 1,\ y'(0) = 0. \tag{4.111}$$

The second and third columns of table 4.1 show the results of applying the 2-point MCRKN method, which we refer to as M2, and the degree 2 Panovsky-Richardson method, which requires approximately the same computational effort, with steplength $h = 0.1$ to this problem. The fourth and fifth columns show the results obtained from the superconvergent 4-point MCRKN method, which we call M4 here, and the degree 4 Panovsky-Richardson method with steplength $h = 0.2$. Notice that the global error for method M4 exhibits a quadratic dependence on the length of integration interval, so that for all reasonable stepsizes we would expect it to be less accurate than the RKN6 method for x sufficiently large.

x	M2	RKN4	M4	RKN6
1	1.36 E-07	4.38 E-08	1.05 E-12	2.78 E-11
2	3.27 E-07	9.47 E-08	1.83 E-12	6.01 E-11
5	9.01 E-07	2.51 E-07	7.63 E-12	1.58 E-10
10	1.48 E-06	4.12 E-07	4.31 E-11	2.62 E-10
20	3.44 E-06	9.50 E-07	1.64 E-10	6.04 E-10
50	9.22 E-06	2.54 E-06	1.09 E-09	1.60 E-09
100	1.87 E-05	5.15 E-06	4.40 E-09	3.27 E-09

Table 4.1: Maximum absolute errors on intervals $[0, x]$ when methods M2, RKN4, M4 and RKN6 are applied to problem (4.111) with steplengths as given in the text.

The two-body problem

As our non-linear test problem we take Kepler's two-body problem

$$y'' + y/r^3 = 0, \qquad y(0) = 1 - e, \qquad y'(0) = 0 \tag{4.112}$$

$$z'' + z/r^3 = 0, \qquad z(0) = 0, \qquad z'(0) = \sqrt{(1+e)/(1-e)} \tag{4.113}$$

with $r^2 = y^2 + z^2$. Table 4.2 is the analogue of table 4.1 for this problem, though here we used the steplength $h = 0.05$ for the two fourth order methods.

x	M2	RKN4	M4	RKN6
1	6.95 E-08	1.54 E-08	1.75 E-10	7.52 E-10
2	3.96 E-07	2.43 E-08	1.25 E-09	7.52 E-10
5	2.65 E-06	6.12 E-08	1.48 E-08	1.15 E-08
10	3.47 E-06	1.77 E-07	3.91 E-08	1.93 E-08
20	1.04 E-05	5.25 E-07	2.26 E-07	5.77 E-08
50	2.65 E-05	1.32 E-06	1.20 E-06	1.47 E-07
100	5.21 E-05	2.62 E-06	2.84 E-06	2.89 E-07

Table 4.2: Maximum absolute errors on intervals $[0, x]$ when methods M2, RKN4, M4 and RKN6 are applied to problem (4.112)-(4.113) with steplengths as given in the text.

It is possible to choose the collocation nodes for the MCRKN methods so that their global errors are smaller than those seen in the Panovsky-Richardson methods,

but only at the cost of reducing the length of the periodicity intervals. Notice that even with the node choices used here, the two Panovsky-Richardson methods have larger intervals of periodicity than the corresponding MCRKN methods.

4.6 Conclusion

We have shown how to construct multistep collocation-based Runge-Kutta-Nyström methods with arbitrary stepnumber k and number of collocation nodes m, and have given expressions for the coefficients of these methods.

The stability polynomial for methods from this class has been derived and used to investigate the stability properties of the two-step symmetric MCRKN methods. In particular we have shown that for the aforementioned methods, intervals of absolute stability are intervals of periodicity. Conditions under which these two-step methods have order $p \geq m + 2$ have also been derived.

For the methods considered in section 4.4 we saw that the conditions imposed by the requirement that the methods should possess a non-vanishing interval of periodicity placed severe restrictions on the range of possible collocation nodes. None of the methods analysed in that section had outstanding stability properties, and in particular we did not succeed in deriving any P-stable methods. The increasing complexity of the coefficients involved leads us to question the practicality of this type of analysis for methods with a greater number of collocation nodes.

The numerical results given in section 4.5 show that, for the problems considered, these methods are inferior to the Panovsky-Richardson methods from the point of view of both accuracy and stability properties.

To obtain these methods we have sacrificed the advantages of one-step methods, and we appear to have gained nothing in return. We will see that this is not the case for the methods considered in the next chapter.

Chapter 5

Multistep collocation methods II: The multistep hybrid methods

In this chapter we present the second of our two classes of multistep collocation methods for second order periodic initial value problems of the form

$$y'' = f(x, y); \quad y(x_0) = y_0, \quad y'(x_0) = z_0. \tag{5.1}$$

These methods, which we shall refer to as MCH (Multistep Collocation-based Hybrid) methods require no derivative data and are aimed specifically at solving problems of the form (5.1).

The unique solvability of the interpolation problem defining each of these methods is discussed in section 5.1.1, and in particular we find that in the case $k = 2$ we need only require the collocation nodes to be distinct in order to guarantee the unique solvability of this problem. In section 5.1.2 we show how to construct MCH methods with arbitrary stepnumber k and number of collocation points m.

The stability polynomial for these methods is found in section 5.2.1 and is used in section 5.2.2 to investigate the stability properties of the two-step symmetric MCH methods. We find that the analysis of the stability properties of these methods is considerably simpler than that for the MCRKN methods from the previous chapter,

and we are able to derive a number of encouraging general results.

The order of the two-step symmetric MCH methods is investigated in section 5.3, and a simple and inexpensive local truncation error estimator is proposed and is shown to be effective for a number of test problems.

Symmetric two-step MCH methods with 1,2,3 and 4 collocation nodes are analysed in detail in section 5.4. In particular we find that it is relatively easy to derive P-stable methods with 2 or 4 nodes. Numerical results in section 5.5 compare selected methods from the previous section with the Panovsky-Richardson methods requiring comparable computational effort.

5.1 Construction

In this section we consider the construction of the MCH methods and give expressions for the coefficients for arbitrary stepnumber k and number of collocation points m. The method of construction we use is the same as was used to construct the MCRKN methods, though due to the reduction in the number of collocation conditions used to define the MCH methods, far less work is required.

First however, we consider the existence of a unique solution to the collocation problem, and give examples of cases where a unique solution is not defined. In order to do this we associate with each MCH method an interpolation problem which is independent of the differential equation under consideration. The uniqueness conditions are derived in the same way as for the MCRKN methods of the previous chapter. We will see that the conditions imposed by the uniqueness criterion are a little less restrictive than those for the MCRKN methods, especially in the case $k = 2$.

5.1.1 Unique solvability of the interpolation problem

In this subsection we define the interpolation problem associated with each MCH method, and derive conditions which ensure its unique solvability. In particular we show that in the case $k = 2$, unique solvability is guaranteed if and only if the

nodes $\{c_i\}_{i=1}^m$ are distinct. Examples of specific methods are given at the end of this subsection.

Let $x_r = x_0 + rh$, for all $r \in \mathbb{R}$, and let $\{c_i\}_{i=1}^m$ $(m \geq 1)$ be distinct real numbers. A k-step m-point MCH method is defined as follows:

Find $u \in \mathcal{P}_{m+k-1}$ such that

$$\begin{aligned} u(x_n - jh) &= y_{n-j} && j = 0, \ldots, k-1 \\ u''(x_n + c_i h) &= f(x_n + c_i h, u(x_n + c_i h)) && i = 1, \ldots, m \end{aligned}$$

then take

$$y_{n+1} = u(x_{n+1})$$

where y_{n+r} is an approximation to $y(x_{n+r})$, for all $r \in \mathbb{R}$.

The solution to this problem will be considered in the next subsection. We associate with this method the following interpolation problem:

Find $u \in \mathcal{P}_{m+k-1}$ such that

$$\begin{aligned} u(x - jh) &= g(x - jh) && j = 0, \ldots, k-1 \\ u''(x + c_i h) &= g''(x + c_i h) && i = 1, \ldots, m \end{aligned}$$

where the function g is assumed to be as differentiable as we please.

In the same way as before, we let $u(x) = \sum_{p=0}^{m+k-1} a_p x^p$ and replace the above interpolation problem by the system of linear equations

$$A\boldsymbol{a} = \boldsymbol{b}$$

where A is the $(m+k) \times (m+k)$ matrix

$$A = \begin{pmatrix} 1 & 0 & 0 & 0 & \dots & 0 \\ 1 & -1 & 1 & -1 & \dots & (-1)^r \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ 1 & (1-k) & (1-k)^2 & (1-k)^3 & \dots & (1-k)^r \\ 0 & 0 & 2 & 6c_1 & \dots & r(r-1)c_1^{r-2} \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 2 & 6c_m & \dots & r(r-1)c_m^{r-2} \end{pmatrix},$$

$\boldsymbol{a} = (a_0, \dots, a_r)^{\mathrm{T}}$, and $\boldsymbol{b} \in \mathbb{R}^r$ is given by:

$$\boldsymbol{b} = (g(0), \dots, g(1-k), g''(c_1), \dots, g''(c_m))^T$$

where for ease of notation we have taken $r = m + k - 1$ and $x = 0$. The above interpolation problem will have a unique solution if and only if the determinant of A is non-zero.

For those methods where k is much larger than m, it might be advantageous to simplify the matrix A using a similar idea to that used in section 4.1. We begin by partitioning A as follows:

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$$

where $A_{11} \in \mathbb{R}^k \times \mathbb{R}^k$, $A_{12} \in \mathbb{R}^k \times \mathbb{R}^m$, $A_{21} \in \mathbb{R}^m \times \mathbb{R}^k$, $A_{22} \in \mathbb{R}^m \times \mathbb{R}^m$. The matrix A_{11} may be viewed as the coefficient matrix arising from a Lagrange interpolation problem in which the values of $g(x)$ are fitted at the nodes $x = 0, \dots, k-1$, and hence must be non-singular. After some algebra (see section 4.2) we obtain:

$$\det A = \alpha \det (A_{22} - A_{21}A_{11}^{-1}A_{12})$$

where α is some real number. When $k = 2$, the matrix A may be row and column

reduced to the coefficient matrix associated with one-step collocation-based Runge-Kutta-Nyström (CRKN) methods, from which we see immediately that we need impose no further constraints on the nodes $\{c_i\}_{i=1}^m$ to guarantee unique solvability.

We close this subsection with a number of examples of specific MCH methods. As was the case for the MCRKN methods, we see that enforcing the uniqueness criteria results in a relatively minor reduction in the range of possible collocation nodes.

Example 1 k=3, m=1.

The coefficient matrix A in this case is given by:

$$A = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & -1 & 1 & -1 \\ 1 & -2 & 4 & -8 \\ 0 & 0 & 2 & 6c_1 \end{pmatrix}$$

and

$$\det A = -12(1 + c_1).$$

So that the interpolation problem will be uniquely solvable provided $c_1 \neq -1$.

Example 2 k=3, m=2.

In this case the coefficient matrix A is given by:

$$A = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & -2 & 4 & -8 & 16 \\ 0 & 0 & 2 & 6c_1 & 12c_1^2 \\ 0 & 0 & 2 & 6c_2 & 12c_2^2 \end{pmatrix}$$

and

$$\det A = -24(c_2 - c_1)(6c_1c_2 + 6(c_2 + c_1) + 7).$$

So that the interpolation problem will be uniquely solvable provided that

$$c_1 \neq c_2 \qquad \text{and} \qquad c_1 \neq -\frac{6c_2+7}{6c_2+6}.$$

If we were to impose the symmetry constraint

$$c_1 + c_2 = -1$$

then our uniqueness conditions would become

$$c_1 \neq -1/2 \qquad \text{and} \qquad c_1 \neq \frac{-1}{2} \pm \sqrt{\frac{5}{12}}.$$

Example 3 k=4, m=2.

The coefficient matrix A in this case is given by:

$$A = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & -2 & 4 & -8 & 16 & -32 \\ 1 & -3 & 9 & -27 & 81 & -243 \\ 0 & 0 & 2 & 6c_1 & 12c_1^2 & 20c_1^3 \\ 0 & 0 & 2 & 6c_2 & 12c_2^2 & 20c_2^3 \end{pmatrix}$$

and

$$\begin{aligned} \det A &= 240(12c_1^2c_2^2 + 36c_1c_2(c_1+c_2) + 22(c_1^2+c_2^2) + 112c_1c_2 + \\ &\quad 72(c_1+c_2) + 51)(c_2 - c_1) \end{aligned}$$

So that the interpolation problem will be uniquely solvable provided that $c_1 \neq c_2$ and

$$c_1 \neq -\frac{18c_2^2 + 56c_2 + 36 \pm \sqrt{60c_2^4 + 360c_2^3 + 744c_2^2 + 612c_2 + 174}}{2(6c_2^2 + 18c_2 + 11)}$$

If we were to impose the symmetry constraint

$$c_1 + c_2 = -2$$

then our uniqueness conditions would become

$$c_1 \neq -1, \qquad c_1 \neq -1 \pm \frac{1}{\sqrt{6}} \qquad \text{and} \qquad c_1 \neq -1 \pm \sqrt{\frac{3}{2}}.$$

5.1.2 Construction of the collocation solution

In this subsection we show how to construct a multistep collocation (MCH) method and show that these methods form a subclass of the multistep hybrid methods.

Let $\{y_n\}_{n=0}^{k-1}$ be given approximations to $\{y(x_n)\}_{n=0}^{k-1}$. For notational convenience we will use the scaled variable

$$s = \frac{x - x_n}{h} \qquad (\text{i.e. } x = x_n + sh)$$

for the remainder of this section. In the same way as before, we define

$$U(s) = u(x_n + sh) \tag{5.2}$$

$$F(s, U(s)) = f(x_n + sh, u(x_n + sh)) \tag{5.3}$$

and let a prime denote differentiation with respect to s. A k-step, m-point MCH collocation method for (5.1) is defined as follows:

Find $U \in \mathcal{P}_{m+k-1}$ such that

$$U(-j) = y_{n-j} \qquad j = 0, \ldots, k-1 \tag{5.4}$$

$$U''(c_i) = h^2 F(c_i, U(c_i)) \qquad i = 1, \ldots, m \tag{5.5}$$

then as an approximation to $y(x_{n+1})$ we take:

$$y_{n+1} = U(1). \tag{5.6}$$

In the following lemma we show that the MCH multistep collocation methods form a subclass of the multistep hybrid methods.

Lemma 5.1 *The MCH multistep collocation method defined by (5.4)-(5.6) may be expressed as the following multistep hybrid method:*

$$Y_i = \sum_{j=0}^{k-1} \lambda_j(c_i) y_{n-j} + h^2 \sum_{l=1}^{m} \nu_l(c_i) F(c_l, Y_l) \qquad i = 1, \ldots, m \tag{5.7}$$

$$y_{n+1} = \sum_{j=0}^{k-1} \lambda_j(1) y_{n-j} + h^2 \sum_{l=1}^{m} \nu_l(1) F(c_l, Y_l) \tag{5.8}$$

where $\lambda_j,\ \nu_i \in \mathcal{P}_{m+k-1}$.

Proof Let $Y_i = U(c_i)$ for $i = 1, \ldots, m$. Then from the collocation conditions (5.4) and (5.5) we must have that

$$U(s) = \sum_{j=0}^{k-1} \lambda_j(s) y_{n-j} + h^2 \sum_{l=1}^{m} \nu_l(s) F(c_l, Y_l) \tag{5.9}$$

for some polynomials λ_j and ν_i of degree at most $m + k - 1$. Expressions (5.7) and (5.8) follow immediately. □

We now show how the polynomials λ_j and ν_i may be constructed. Without loss of generality we let $x_n = 0$ and $h = 1$ for the remainder of this section.

The polynomials $\lambda_j,\ j = 0, \ldots, k-1$

From the collocation conditions (5.4) and (5.5) we see that the polynomial λ_j must satisfy the following conditions:

$$\lambda_j(-r) = \delta_{jr} \qquad r = 0, \ldots, k-1 \tag{5.10}$$

$$\lambda_j''(c_i) = 0 \qquad i = 1, \ldots, m \tag{5.11}$$

When $k = 2$, we have that $\lambda_j'' \in \mathcal{P}_{m-1}$, but since we require it to vanish at m different points, it must be identically zero. Thus in this case

$$\lambda_0(s) = 1 + s \qquad \text{and} \qquad \lambda_1(s) = -s \tag{5.12}$$

Suppose now that $k \geq 3$. Condition (5.5) may be satisfied by a polynomial of the form

$$\lambda_j''(s) = M(s) \sum_{p=0}^{k-3} a_{jp} s^p$$

where $M(s)$ is as defined in the previous chapter. Integrating twice we obtain:

$$\lambda(s) = \sum_{p=0}^{k-3} a_{jp} \int_0^s (s - \tau)\tau^p M(\tau) d\tau + a_{j\,k-2} s + \delta_{j0} \tag{5.13}$$

for some $a_{j\,k-2} \in \mathbb{R}$. The collocation conditions (5.10) may now be written as:

$$\sum_{p=0}^{k-3} a_{jp} \int_{-r}^0 (r + \tau)\tau^p M(\tau) d\tau - r\, a_{j\,k-2} = \delta_{jr} - \delta_{j0} \qquad r = 1, \ldots, k-1 \tag{5.14}$$

Using Cramer's Rule to solve this $(k-1) \times (k-1)$ system of linear equations we obtain:

$$\lambda(s) = \sum_{p=0}^{k-3} \frac{D_{jp}^{(\lambda)}}{D_{k-1}} \int_0^s (s - \tau)\tau^p M(\tau) d\tau + \frac{D_{j\,k-2}^{(\lambda)}}{D_{k-1}} s + \delta_{j0} \tag{5.15}$$

where

$$D_{k-1} = \det \begin{pmatrix} \int_{-1}^0 (1 + \tau) M(\tau) d\tau & \ldots & \int_{-1}^0 (1 + \tau)\tau^{k-3} M(\tau) d\tau & -1 \\ \vdots & & \vdots & \vdots \\ \int_{1-k}^0 (k - 1 + \tau) M(\tau) d\tau & \ldots & \int_{1-k}^0 (k - 1 + \tau)\tau^{k-3} M(\tau) d\tau & 1 - k \end{pmatrix} \tag{5.16}$$

and $D_{jp}^{(\lambda)}$ is the determinant obtained when the p^{th} column of D_{k-1} is replaced by the vector

$$\boldsymbol{v}_j^{(\lambda)} = \begin{cases} -\mathbf{1}^T & j = 0 \\ \boldsymbol{e}_j^T & j > 0 \end{cases} \tag{5.17}$$

where $\mathbf{1} \in \mathbb{R}^{k-1} = (1, \ldots, 1)$ and $\boldsymbol{e}_j \in \mathbb{R}^{k-1}$ has 1 as its j^{th} entry, and all other entries zero.

The polynomials $\nu_i,\ i = 1, \ldots, m$

From the collocation conditions (5.4) and (5.5) we see that the following conditions are imposed on ν_i:

$$\nu_i(-r) = 0 \qquad r = 0, \ldots, k-1 \tag{5.18}$$

$$\nu_i''(c_j) = \delta_{ij} \qquad j = 1, \ldots, m \tag{5.19}$$

We will deal with the special case $k = 2$ in a moment, but for now we assume that $k \geq 3$. Condition (5.19) can be satisfied by a polynomial of the form

$$\nu_i''(s) = l_i(s) + M(s) \sum_{p=0}^{k-3} b_{ip} s^p \tag{5.20}$$

where, for $m > 1$, $l_i(s)$ is the i^{th} fundamental Lagrange basis function based on the nodes $\{c_i\}_{i=1}^m$, and $l_1(s) \equiv 1$ when $m = 1$. Integrating twice, and using condition (5.18) we obtain:

$$\nu_i(s) = \sum_{p=0}^{k-3} b_{ip} \int_0^s (s-\tau)\tau^p M(\tau) d\tau + \int_0^s (s-\tau) l_i(\tau) d\tau + b_{i\,k-2} s \tag{5.21}$$

Rewriting the remaining collocation conditions as a system of linear equations, and using Cramer's Rule we readily obtain:

$$\nu_i(s) = \int_0^s (s-\tau) l_i(\tau) d\tau + \sum_{p=0}^{k-3} \frac{D_{ip}^{(\nu)}}{D_{k-1}} \int_0^s (s-\tau)\tau^p M(\tau) d\tau + \frac{D_{i\,k-2}^{(\nu)}}{D_{k-1}} s \tag{5.22}$$

where $D_{ip}^{(\nu)}$ is the determinant obtained when the p^{th} column of D_{k-1} is replaced by the vector

$$\boldsymbol{v}_i^{(\nu)} = \left(\int_{-1}^{0} (1+\tau) l_i(\tau) d\tau, \ldots, \int_{1-k}^{0} (k-1+\tau) l_i(\tau) d\tau \right)^T \tag{5.23}$$

Now suppose that $k = 2$. From condition (5.19) we must have that

$$\nu_i''(s) = l_i(s)$$

Integrating twice and using (5.18) gives:

$$\nu_i(s) = \int_0^s (s-\tau) l_i(\tau) d\tau + s \int_{-1}^{0} (1+\tau) l_i(\tau) d\tau \tag{5.24}$$

We close this section with two examples of MCH methods.

Example 1 $k = 3$, $m = 1$

From the previous subsection we have that the interpolation problem is uniquely solvable provided that $c_1 \neq -1$. Assuming that this condition holds, the method is given by

$$\begin{aligned} 6y_{n+c_1} &= (2c_1^2 + 7c_1 + 6)y_n - 2c_1(c_1+2)y_{n-1} + c_1(2c_1+1)y_{n-2} \\ &\quad + h^2 c_1(c_1+2) f_{n+c_1} \\ (1+c_1)y_{n+1} &= (3c_1+2)y_n - (3c_1+1)y_{n-1} + c_1 y_{n-2} + h^2 f_{n+c_1} \end{aligned}$$

This method has order at least 2 by construction, and has order 3 when $c_1 = (\sqrt{15} - 3)/6$. For absolute stability we must have $c_1 \geq -1/2$. The method has an interval of periodicity $\nu^2 \in (0, 8/3)$ when $c_1 = -1/2$, and is unconditionally stable whenever $c_1 \geq (\sqrt{7} - 1)/2$. When $c_1 = (\sqrt{15} - 3)/6$ the method is absolutely stable for $\nu^2 \in (0, 9/2)$.

Example 2 $k = 2$, $m = 2$, symmetric nodes.

Later in this chapter we will restrict our attention to 2-step MCH methods whose nodes are symmetrically distributed in the interval $[-1, 1]$. In this example we give

the general form of a 2-point method from this family and outline some of its more desirable properties. The analysis used to derive these results may be found in later sections of this chapter. The general 2-point 2-step symmetric MCH method is given by

$$\begin{aligned} y_{n\pm c_1} &= (1 \pm c_1)y_n \mp c_1 y_{n-1} + \\ &\quad \frac{h^2}{12}\left((4c_1^2 \pm 3c_1 - 1)f_{n\pm c_1} + (2c_1^2 \pm 3c_1 + 1)f_{n\mp c_1}\right) \\ y_{n+1} &= 2y_n - y_{n-1} + \frac{h^2}{2}(f_{n+c_1} + f_{n-c_1}) \end{aligned}$$

By construction, this method has order 2, it is possible to increase this to 4 by taking $c_1 = 1/\sqrt{6}$, in which case the method is periodic for all $\nu^2 \in (0, 6)$. The method has a single, non-empty interval of periodicity whenever $c_1 \in (0, 1/\sqrt{2})$ and is P-stable whenever $c_1 \in [1/\sqrt{2}, 1]$.

5.2 Stability analysis

In section 5.2.1 we present two methods by which the stability polynomial for a general k-step, m-point MCH method may be constructed. The first method is based on the use of the variation of constants approach used in section 4.4, while the second is based on the repeated differentiation approach used by Wright [69].

In section 5.2.2 we restrict our attention to 2-step, m-point MCH methods whose collocation nodes are symmetrically distributed in [-1,1]. We show that for these methods, any interval of absolute stability is also an interval of periodicity, then go on to derive conditions under which these methods possess a non-empty interval of periodicity, or are almost P-stable in the sense of Thomas [60].

5.2.1 Construction of the stability polynomial

The variation of constants approach

The normal way to analyse the stability properties of a method is to apply it to the standard scalar test problem

$$\frac{d^2y}{dx^2} = -\omega^2 y, \qquad y(x_0) = y_0, \ \frac{dy}{dx}(x_0) = z_0 \tag{5.25}$$

We cannot use this approach directly here, since the MCH methods contain no derivative approximation stages. A more natural choice of test problem in this case might be the following boundary value problem:

$$\frac{d^2y}{dx^2} = -\omega^2 y, \qquad y(x_0) = y_0, \ y(x_1) = y_1 \tag{5.26}$$

This may be reposed as the equivalent initial problem

$$\frac{d^2y}{dx^2} = -\omega^2 y, \qquad y(x_0) = y_0, \ \frac{dy}{dx}(x_0) = Z(y_0, y_1) \tag{5.27}$$

where Z is the value of $dy(x_0)/dx$ required to ensure that $y(x_0 + h) = y_1$. Problem (5.27) is just (5.25) with different initial conditions. In what follows we will use the formulations (5.26) and (5.27) interchangeably.

When a k-step MCH method is applied to the problem (5.26) with constant stepsize h we obtain a numerical solution of the form:

$$\boldsymbol{u}_n = A^{n-(k-1)}\boldsymbol{y}_{k-1} \qquad n = k-1, k, \ldots$$

where A is a $k \times k$ matrix whose entries are independent of n, and whose eigenvalues are functions of $\nu = \omega h$,

$$\begin{aligned} \boldsymbol{u}_n &= (u(x_n), \ldots, u(x_{n-k+1}))^T \\ \boldsymbol{y}_n &= (y_n, \ldots, y_{n-k+1})^T \qquad n = k-1, k, \ldots \end{aligned}$$

and $\{y_0, \ldots, y_{k-1}\}$ are approximations to $\{y(x_0), \ldots, y(x_{k-1})\}$ obtained using a suitable starting procedure. The collocation conditions (5.4) and (5.5) in this case become:

Find $u \in \mathcal{P}_{m+k-1}$ such that

$$\begin{aligned} u(x_n - jh) &= y_{n-j} \qquad j = 0, \ldots, k-1 \qquad (5.28) \\ \frac{d^2u}{dx^2}(x_n + c_i h) &= -\omega^2 u(x_n + c_i h) \qquad i = 1, \ldots, m \qquad (5.29) \end{aligned}$$

The function $d^2u(x)/dx^2 + \omega^2 u(x)$ is a polynomial of degree $m + k - 1$ which has simple roots at the collocation nodes $\{c_i\}_{i=1}^m$. Using this, and the above collocation conditions, we see that $u(x)$ is a solution of the following initial value problem:

$$\begin{aligned} \frac{d^2u}{dx^2}(x) + \omega^2 u(x) &= R(x) \sum_{p=0}^{k-2} \alpha_p x^p, \\ u(x_{n-k+1}) &= y_{n-k+1} \\ \frac{du}{dx}(x_{n-k+1}) &= Z \end{aligned} \qquad (5.30)$$

where Z is such that $u(x_{n-k+2}) = y_{n-k+2}$, $\alpha_p \in \mathbb{R}$, for $p = 0, \ldots, k-1$, and $R(x)$ is as defined in section 4.3. In what follows it will be convenient to replace x by the scaled variable

$$s = \frac{x - x_{n-k+1}}{h},$$

and to let a prime denote differentiation with respect to s. Take $n = k-1$, so that we are considering the first step in which the MCH method will be applied. The initial value problem (5.30) is easily solved using the method of variation of constants to give:

$$\begin{aligned} u(sh) &= y_0 \cos(\nu s) + \frac{Z}{\omega} \sin(\nu s) + \\ &\quad \frac{1}{\omega} \int_0^s \sin[(s-\tau)\nu] \tilde{M}(\tau) \sum_{p=0}^{k-1} a_p \tau^p d\tau \end{aligned} \qquad (5.31)$$

where $a_p = \alpha_p h^{m+1+p}$, for $p = 0, \ldots, k-1$ and $\tilde{M}(\tau)$ is as defined in section 4.3. Our first task is to eliminate the unknown starting derivative value Z from our expression for $u(sh)$. To do this we enforce the collocation condition $u(h) = y_1$, from which we obtain:

$$\frac{Z}{\omega} = \operatorname{cosec}(\nu)\left(-y_0\sin(\nu) + y_1 - \frac{1}{\omega}\int_0^1 \sin[(1-\tau)\nu]\tilde{M}(\tau)\sum_{p=0}^{k-1} a_p\tau^p d\tau\right) \tag{5.32}$$

After substituting (5.32) into (5.31) and re-arranging we obtain the following expression for $u(sh)\sin(\nu)$:

$$\begin{aligned} u(sh)\sin(\nu) \;=\; & y_0(\sin(\nu)\cos(\nu s) - \cos(\nu)\sin(\nu s)) + y_1\sin(\nu s) - \\ & \frac{\sin(\nu s)}{\omega}\int_0^1 \sin[(1-\tau)\nu]\tilde{M}(\tau)\sum_{p=0}^{k-1} a_p\tau^p d\tau + \\ & \frac{\sin(\nu)}{\omega}\int_0^s \sin[(s-\tau)\nu]\tilde{M}(\tau)\sum_{p=0}^{k-1} a_p\tau^p d\tau \end{aligned} \tag{5.33}$$

Using the identity

$$\sin(A)\sin(B-C) - \sin(B)\sin(A-C) = \sin(C)\sin(B-A)$$

along with the standard double-angle formulae to simplify (5.33) we obtain:

$$\begin{aligned} u(sh)\sin(\nu) \;=\; & y_0(\sin(\nu(1-s)) + y_1\sin(\nu s) + \\ & \frac{\sin(\nu(s-1))}{\omega}\int_0^1 \sin[\nu\tau]\tilde{M}(\tau)\sum_{p=0}^{k-1} a_p\tau^p d\tau + \\ & \frac{\sin(\nu)}{\omega}\int_1^s \sin[(s-\tau)\nu]\tilde{M}(\tau)\sum_{p=0}^{k-1} a_p\tau^p d\tau \end{aligned} \tag{5.34}$$

Our next task is to evaluate the integrals contained in the above equation, to do this we will use the following lemma:

Lemma 5.2 *Let $g \in \mathcal{P}_n$, $n \geq 0$, and let $q = \lfloor n/2 \rfloor$, then*

$$\begin{aligned}\int_0^1 \sin[\nu\tau]g(\tau)d\tau &= \sum_{j=0}^{q} \frac{(-1)^j g^{(2j)}(0)}{\nu^{2j+1}} - \\ &\quad \cos(\nu)\sum_{j=0}^{q} \frac{(-1)^j g^{(2j)}(1)}{\nu^{2j+1}} + \\ &\quad \sin(\nu)\sum_{j=0}^{q} \frac{(-1)^j g^{(2j+1)}(1)}{\nu^{2j+2}} \qquad (5.35)\\ \int_1^s \sin[\nu(s-\tau)]g(\tau)d\tau &= \sum_{j=0}^{q} \frac{(-1)^j g^{(2j)}(s)}{\nu^{2j+1}} - \\ &\quad \cos(\nu(s-1))\sum_{j=0}^{q} \frac{(-1)^j g^{(2j)}(1)}{\nu^{2j+1}} - \\ &\quad \sin(\nu(s-1))\sum_{j=0}^{q} \frac{(-1)^j g^{(2j+1)}(1)}{\nu^{2j+2}} \qquad (5.36)\end{aligned}$$

Proof Use induction on n, and integration by parts. □

Let

$$I_p = \int_0^1 \sin[\nu\tau]\tilde{M}(\tau)\sum_{p=0}^{k-1} a_p\tau^p d\tau$$

and

$$J_p(s) = \int_1^s \sin[\nu(s-\tau)]\tilde{M}(\tau)\sum_{p=0}^{k-1} a_p\tau^p d\tau$$

Now define $A, B, C, D \in \mathbb{R}$ so that

$$I_p = A - B\cos(\nu) + C\sin(\nu)$$

and

$$J_p(s) = D - B\cos(\nu(s-1)) - C\sin(\nu(s-1))$$

Substituting these expressions back into (5.33) gives:

$$\begin{aligned}u(sh)\sin(\nu) &= -y_0\sin(\nu(s-1)) + y_1\sin(\nu s) + \\ &\quad \omega^{-1}[A\sin(\nu(s-1)) + D\sin(\nu) -\end{aligned}$$

$$
\begin{aligned}
& B\{\sin(\nu(s-1))\cos(\nu)+\sin(\nu)\cos(\nu(s-1))\}+ \\
& C\{\sin(\nu(s-1))\sin(\nu)-\sin(\nu)\sin(\nu(s-1))\}] \\
= \; & \sin(\nu(s-1))\{-y_0+\omega^{-1}A\}+\sin(\nu s)\{y_1-\omega^{-1}B\}+ \\
& \omega^{-1}D\sin(\nu)
\end{aligned}
$$

We know that u is a polynomial, so that the coefficients of $\sin(\nu s)$ and $\sin(\nu(s-1))$ in the above expression must vanish. Let the functions $\Psi_p(s)$ and $\Phi_p^{(r)}(s)$ be as defined in section 4.4, then we have that

$$u(sh) = h\sum_{p=0}^{k-1} a_p \Psi_p(s) \tag{5.37}$$

With u in this form we may now easily enforce the collocation conditions

$$u(jh) = y_j \qquad j = 0,\ldots,k-1$$

and hence obtain the following equations expressing $\boldsymbol{a} = (a_0,\ldots,a_{k-1})^{\mathrm{T}}$ in terms of $\boldsymbol{y}_{k-1}$:

$$\boldsymbol{y}_{k-1} = hP\boldsymbol{a} \tag{5.38}$$

where P is given by:

$$P = \begin{pmatrix} \Psi_0(k-1) & \ldots & \Psi_{k-1}(k-1) \\ \vdots & & \vdots \\ \Psi_0(0) & \ldots & \Psi_{k-1}(0) \end{pmatrix}$$

Evaluating $u(sh)$ at $s = k$ to find our approximation for y_k gives:

$$
\begin{aligned}
u(kh) &= h\boldsymbol{q}^T\boldsymbol{a} \\
&= \boldsymbol{q}^T P^{-1}\boldsymbol{y}_{k-1}
\end{aligned} \tag{5.39}
$$

where $\boldsymbol{q}$ is given by:

$$\boldsymbol{q} = (\Psi_0(k), \ldots, \Psi_{k-1}(k))^T$$

We now have an explicit expression for our y approximations at step 1 in terms of the information carried forward from step 0. Using the same idea we can write the approximations at step 2 in terms of the information carried forward from step 1, and so on. The iteration matrix A such that $\boldsymbol{y}_n = A^{n-k+1}\boldsymbol{y}_{k-1}$, $n = k-1, k, \ldots$ is now trivial to form, and is given by:

$$A = \begin{pmatrix} \boldsymbol{q}^T P^{-1} \\ I_{k-2} \quad \mathbf{0}_{k-2} \end{pmatrix} \tag{5.40}$$

where I_{k-2} is the $(k-2) \times (k-2)$ identity matrix, and $\mathbf{0}_{k-2}$ is a $(k-2)$-dimensional vector of zeroes. Let $\boldsymbol{w}^{\mathrm{T}} = \boldsymbol{q}^{\mathrm{T}} P^{-1}$, then the stability polynomial $\pi(\lambda)$ for the k-step, m-point MCH method is given by:

$$\pi(\lambda) = \lambda^k - \sum_{i=0}^{k} w_i \lambda^{k-i} \tag{5.41}$$

where $\boldsymbol{w}^{\mathrm{T}} = (w_0, \ldots, w_k)$. To see this notice that A takes the form of a companion matrix.

The repeated differentiation approach

Let $G(s) = \sum_{p=0}^{k-1} a_p s^p$, where $a_p \in \mathbb{R}$, for $p = 0, \ldots, k-1$ and let $N(s) = G(s)\tilde{M}(s)$, where $\tilde{M}(s)$ is as defined previously. Without loss of generality we take $h = 1$ and $n = k-1$. From above we have that the polynomial $u(s)$ satisfies the following differential equation:

$$u''(s) + \nu^2 u(s) = N(s) \tag{5.42}$$

Differentiate this twice with respect to s to obtain:

$$u^{(4)}(s) + \nu^2 u''(s) = N''(s) \tag{5.43}$$

Using (5.42) we can eliminate $u''(s)$ from the above equation to get

$$u^{(4)}(s) - \nu^4 u(s) = -\nu^2 N(s) + N''(s) \tag{5.44}$$

We now repeat this process until eventually we find:

$$-(-\nu^2)^r u(s) = \sum_{j=0}^{r-1} N^{(2j)}(s)(-\nu^2)^{r-1-j}, \qquad m+k=2r \tag{5.45}$$

$$-(-\nu^2)^{r+1} u(s) = \sum_{j=0}^{r} N^{(2j)}(s)(-\nu^2)^{r-j}, \qquad m+k=2r+1 \tag{5.46}$$

Recall from the previous chapter:

$$\Phi_p^{(i)}(s) = \frac{d^i}{ds^i}\left[\tilde{M}(s)s^p\right], \qquad p, i \geq 0$$

and

$$\Psi_p = \frac{1}{\nu^2}\sum_{j=0}^{N_p}\left(\frac{1}{\nu^2}\right)^j \Phi_p^{(2j)}(s), \qquad N_p = \lfloor \tfrac{1}{2}(m+p) \rfloor, \quad p \geq 0$$

From these we see immediately that $N^{(2j)}(s)$ may be written as

$$N^{(2j)}(s) = \sum_{p=0}^{k-1} a_p \Phi^{(2j)}(s), \qquad j = 0, \ldots$$

and hence $u(s)$ may be written as

$$u(s) = \sum_{p=0}^{k-1} a_p \Psi_p(s).$$

This expression is identical to that obtained from the variation of constants approach. The construction of the stability polynomial now proceeds as before.

As an example we now use our stability polynomial to analyse the stability properties of the general 2-step, 1-point MCH method.

Example $k = 2,\ m = 1.$

The general 2-step, 1-point MCH method is defined for all c_1 and is given by:

$$\begin{aligned} y_{n+c_1} &= (1+c_1)y_n - c_1 y_{n-1} + \frac{h^2}{2}c_1(1+c_1)f_{n+c_1} \\ y_{n+1} &= 2y_n - y_{n-1} + h^2 f_{n+c_1} \end{aligned}$$

The stability polynomial for this method is:

$$\pi(\lambda) = \lambda^2(c_1(1+c_1)\nu^2 + 2) + 2\lambda((1-c_1^2)\nu^2 - 2) + c_1(c_1-1)\nu^2 + 2$$

After applying the Routh-Hurwitz transformation, we obtain the following Routh-Hurwitz polynomial:

$$R(\zeta) = 2\zeta^2((2c_1^2-1)\nu^2 + 4) + 4\zeta c_1\nu^2 + 2\nu^2$$

The Routh-Hurwitz criteria for this problem are that all the coefficients of $R(\zeta)$ must have the same sign, i.e.

$$c_1 \geq 0 \qquad \text{and} \qquad (2c_1^2-1)\nu^2 + 4 \geq 0$$

In particular, the method will be unconditionally stable whenever $c_1 \geq 1/\sqrt{2}$, and periodic with periodicity interval $\nu^2 \in (0,4)$ if and only if $c_1 = 0$. The method has order 1 unless $c_1 = 0$, in which case its order is 2, and the leading error coefficient is $1/12$.

5.2.2 The symmetric two-step, m-point MCH methods

In this section we restrict our attention to the two-step symmetric MCH methods whose collocation nodes $\{c_i\}_{i=1}^m$ are symmetrically distributed in the interval $[-1,1]$. We show that for these methods, intervals of absolute stability are intervals of periodicity, and then go on to derive conditions under which a $2N$-point method from this family is almost P-stable in the sense of Thomas. In particular we find that, for

$m = 2, 4$, there are many P-stable methods from this family.

In order to show more clearly any possible symmetry properties in the stability polynomial we will change variable from s to the shifted variable $t = s - 1$. Before we begin our analysis we give again the definition of the functions $\gamma_i(t)$ used in section 4.3. We will find it convenient to append the suffix m to the $\gamma_i(t)$ to get:

$$\gamma_{m,i}(t) = \begin{cases} \left(\frac{-1}{\nu^2}\right)^{\frac{1}{2}i} \sum_{j=0}^{N} \left(\frac{-1}{\nu^2}\right)^j \frac{(2j+i)!}{(2j)!} M^{(2j)}(t) & i \text{ even}, \\ \left(\frac{-1}{\nu^2}\right)^{\frac{1}{2}(i+1)} \sum_{j=0}^{N} \left(\frac{-1}{\nu^2}\right)^j \frac{(2j+i+1)!}{(2j+1)!} M^{(2j+1)}(t) & i \text{ odd} \end{cases}$$

From above, the matrix P and vector $\boldsymbol{q}^{\mathrm{T}}$ for these methods are given by:

$$P = \begin{pmatrix} \gamma_{m,0}(0) & \gamma_{m,1}(0) \\ \gamma_{m,0}(-1) & -\gamma_{m,0}(-1) + \gamma_{m,1}(-1) \end{pmatrix}$$

$$\boldsymbol{q}^T = \begin{pmatrix} \gamma_{m,0}(1) & \gamma_{m,0}(1) + \gamma_{m,1}(1) \end{pmatrix}$$

We now assume that the collocation nodes $\{c_i\}_{i=1}^m$ satisfy the following symmetry constraint:

$$c_i + c_{m+1-i} = 0 \qquad i = 1, \ldots, \lceil \tfrac{1}{2}m \rceil$$

We will see in example 1 of this section that the 2-point method has far better stability properties than the 1-point method. We will see that this is no coincidence, and that, in general, it is far easier to find almost P-stable methods if the number of collocation points is even. We consider the cases $m = 2N$ and $m = 2N + 1$ $(N \geq 0)$ separately.

The 2N-point MCH methods

When $m = 2N$ the polynomial $M(t)$ satisfies the identity

$$M^{(r)}(-t) = (-1)^r M^{(r)}(t) \qquad r \geq 0$$

So that

$$\begin{aligned} \gamma_{2N,0}(-1) &= \gamma_{2N,0}(1) \\ \gamma_{2N,1}(-1) &= -\gamma_{2N,1}(1) \\ \gamma_{2N,1}(0) &= 0 \end{aligned}$$

Using the above relations, we may simplify $\boldsymbol{w}^{\mathrm{T}} = \boldsymbol{q}^{\mathrm{T}} P^{-1}$ to get

$$\boldsymbol{w}^T = \begin{pmatrix} 2\dfrac{\gamma_{2N,0}(1)}{\gamma_{2N,0}(0)} & -1 \end{pmatrix}$$

and thus the stability polynomial $\pi(\lambda)$ is given by:

$$\pi(\lambda) = \lambda^2 - 2\frac{\gamma_{2N,0}(1)}{\gamma_{2N,0}(0)}\lambda + 1 \tag{5.47}$$

Many numerical methods for second order differential equations, e.g. CRKN methods and the hybrid methods of Cash, Chawla and others, have stability polynomials of the form (5.47). A general framework for analysing the stability properties and order of dispersion of such methods is given in Coleman [21]. We will go on to derive some general results regarding the stability properties of the 2-step, $2N$-point MCH methods in a moment, but first we look at the stability polynomial in the case $m = 2N + 1$.

The 2N+1-point MCH methods

The polynomial $M(t)$ in this case satisfies

$$M^{(r)}(-t) = (-1)^{r+1} M^{(r)}(t) \qquad r \geq 0$$

So that

$$\gamma_{2N+1,0}(-1) = -\gamma_{2N+1,0}(1)$$

$$\begin{aligned}\gamma_{2N+1,1}(-1) &= \gamma_{2N+1,1}(1)\\ \gamma_{2N+1,0}(0) &= 0\end{aligned}$$

Using these relations we may write the vector $\boldsymbol{w}^{\mathrm{T}}$ as:

$$\boldsymbol{w}^T = \left(2\frac{\gamma_{2N+1,0}(1)+\gamma_{2N+1,1}(1)}{\gamma_{2N+1,1}(0)} \quad -1 \right)$$

From which we see that the stability polynomial $\pi(\lambda)$ takes the same form as before, and is given by:

$$\pi(\lambda) = \lambda^2 - 2\frac{\gamma_{2N+1,0}(1)+\gamma_{2N+1,1}(1)}{\gamma_{2N+1,1}(0)}\lambda - 1 \tag{5.48}$$

Using the fact that

$$M(t) = tM_{2N}(t) \quad \text{where} \quad M_{2N}(t) = \prod_{i=1}^{N}(t^2 - c_i^2)$$

we can write

$$\begin{aligned}M^{(2p)}(0) &= 0\\ M^{(2p+1)}(0) &= (2p+1)M_{2N}^{(2p)}(0) \qquad p = 0,1,\ldots\\ M^{(r)}(-1) &= (-1)^r M_{2N}^{(r)}(1) \qquad r = 0,1,\ldots\end{aligned}$$

These relations can be used to re-express the $\gamma_{2N+1,i}(t)$ in terms of the $\gamma_{2N,i}$ arising from the method obtained by discarding the node $c_{N+1} = 0$, to get:

$$\begin{aligned}\gamma_{2N+1,0}(t) &= t\gamma_{2N,0}(t) + \gamma_{2N,1}(t)\\ \gamma_{2N+1,1}(t) &= t\gamma_{2N,1}(t) + \gamma_{2N,2}(t)\end{aligned}$$

so that the stability polynomial may be written as

$$\pi(\lambda) = \lambda^2 - 2\frac{\gamma_{2N,0}(1)+2\gamma_{2N,1}(1)+\gamma_{2N,2}(1)}{\gamma_{2N,2}(0)}\lambda - 1 \tag{5.49}$$

We will now use the stability polynomials above to derive some sufficient conditions for these methods to possess a non-empty interval of periodicity, and to be almost P-stable in the sense of Thomas [60]. Define $\alpha_m(\nu^2)$ such that

$$\pi(\lambda) = \lambda^2 - 2\alpha_m(\nu^2)\lambda + 1$$

Following Coleman [21], since our aim is to draw conclusions regarding the stability properties of these methods using only the above characteristic or stability polynomial, we take $|\alpha_m(\nu^2)| < 1$ as our condition for periodicity.

Theorem 5.3 *A symmetric 2-step $2N+1$-point MCH method can be almost P-stable only if $\exists\ i \in \{1, \ldots, N\}$ such that $c_i = 1$.*

Proof We look at the behaviour of $\alpha_{2N+1}(\nu^2)$ as ν^2 becomes large. For the method to be almost P-stable we must have that $|\alpha_{2N+1}(\nu^2)| < 1$ as $\nu^2 \to \infty$. For large ν^2, $\alpha_{2N+1}(\nu^2)$ is given by

$$\alpha_{2N+1}(\nu^2) = \frac{M_{2N}(1) + O(\nu^{-2})}{2M_{2N}(0)(-\nu^{-2}) + O(\nu^{-4})}$$

Clearly this will grow without bound as ν^2 increases unless $M_{2N}(1) = 0$ □

Theorem 5.4 *Every symmetric 2-step, $2N$-point MCH method possesses a non-empty interval of periodicity. Furthermore, for each method from this class there exist infinitely many choices of the collocation nodes $\{c_i\}_{i=1}^m$ such that the method is almost P-stable.*

Proof We begin by showing that every 2-step, $2N$-point MCH method possesses a non-empty interval of periodicity. To do this we will look at the behaviour of $\alpha_{2N}(\nu^2)$ for small ν^2. For small ν^2, the function $\alpha_{2N}(\nu^2)$ may be written as

$$\alpha_{2N}(\nu^2) = \frac{M^{(2N)}(1) - \nu^2 M^{(2N-2)}(1) + O(\nu^4)}{M^{(2N)}(0) - \nu^2 M^{(2N-2)}(0) + O(\nu^4)}$$

where we have multiplied the top and bottom of $\alpha_{2N}(\nu^2)$ by ν^{2N}. Now

$$M(t) = t^{2N} - \sum_{i=1}^{N} c_i^2 t^{2N-2} + \ldots + \prod_{i=1}^{N}(-c_i^2)$$

so that with

$$\eta = \frac{1}{(2N)(2N-1)} \sum_{i=1}^{N} c_i^2$$

we have that

$$\begin{aligned} \alpha_{2N}(\nu^2) &= \frac{1 - \nu^2(\frac{1}{2} - \eta) + O(\nu^4)}{1 + \nu^2\eta + O(\nu^4)} \\ &= (1 - \nu^2(\tfrac{1}{2} - \eta) + O(\nu^4))(1 - \nu^2\eta + O(\nu^4)) \\ &= 1 - \tfrac{1}{2}\nu^2 + O(\nu^4) \end{aligned}$$

Clearly there exists some $\nu_0^2 > 0$ such that $|\alpha_{2N}(\nu^2)| < 1$ for all $\nu^2 \in (0, \nu_0^2)$.

We now look at the behaviour of $\alpha_{2N}(\nu^2)$ as ν^2 becomes large. For large ν^2, we may write $\alpha_{2N}(\nu^2)$ as

$$\alpha_{2N}(\nu^2) = \frac{M(1) + O(\nu^{-2})}{M(0) + O(\nu^{-2})}$$

So that if

$$M(1) = 0 \qquad \text{or} \qquad |M(1)| \leq |M(0)| \tag{5.50}$$

then there will exist some β^2 such that the method is periodic for all $\nu^2 \in (\beta^2, \infty)$. Let

$$\sigma_i = \left| \frac{1 - c_i^2}{-c_i^2} \right| \qquad i = 1, \ldots, N$$

so that $|M(1)| = \prod_{i=1}^{N} \sigma_i |M(0)|$. It is now easy to show that $\sigma_i < 1$ provided that $c_i \in (1/\sqrt{2}, 1]$. This completes our proof. □

In the following lemma we give slightly better bounds for the range of collocation nodes which give rise to almost P-stable symmetric 2-step, $2N$-point MCH methods.

Lemma 5.5 *If the collocation nodes $\{c_i\}_{i=1}^{m}$ of a symmetric 2-step, $2N$-point MCH*

method satisfy the following constraints:

$$\begin{aligned} c_{N+1-i} &> \sqrt{1-c_i^2} \qquad i=1,\ldots,p \quad \textit{with } p=\lfloor \tfrac{1}{2}N \rfloor, \\ c_{p+1} &> \frac{1}{\sqrt{2}} \qquad \textit{if } N=2p+1 \end{aligned}$$

and $\{c_i\}_{i=1}^N \subset (0,1]$, *then the method will be almost P-stable.*

Proof Assume that $\{c_i\}_{i=1}^N \subset (0,1]$. Let $N=2p$, with $p \geq 0$, then we may write

$$\frac{M(1)}{M(0)} = \prod_{i=1}^{p} \left(\frac{(1-c_1^2)(1-c_{N+1-i}^2)}{c_i^2 c_{N+1-i}^2} \right)$$

We require this ratio to be less than one. Let

$$\sigma_i = \left| \frac{(1-c_1^2)(1-c_{N+1-i}^2)}{c_i^2 c_{N+1-i}^2} \right| \qquad i=1,\ldots,p$$

then a sufficient condition for $M(1)/M(0) < 1$ is $\sigma_i < 1$, for $i=1,\ldots,p$, i.e.

$$\begin{aligned} (1-c_i^2-c_{N+1-i}^2+c_i^2c_{N+1-i}^2) &< c_i^2 c_{N+1-i}^2 \\ c_{N+1-i} &> \sqrt{1-c_i^2} \qquad \text{for } i=1,\ldots,p \end{aligned}$$

When $N=2p+1$ we may write

$$\left| \frac{M(1)}{M(0)} \right| = \left| \frac{1-c_{p+1}^2}{-c_{p+1}^2} \right| \prod_{i=1}^{p} \sigma_i$$

from which the lemma follows immediately.

□

To illustrate the results of this section we analyse in detail the stability properties of the general 2-step, 2-point and 3-point MCH methods with symmetric nodes. Analysis of the symmetric 2-step 4-point MCH method is given in section 5.4.

Example 1 $k=2,\ m=2,$ symmetric nodes.

The stability polynomial for these methods is

$$\pi(\lambda) = \lambda^2 - 2\frac{\nu^2(1-c_1^2)-2}{c_1^2\nu^2+2}\lambda + 1$$

The corresponding Routh-Hurwitz polynomial is given by

$$R(\zeta) = 2\left((4+\nu^2(2c_1^2-1))\zeta^2 + \nu^2\right)$$

Applying the Routh-Hurwitz conditions we find immediately that when $c_1 \in (0, 1/\sqrt{2})$ the method is periodic provided that $\nu^2 \in (0, 4(1-2c_1^2)^{-1})$, and when $c_1 \in [1/\sqrt{2}, 1]$ the method is P-stable.

Example 2 $k = 2,\ m = 3,$ symmetric nodes.

The stability polynomial for these methods is

$$\pi(\lambda) = \lambda^2 - 2\frac{\nu^4(c_1^2-1)+2(6-c_1^2)\nu^2-24}{2c_1^2\nu^2+24}\lambda - 1$$

After applying the Routh-Hurwitz transformation we obtain the following Routh-Hurwitz polynomial:

$$R(\zeta) = (\nu^4(1-c_1^2) - 4\nu^2(3-c_1^2) + 48)\zeta^2 - \nu^2((1-c_1^2)\nu^2 - 12)$$

The Routh-Hurwitz conditions are thus

$$\nu^2 < \frac{12}{(1-c_1^2)} \tag{5.51}$$

and

$$\nu^4(1-c_1^2) - 4\nu^2(3-c_1^2) + 48 > 0) \tag{5.52}$$

Assume $c_1 \neq 1$. The above quadratic in ν^2 has roots $r_\pm$ given by

$$r_\pm = \frac{2}{c_1^2-1}\left(c_1^2 - 3 \pm \sqrt{c_1^4 + 6c_1^2 - 3}\right)$$

When $c_1^2 < 2\sqrt{3} - 3$, the roots $r_\pm$ are complex, and so condition (5.52) holds for all ν^2. When $c_1^2 \geq 2\sqrt{3} - 3$, then the quadratic has real roots, and so (5.52) holds for $\nu^2 \in (0, r_-) \cup (r_+, \infty)$. When $c_1 = 1$, the method becomes Numerov's method. To summarize, the periodicity intervals for these methods are as follows:

$$\begin{aligned} c_1^2 \in (0, 2\sqrt{3} - 3): &\quad \nu^2 \in (0, \tfrac{12}{1-c_1^2}) \\ c_1^2 \in (2\sqrt{3} - 3, 1): &\quad \nu^2 \in (0, r_-) \cup (r_+, \tfrac{12}{1-c_1^2}) \\ c_1^2 = 1: &\quad \nu^2 \in (0, 6) \end{aligned}$$

5.3 Order and local truncation error

In the previous chapter on MCRKN methods we were able to derive order conditions for the two-step methods with arbitrary number of collocation nodes using the Gröbner-Alekseev theorem. This derivation relied heavily on the fact that we had information about the quantities $u(x) - y(x)$ and $u'(x) - z(x)$ at the previous step-points x_{n-1} and x_n. The MCH methods of this chapter are designed so as to contain no explicit first derivative evaluations, since they are intended to be used solely for the special second order differential equation $y'' = f(x, y)$; $y(x_0) = y_0$, $y'(x_0) = z_0$. This means that we have no information about the quantities $u'(x) - z(x)$ at the previous step-points, and so the previous derivation of the order conditions may not be used here.

We begin by restricting our attention to the two-step symmetric methods once again. Using a Taylor series approach and properties of the coefficients of these methods, we derive conditions for methods with an even number of collocation nodes to have order at least $m + 4$, and those with an odd number of nodes to have order at least $m + 3$.

In section 5.3.2 we examine an approach used by Nørsett & Lie [47] to derive order conditions for their multistep collocation methods for first order systems, and show that it is not applicable to our methods.

Finally, in section 5.3.3 we present a simple, cheap and effective local truncation

error estimator for the $2N$-point methods of order $2N$.

5.3.1 Taylor series approach

In this subsection we consider the two-step m-point MCH methods, and later restrict our attention to those methods whose nodes are distributed symmetrically in $[-1,1]$, which for brevity we will call 2CHS methods. We adopt the approach used by Lambert [45] for linear multistep methods and associate with each two-step MCH method a number of linear operators. Using these operators we examine the leading terms in the local truncation error expansion. We show that the minimum order of an m-point 2CHS method is m if m is even, and $m+1$ if m is odd, we then go on to derive conditions under which a $2N$-point 2CHS method will have order at least $m+2$.

We begin by writing the general 2-step m-point MCH method as

$$y_{n+c_i} = (1+c_i)y_n - c_i y_{n-1} + h^2 \sum_{j=1}^{m} A_{ij} f_{n+c_j} \quad i = 1,\ldots,m \tag{5.53}$$

$$y_{n+1} = 2y_n - y_{n-1} + h^2 \sum_{j=1}^{m} A_{m+1,j} f_{n+c_j} \tag{5.54}$$

where

$$A_{ij} = \int_0^{c_i} \int_0^{\tau} l_j(\sigma) d\sigma d\tau - c_i \int_{-1}^{0} \int_0^{\tau} l_j(\sigma) d\sigma d\tau \quad i = 1,\ldots,m+1,\ j = 1,\ldots,m \tag{5.55}$$

and where we have taken $c_{m+1} = 1$. With each method from this class we associate the following linear operators:

$$\begin{aligned} \mathcal{L}_i[y(x)] &= y(x+c_i h) - (1+c_i)y(x) + c_i y(x-h) \\ &\quad -h^2 \sum_{j=1}^{m} A_{ij} y''(x+c_j h) \qquad i = 1\ldots,m \end{aligned} \tag{5.56}$$

$$\mathcal{L}_{m+1}[y(x)] = y(x+h) - 2y(x) + y(x-h) - h^2 \sum_{j=1}^{m} A_{m+1,j} y''(x+c_j h) \tag{5.57}$$

where y is an arbitrary test function, assumed to be as differentiable as we please. By

expanding the functions $y(x \pm h)$, $y(x + c_i h)$ and the second derivatives $y''(x + c_i h)$ (for $i = 1, \ldots, m$) as Taylor series about x, we may re-express the operators $\mathcal{L}_i[y(x)]$ as

$$\mathcal{L}_i[y(x)] = \sum_{p=0}^{r} \frac{h^{p+2} B_p^i y^{(p+2)}(x)}{p!} + O(h^{r+3}) \quad i = 1, \ldots, m+1 \tag{5.58}$$

for some $r < \infty$, where

$$B_p^i = \frac{c_i^{p+2} + (-1)^p c_i}{(p+1)(p+2)} - \sum_{j=1}^{m} A_{ij} c_j^p \tag{5.59}$$

We know that the order of methods from this class is at least m. This result follows directly from the method by which they are constructed, or, as we show here, using expressions (5.58) and (5.59), and basic properties of Lagrange interpolation. A two-step MCH method will have order at least m if the coefficients B_p^i satisfy the following conditions:

$$B_p^i = 0 \qquad \text{for } i = 1, \ldots m, \; p = 0, \ldots m-3 \tag{5.60}$$

$$B_p^{m+1} = 0 \qquad \text{for } p = 0, \ldots, m-1 \tag{5.61}$$

Let g be a function, assumed to be as differentiable as we please. The error in Lagrange interpolation for g at the nodes $\{c_i\}_{i=1}^m$ may be written as

$$g(x) - \sum_{j=1}^{m} g(c_j) l_j(x) = \frac{M(x) g^{(m)}(\eta(x))}{m!} \qquad \text{for all } x \tag{5.62}$$

where $M(x) = \prod_{i=1}^{m}(x - c_i)$, and η is some number that depends on x. Now let $g(x) = x^p$, for some $p \in \{0, \ldots, m-1\}$. Using (5.62) we have that

$$\sum_{j=1}^{m} c_j^p l_j(x) \equiv x^p \qquad \text{for all } x$$

Using this we may write

$$\begin{aligned}\sum_{j=1}^{m} A_{ij}c_j^p &= \int_0^{c_i}(c_i-\tau)\sum_{j=1}^{m} c_j^p l_j(\tau)d\tau + \\ &\quad c_i\int_0^{-1}(-1-\tau)\sum_{j=1}^{m} c_j^p l_j(\tau)d\tau \\ &= \int_0^{c_i}(c_i-\tau)\tau^p d\tau + c_i\int_0^{-1}(-1-\tau)\tau^p d\tau \\ &= \frac{c_i^{p+2}+(-1)^p c_i}{(p+1)(p+2)}\end{aligned}$$

We see immediately from this that $B_p^i = 0$ for $p < m$ and $i = 1,\ldots,m+1$, and hence the required result follows.

When 2-step m-point MCH method is applied to the differential equation

$$y''(x) = f(x,y), \quad y(x_0) = y_0,\ y'(x_0) = z_0 \tag{5.63}$$

the local truncation error in the approximation y_{n+1} is defined to be

$$\delta_{m+1}[y(x_n)] = y(x_{n+1}) - y_{n+1} \tag{5.64}$$

where $y(x)$ is a solution of (5.63), and y_{n+1} is obtained from the MCH method under the assumptions $y_n = y(x_n)$ and $y_{n-1} = y(x_{n-1})$. Similarly we define the local truncation error in the i^{th} corresponding off-step value y_{n+c_i} to be

$$\delta_i[y(x_n)] = y(x_{n+c_i}) - y_{n+c_i} \qquad \text{for } i = 1,\ldots,m \tag{5.65}$$

under the above localising assumptions. The operators $\delta_i[y(x_n)]$ may be re-expressed using the $\mathcal{L}_i[y(x_n)]$ operators as follows:

$$\begin{aligned}\delta_i[y(x_n)] &= \mathcal{L}_i[y(x_n)] - h^2\sum_{j=1}^{m} A_{ij}y''(x_{n+c_j}) \\ &\quad + h^2\sum_{j=1}^{m} A_{ij}f(x_{n+c_j}, y(x_{n+c_j}) - \delta_j[y(x_n)])\end{aligned}$$

$$
\begin{aligned}
&= \mathcal{L}_i[y(x_n)] \\
&\quad + h^2 \sum_{j=1}^{m} A_{ij} \sum_{l=1} \frac{(-1)^l}{l!} (\delta_j[y(x_n)])^l \frac{\partial^l f}{\partial y^l}(x_{n+c_j}, y(x_{n+c_j})) \qquad (5.66) \\
&= \frac{B_m^i y^{(m+2)}(x_n)}{m!} h^{m+2} + \frac{B_{m+1}^i y^{(m+3)}(x_n)}{(m+1)!} h^{m+3} + \\
&\quad \left(\frac{B_{m+2}^i y^{(m+4)}(x_n)}{(m+2)!} + \frac{\partial f}{\partial y}(x_n, y(x_n)) \frac{y^{(m+2)}(x_n)}{m!} \sum_{j=1}^{m} A_{ij} B_m^j \right) h^{m+4} \\
&\quad + O(h^{m+5}) \qquad (5.67)
\end{aligned}
$$

Before proceeding any further with our error analysis we impose the symmetry constraints

$$c_i + c_{m+1-i} = 0 \qquad \text{for } i = 1, \ldots, N+1, \quad \text{with } N = \lfloor \tfrac{1}{2} m \rfloor \qquad (5.68)$$

and restrict our attention to the 2CHS methods. When the conditions (5.68) are satisfied, a number of identities involving the A_{ij} and B_p^i may be derived. These identities may then be used to simplify the definition of the method given in (5.53) and (5.54), and the local truncation error as given by (5.67). Let $j \in \{1, \ldots, N\}$ then

$$
\begin{aligned}
l_j(-x) &= \prod_{\substack{l=1 \\ l \neq j}}^{m} \left(\frac{-x - c_l}{c_j - c_l} \right) \\
&= \prod_{\substack{l=1 \\ l \neq j}}^{m} \left(\frac{-(x - c_{m+1-l})}{-(c_{m+1-j} - c_{m+1-l})} \right) \\
&= l_{m+1-j}(x)
\end{aligned}
$$

Using the above identity, consider $A_{m+1,j}$ with $j \in \{1, \ldots, N\}$:

$$
\begin{aligned}
A_{m+1,j} &= \int_0^1 (1-\tau) l_j(\tau) d\tau + \int_0^{-1} (-1-\tau) l_j(\tau) d\tau \\
&= \int_0^{-1} (-1-\sigma) l_{m+1-j}(\sigma) d\sigma + \int_0^1 (1-\sigma) l_{m+1-j}(\sigma) d\sigma \\
&= A_{m+1,m+1-j} \qquad (5.69)
\end{aligned}
$$

where we have changed the integration variable from τ to $\sigma = -\tau$. Using the same

idea we can also show that

$$A_{ij} + A_{m+1-i,j} = A_{i,m+1-j} + A_{m+1-i,m+1-j} \qquad i,j = 1,\ldots,N$$

In view of these identities we might be tempted to write the 2CHS method in the same form as the Panovsky-Richardson methods. Take $m = 2N$, and let $a_{ij} = A_{ij} + A_{m+1-i,j}$ for $i,j = 1,\ldots,N$, then we might write the general $2N$-point 2CHS method as

$$\begin{aligned} y_{n+c_i} - 2y_n + y_{n-c_i} &= h^2 \sum_{j=1}^{N} a_{ij}(f_{n+c_j} + f_{n-c_j}) \qquad i = 1,\ldots,N \\ y_{n+1} - 2y_n + y_{n-1} &= h^2 \sum_{j=1}^{N} A_{m+1,j}(f_{n+c_j} + f_{n-c_j}) \end{aligned}$$

The problem now is, how do we generate the values y_{n-c_i}? We could provide these values in the first step, in the same way as for the Panovsky-Richardson methods, but this would not help us in step 2. In addition we could force the positive nodes $\{c_i\}_{i=1}^{N}$ to be symmetrically distributed in the interval $(0,1)$, and try the same method of advancing as used by those methods. Unfortunately this does not work either. For the Panovsky-Richardson method of advancing to work, we must have that for each $i \in \{1,\ldots,N\}$,

$$y_{(n+1)-c_i} = y_{n+c_j} \qquad \text{for some } j \in \{1,\ldots,N.\} \tag{5.70}$$

This was the case for the Panovsky-Richardson methods, since, now that we know them to be one-step collocation methods, we see that the same collocation polynomial $u(x)$ is used to calculate both $y_{(n+1)-c_i}$ and y_{n+c_j}. However this is not the case for the 2CHS methods. The collocation polynomial used to calculate y_{n+c_j}, $u_n(x)$ say, is defined by incomplete Hermite interpolation over the interval $x \in [x_{n-1}, x_{n+1}]$, whereas the polynomial $u_{n+1}(x)$ used to calculate $y_{(n+1)-c_i}$ is defined by interpolation over the interval $x \in [x_n, x_{n+2}]$, and so it is clear that $u_n \not\equiv u_{n+1}$. This means that in general, we will not be able to satisfy condition (5.70). It is due to difficulties such as this that we have so far been unable to derive a complete set of order conditions

for the MCH methods with arbitrary k and m.

Let us now look at the coefficients B_m^i. Using our expression (5.62) for the error in Lagrange interpolation, with $g(x) = x^m$ we have that

$$\sum_{j=1}^{m} l_j(x) c_j^m \equiv x^m - M(x) \quad \text{for all } x$$

Using this to simplify B_m^i gives

$$B_m^i = \int_0^{c_i} (c_i - \tau) M(\tau) d\tau + c_i \int_0^{-1} (-1 - \tau) M(\tau) d\tau \quad i = 1, \ldots, m$$

and, using $M(-x) = (-1)^m M(x)$,

$$B_m^{m+1} = (1 + (-1)^m) \int_0^1 (1 - \tau) M(\tau) d\tau$$

Thus we see that the minimum order of an arbitrary 2CHS method is m when m is even, and $m+1$ when m is odd. So far we have been able to obtain sufficient, but by no means necessary, conditions for an arbitrary m-point 2CHS method to have order at least $m+2$, and for an arbitrary $2N$-point method to have order at least $m+4$. These results are summarised in the theorems below.

Theorem 5.6 *The minimum order, p_0, of an arbitrary m-point 2CHS method is m if m is even, and $m+1$ if m is odd. If the conditions*

$$\int_0^1 (1 - \tau) M(\tau) d\tau = 0 \qquad m = 2N \tag{5.71}$$

$$\sum_{j=1}^{N} A_{m+1,j} c_j^{2N+2} = \frac{1}{(2N+3)(2N+4)} \qquad m = 2N+1 \tag{5.72}$$

are satisfied, with

$$A_{m+1,j} = \int_0^1 (1 - \tau)(l_j(\tau) + l_j(-\tau)) d\tau \qquad j = 1, \ldots, m$$

then the method will have order $p_0 + 2$. If in addition the nodes of a $2N$-point 2CHS

method satisfy the conditions

$$\sum_{j=1}^{N} A_{m+1,j} c_j^{2N+2} = \frac{1}{(2N+3)(2N+4)} \tag{5.73}$$

$$\sum_{j=1}^{N} A_{m+1,j} \int_0^{c_j} (c_j - \tau) M(\tau) d\tau = 0 \tag{5.74}$$

then the method will have order $2N+4$.

Proof NED □

Theorem 5.7 *If the nodes of a* $2N$*-point* 2*CHS method are chosen so that condition (5.71) is satisfied, then there exists at least one* $j \in \{1, \ldots, 2N\}$ *such that*

$$\int_0^{c_j} (c_j - \tau) M(\tau) d\tau \neq 0. \tag{5.75}$$

Proof Postponed until the end of section 5.3.2. □

Observe that this result means that at least one of the off-step approximations, y_{n+c_i}, from a $2N$-point 2CHS method has order at most $2N$ whenever the nodes are chosen so that the method itself is of order $2N+2$.

The Taylor series analysis in this subsection, though not as elegant as we would have liked, has proved useful in analysing the 2CHS methods with 1,2,3 and 4 nodes. The analysis of these methods may be found in section 5.4. In order to make any further progress in deriving a full set of order conditions for MCH methods with arbitrary stepnumber and number of collocation nodes, we believe that a formulation similar to that used in the previous chapter must be found. One avenue which we pursued was to attempt to extend the 'Collocation approach' used by Lie & Nørsett [47] for their methods.

5.3.2 Lie & Nørsett's 'Collocation approach'

Once again we restrict our attention to the symmetric two-step MCH methods. Before we begin our analysis, we will change variable from x to

$$s = \frac{x - x_n}{h}$$

As before we define

$$\begin{aligned} u(x_n + sh) &= U(s) \\ y(x_n + sh) &= Y(s) \\ f(x_n + sh, y(x_n + sh)) &= F(s, Y(s)) \end{aligned}$$

and let a prime denote differentiation with respect to s. We consider the approximation of an arbitrary test function Y, assumed to be as differentiable as we please, by a polynomial U using our interpolation scheme. Let

$$\Psi = Y - U.$$

Lie & Nørsett begin with the assertion that, for their methods, order p corresponds to

$$\Psi(1) = 0 \qquad \text{for all } Y \in \mathcal{P}_p,$$

i.e. the error in interpolating Y by U is zero for polynomials up to degree p. We feel that this assertion is incorrect. To see why, let us consider the application of the simple implicit Runge-Kutta method

$$y_{n+1} = y_n + hf(x_n + \tfrac{1}{2}h, \tfrac{1}{2}(y_n + y_{n+1})) \tag{5.76}$$

to the first order initial value problem

$$y' = \frac{2y}{x}, \quad y(x_0) = x_0^2 \tag{5.77}$$

which has solution $y(x) = x^2$. Take $x_0 = 1$, then

$$\begin{aligned} y_1 &= 1 + \frac{h(1+y_1)}{1+\frac{1}{2}h} \\ &= \frac{1+\frac{3}{2}h}{1-\frac{1}{2}h} \end{aligned}$$

Expand this as a Taylor series to get

$$\begin{aligned} y_1 &= (1+\tfrac{3}{2}h)(1+\tfrac{1}{2}h+\tfrac{1}{4}h^2+O(h^3)) \\ &= x_1^2 + \tfrac{1}{2}h^3 + O(h^4) \end{aligned}$$

In this example we clearly see that, though the method has order 2, the solution $y(x) = x^2$ is not reproduced exactly. Having said this, Lie & Nørsett's approach does seem to work for their methods, though this appears to be more by luck than by design. One possible reason for this might be that their methods satisfy the simplifying assumptions of Burrage & Moss [3] which ensure that the only Butcher trees which contribute to the order conditions are the quadrature trees (see Hairer et al. [35] pp203-4).

We now extend this approach to cover our 2CHS methods. To begin with we will proceed as Lie & Nørsett, and ignore the above flaw. After generating the 'order conditions', we will use them to analyse a number of examples and compare our results with those obtained from the Taylor series approach from the previous subsection. Following Lie & Nørsett we begin with the assertion that order p corresponds to

$$\Psi(1) = 0 \qquad \text{for all } Y \in \mathcal{P}_{p+1}$$

We know already that such methods have order at least m, so we can take $p = m + \rho$

with $\rho \geq 0$. The interpolation conditions defining $U(s)$ are as follows:

$$U(-j) = Y(-j) \qquad j = 0, 1 \tag{5.78}$$

$$U''(c_i) = Y''(c_i) \qquad i = 1, \ldots, m \tag{5.79}$$

Let $\Phi_r(s) \in \mathcal{P}_{m+1}$ be the polynomial which interpolates to s^r using our interpolation scheme, for $r = 0, 1, \ldots$, and let $Y(s)$ be given by

$$Y(s) = \sum_{r=0}^{p+1} a_r s^r \qquad a_r \in \mathbb{R},\ r = 0, \ldots, p+1$$

We may now write $\Psi(s)$ as

$$\Psi(s) = \sum_{r=0}^{p+1} a_r (s^r - \Phi_r(s))$$

Since there are $m+2$ interpolation conditions in (5.78) and (5.79), we must have that $s^r \equiv \Phi_r(s)$ for $r = 0, \ldots, m+1$, and hence

$$\Psi(s) = \sum_{r=m+2}^{p+1} a_r (s^r - \Phi_r(s)). \tag{5.80}$$

In order to proceed with our analysis we will need to re-express $\Psi(s)$ in a more convenient form. Using the interpolation conditions (5.78) and forcing $\Psi(1) = 0$ we can write

$$\Psi(s) = s(s-1)(s+1)R_{p-2}(s) \qquad \text{with } R_{p-2}(s) \in \mathcal{P}_{p-2} \tag{5.81}$$

The remaining interpolation conditions (5.79) may now be expressed as

$$\Psi''(c_i) = 0 \qquad \text{for } i = 1, \ldots, m. \tag{5.82}$$

Let $R_{p-2}(s)$ be given by

$$R_{p-2}(s) = \sum_{r=0}^{p-2} \eta_r s^r \qquad \text{with } \eta_r \in \mathbb{R},\ r = 0, \ldots, p-2$$

Then we seek values of $\eta_0, \ldots, \eta_{p-2}$ such that conditions (5.82) are satisfied for polynomials R_{p-2} of degree $p-2$. From equation (5.80) above, we see that the only free parameters in $R_{p-2}(s)$ are the numbers $\eta_{m-1}, \ldots, \eta_{p-2}$, the remaining η's are just linear combinations of these. We now attempt to simplify the conditions $\Psi''(c_i) = 0,\ i = 1 \ldots, m$ by making use of the symmetry properties of the 2CHS methods. Let

$$\Gamma_r(s) = s^r((r+3)(r+2)s^2 - r(r+1)) \qquad \text{for } r = 0, 1, \ldots$$

Then the conditions $\Psi''(c_i) = 0$ may be written as

$$\sum_{r=0}^{p-2} \eta_r \Gamma_r(c_i) = 0 \qquad i = 1, \ldots, m$$

Using the symmetry of the nodes $\{c_i\}_{i=1}^m$, and noting that Γ_r is even if r is even, and odd otherwise, we may rewrite the above conditions as

$$\sum_{\substack{r=0 \\ r \text{ odd}}}^{p-2} \eta_r \Gamma_r(c_i) = 0 \qquad i = 1, \ldots, N \tag{5.83}$$

$$\sum_{\substack{r=0 \\ r \text{ even}}}^{p-2} \eta_r \Gamma_r(c_i) = 0 \qquad i = 1, \ldots, N \tag{5.84}$$

$$\eta_1 = 0 \qquad \text{when } m = 2N+1 \tag{5.85}$$

where equation (5.85) represents the condition $\Psi''(0) = 0$. Notice in particular that this condition means that the order of a 1-point 2CHS method may not exceed 2.

As examples of how to apply these conditions we consider the general 2-, 3- and 4-point 2CHS methods.

Example 1 $m = 2, c_2 = -c_1, \quad p \geq 2.$

We seek the largest value of p such that a non-trivial solution to the system (5.83)-(5.85) exists and has $\eta_{p-2} \neq 0$.

(i) p=3. The conditions (5.83)-(5.85) in this case are as follows:

$$\begin{aligned} 6c_1\eta_0 &= 0 \\ 2(6c_1^2 - 1)\eta_1 &= 0 \end{aligned}$$

We require that this system be solvable for all η_1, i.e. that $c_1 = 1/\sqrt{6}$.

(ii) p=4. Take $c_1 = 1/\sqrt{6}$. The conditions (5.83)-(5.85) now become:

$$\sqrt{6}\eta_0 - \frac{4\sqrt{6}}{9}\eta_2 = 0$$

which is clearly solvable for all η_2.

(iii) p=5. The condition (5.84) remains unchanged from the $p = 4$ case. Condition (5.84) is now

$$\frac{-7}{6}\eta_3 = 0$$

The only solution to this equation is $\eta_3 = 0$.

We have shown that the conditions (5.82) can be satisfied with $R(s)$ a polynomial of degree at most 2 by choosing $c_1 = 1/\sqrt{6}$. By applying our Taylor analysis above, we see that this value of c_1 does indeed result in an increase in the order of the method from 2 to 4. For the stability analysis for these methods we refer the reader to section 5.4, numerical results may be found in section 5.5.

Example 2 $m = 3, c_3 = -c_1, c_2 = 0, \quad p \geq 3.$

From our Taylor series analysis above, we know that the minimum order of these methods is in fact 4, so that we need only consider $p \geq 5$ here.

(i) $p = 5$. The conditions (5.83)-(5.85) in this case are given by

$$\begin{aligned} 6c_1\eta_0 + c_1(20c_1^2 - 6)\eta_2 &= 0 \\ 6c_1^2(5c_1^2 - 2) &= 0 \end{aligned}$$

The first of these equations remains unchanged from the $p = 4$ case, and so we know that it is solvable for all η_2. The second equation has a non-trivial solution if and only if $5c_1^2 - 2 = 0$, note that $c_1 = 0$ is not permitted.

(ii) $p = 6$. The condition (5.83) remains unchanged from the $p = 5$ case above. Condition (5.84) is now

$$6\eta_0 + 2\eta_2 - \frac{32}{25}\eta_4 = 0$$

which certainly possesses solutions with η_2 and η_4 both non-zero.

(iii) $p = 7$. The condition (5.84) remains unchanged from the $p = 6$ case above. Condition (5.83) now becomes

$$\frac{152}{125}\eta_5 = 0$$

Clearly the only solution to this equation is $\eta_5 = 0$.

When $m = 3$ we have shown that the condition (5.82) can be satisfied by a polynomial $R(s)$ of degree at most 4 by choosing $c_1 = \sqrt{2/5}$. From our Taylor series analysis above, we find that this value of c_1 does in fact result in an increase in the order of the method from 4 to 6.

There is evidence from these examples to support the conjecture that the maximum attainable order of an m-point 2CHS method is $2m$. In the next example we will see that this is in fact not the case. We will also see that this collocation approach to the order analysis fails to find correct order conditions for $p > p_0 + 2$. By relating this analysis back to the Taylor analysis above, we see that this failure is due to the fact that the operators $\mathcal{L}_1[y], \ldots, \mathcal{L}_m[y]$ are not taken into consideration. We might then ask why this approach works for Lie & Nørsett's methods, but not for these? Unfortunately we have been unable to find an answer to this question. One approach

which we have not pursued might be to extend the Butcher theory of trees to cover General Linear Methods for our special second order differential equation, and then to try to find simplifying assumptions similar to those used by Burrage & Moss [3].

Example 4 $m = 4,\ c_4 = -c_1,\ c_3 = -c_2, \quad p \geq 4.$

(i) $p = 5$. The conditions (5.83)-(5.85) in this case are given by

$$\begin{aligned} 6c_i\eta_0 + 2c_i(10c_i^2 - 3)\eta_2 &= 0 \qquad i = 1,2 \\ 2(6c_i^2 - 1)\eta_1 + 6c_i^2(5c_i^2 - 2)\eta_3 &= 0 \qquad i = 1,2 \end{aligned}$$

We require that there be a non-trivial solution to this system with $\eta_3 \neq 0$. Writing the second pair of equations in matrix form we have

$$A(\eta_1, \eta_3)^T = 0$$

where

$$A = \begin{pmatrix} 6c_1^2 - 1 & 3c_1^2(5c_1^2 - 2) \\ 6c_2^2 - 1 & 3c_2^2(5c_2^2 - 2) \end{pmatrix}.$$

Our requirement now becomes det(A)=0.

$$\det\,(A) = 12(c_2^2 - c_1^2)(30c_1^2c_2^2 - 5(c_1^2 + c_2^2) + 2)$$

This determinant will vanish provided that the nodes $\{c_1, c_2\}$ satisfy

$$c_1^2 = \frac{5c_2^2 - 2}{5(6c_2^2 - 1)}$$

(ii) $p = 6$. The conditions (5.83) remain unchanged from the previous case. Conditions (5.84) now become

$$6c_i\eta_0 + 2c_i(10c_i^2 - 3)\eta_2 + 2c_i^3(21c_i^2 - 10)\eta_4 = 0 \qquad i = 1,2$$

We require that a non-trivial solution to this system exists and has $\eta_4 \neq 0$ Write this system in matrix form as

$$B(\eta_0, \eta_2)^T = -\boldsymbol{b}\eta_4$$

Our requirement now becomes $\det(B) \neq 0$.

$$\det(B) = 120 c_1 c_2 (c_2^2 - c_1^2)$$

Since we have chosen the collocation nodes to be distinct, this determinant can never vanish.

(iii) $p = 7$. The conditions from (5.84) remain unchanged from the previous case. Conditions (5.83) are now given by

$$2(6c_i^2 - 1)\eta_1 + 6c_i^2(5c_i^2 - 2)\eta_3 + 2c_i^4(28c_i^2 - 15)\eta_5 = 0 \qquad i = 1, 2$$

We require this system to have a non-trivial solution with $\eta_5 \neq 0$. Let $\{c_1, c_2\}$ be chosen so that the matrix A from the $p = 5$ case is singular. There must now exist a constant ξ such that the second column of A is ξ times the first column. Letting

$$\alpha = \eta_1 + \xi\eta_3$$

we may now rewrite the above system of equations as

$$2(6c_i^2 - 1)\alpha + 2c_i^4(38c_i^2 - 15)\eta_5 = 0 \qquad i = 1, 2$$

Write this as a matrix system:

$$C(\alpha, \eta_5)^T = 0$$

with

$$C = \begin{pmatrix} 2(6c_i^2 - 1) & 2c_i^4(28c_i^2 - 15) \\ 2(6c_i^2 - 1) & 2c_i^4(28c_i^2 - 15) \end{pmatrix}$$

We now require that det(C)=0.

$$\det\,(C) = 4(c_2^2 - c_1^2)(168(c_1^2c_2^2 + 15)(c_1^2 + c_2^2) - 28(c_1^4 + c_2^4) - 118c_1^2c_2^2)$$

After enforcing det(A)=0 this becomes

$$\det\,(C) = \frac{4(490c_2^4 - 310c_2^2 + 19)(15c_2^4 - 5c_2^2 + 1)}{125(6c_2^2 - 1)^2}$$

The matrix C is thus singular whenever

$$c_2^2 = \frac{155 \pm \sqrt{1635}}{490}$$

By checking with our Taylor series analysis from the previous section we find that the condition on the nodes arising from the $p = 5$ case does indeed guarantee that the method is of order 6. However the condition from the $p = 7$ case is not sufficient for the method to have order greater than 6. Though we cannot achieve order 8 for general non-linear problems, it is possible to choose the node c_2 so that the method has order of dispersion 8, for this analysis we refer the reader to section 5.4.

Before moving on to look at some examples of 2CHS methods, we return to the proof of Theorem 5.7.

Proof (Theorem 5.7) Suppose that $Y \in \mathcal{P}_{2N+2}$, and let the polynomial Ψ be as defined above. We suppose that $\Psi(s) = 0$ whenever $s \in \{-1, 0, 1, c_1, \ldots, c_{2N}\}$ and show that this must imply that Ψ is identically zero. Observe that this is equivalent to asking that all of the off-step approximations y_{n+c_i}, for $i = 1, \ldots, 2N$, have order at least $2N + 2$.

We present two methods by which this theorem may be proved. The first method works whatever the values of the nodes $\{c_i\}_{i=1}^{2N}$, while the second is considerably shorter but works only if none of the nodes is equal to 1.

Suppose that $\Psi(1) = 0$ and $\Psi(c_i) = 0$, for $i = 1, \ldots, 2N$, whenever $Y \in \mathcal{P}_{m+2}$.

Method (i)

Let

$$\Psi(s) = s(s+1)R(s)$$

where $R \in \mathcal{P}_{2N}$ is given by $R(s) = \sum_{r=0}^{2N} \eta_r s^r$. Suppose that for each $l \in \{1, \ldots, 2N\}$ there exists a polynomial $R_l \not\equiv 0$ given by

$$R_l(s) = \sum_{r=0}^{2N-1} \eta_{r,l} s^r$$

such that $R(s) = (s - c_l)R_l(s)$. Write

$$\Psi_l(s) = s(s+1)(s-c_l)R_l(s) \qquad \text{for } l = 1, \ldots, 2N$$

Differentiating twice with respect to s we obtain

$$\begin{aligned} \Psi_l''(s) &= \sum_{r=0}^{2N-1} \eta_{r,l} s^{r-1} \Big((r+3)(r+2)s^2 + (r+2)(r+1)s \Big) \\ &\quad -c_l \sum_{r=0}^{2N-1} \eta_{r,l} s^{r-1} \left((r+2)(r+1)s + r(r+1) \right) \end{aligned}$$

We now attempt to enforce the conditions (5.82). Using the symmetry properties of the nodes $\{c_i\}_{i=1}^{2N}$ to simplify these conditions, and writing them in matrix form we obtain

$$(A - c_l B)\boldsymbol{\eta}_l = 0 \tag{5.86}$$

where

$$A = \begin{pmatrix} 2 & 12c_1^2 & 12c_1^2 & \ldots & 2N(2N-1)c_1^{2N-2} & (2N+1)(2N+2)c_1^{2N} \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 2 & 12c_N^2 & 12c_N^2 & \ldots & 2N(2N-1)c_N^{2N-2} & (2N+1)(2N+2)c_N^{2N} \\ 6c_1 & 6c_1 & 20c_1^3 & \ldots & 2N(2N+1)c_1^{2N-1} & 2N(2N+1)c_1^{2N-1} \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 6c_N & 6c_N & 20c_N^3 & \ldots & 2N(2N+1)c_N^{2N-1} & 2N(2N+1)c_N^{2N-1} \end{pmatrix}$$

$$B = \begin{pmatrix} 2 & 2 & 12c_1^2 & \dots & 2N(2N-1)c_1^{2N-2} & 2N(2N-1)c_1^{2N-2} \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 2 & 2 & 12c_N^3 & \dots & 2N(2N-1)c_N^{2N-2} & 2N(2N-1)c_N^{2N-2} \\ 0 & 6c_1 & 6c_1 & \dots & (2N-1)(2N-2)c_1^{2N-3} & 2N(2N+1)c_1^{2N-1} \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 6c_N & 6c_N & \dots & (2N-1)(2N-2)c_N^{2N-3} & 2N(2N+1)c_N^{2N-1} \end{pmatrix}$$

$$\boldsymbol{\eta}_l = \begin{pmatrix} \eta_{0,l} & \dots & \eta_{2N-1,l} \end{pmatrix}^T$$

If our assumptions are correct then we must have that $\det(A - c_l B) = 0$ for each $l \in \{1, \dots, 2N\}$. Before we look at $\det(A - c_l B)$, let us first investigate the determinants of A and B individually. By performing elementary column operations on the matrix A we can simplify its determinant somewhat to get

$$\begin{aligned} \det A &= \alpha \begin{vmatrix} \Gamma_1(c_1) & \dots & \Gamma_{2N-1}(c_1) & 0 & \dots & 0 \\ \vdots & & \vdots & \vdots & & \vdots \\ \Gamma_1(c_N) & \dots & \Gamma_{2N-1}(c_N) & 0 & \dots & 0 \\ 0 & \dots & 0 & \Gamma_0(c_1) & \dots & \Gamma_{2N-2}(c_1) \\ \vdots & & \vdots & \vdots & & \vdots \\ 0 & \dots & 0 & \Gamma_0(c_N) & \dots & \Gamma_{2N-2}(c_N) \end{vmatrix} \\ &= \alpha \begin{vmatrix} \Gamma_1(c_1) & \dots & \Gamma_{2N-1}(c_1) \\ \vdots & & \vdots \\ \Gamma_1(c_N) & \dots & \Gamma_{2N-1}(c_N) \end{vmatrix} \begin{vmatrix} \Gamma_0(c_1) & \dots & \Gamma_{2N-2}(c_1) \\ \vdots & & \vdots \\ \Gamma_0(c_N) & \dots & \Gamma_{2N-2}(c_N) \end{vmatrix} \end{aligned}$$

for some $\alpha \neq 0$ independent of the nodes $\{c_i\}_{i=1}^{2N}$. Since we have enforced the condition $\Psi(1) = 0$, we see from above that the first of these two determinants must vanish, and so A must be singular. It can be shown that

$$\det B = \beta \prod_{i=1}^{N} c_i \prod_{\substack{r=1 \\ r \neq i}}^{N} (c_i^2 - c_r^2)$$

for some $\beta \neq 0$ independent of the nodes $\{c_i\}_{i=1}^{2N}$. From the restrictions we have placed on the nodes, we see immediately that B must be non-singular. Let us now look at the determinant of $A - c_l B$. Since B is non-singular we can write

$$\det\,(A - c_l B) = \det\, B\, \det\,(B^{-1}A - c_l I_{2N})$$

where I_{2N} is the $2N \times 2N$ identity matrix. The idea now is to view this as an eigenvalue problem. The above determinant will vanish if and only if c_l is an eigenvalue of $B^{-1}A$. Since the nodes $\{c_i\}_{i=1}^{2N}$ are distinct and non-zero, our assumption that $\Psi(c_l) = 0$ for each $l \in \{1, \ldots, 2N\}$ is equivalent to the assumption that the eigenvalues of $B^{-1}A$ are $\{c_1, \ldots, c_{2N}\}$. A simple result from Linear Algebra states that the determinant of a matrix is equal to the product of its eigenvalues. Applying this result to the matrix $B^{-1}A$ gives

$$\prod_{i=1}^{2N} c_i = 0$$

which is nonsense in view of the conditions we have imposed on the nodes. Hence $\Psi(c_l)$ must be non-zero for at least one value of l in $\{1, \ldots, 2N\}$.

Method (ii) (when $c_i \neq 1$ for all $i \in \{1, \ldots, 2N\}$).

The polynomial Ψ now has $m + 3$ roots, namely $\{-1, 0, 1, c_1, \ldots, c_{2N}\}$. Since Ψ has degree at most $2N + 2$, we must have that $\Psi \equiv 0$. □

5.3.3 A simple error estimation technique

Before closing this section on order conditions we present a simple and cheap method of estimating the local truncation error in an arbitrary $2N$-point 2CHS method of order $2N$. Numerical results which show the effectiveness of this estimator are given at the end of this subsection.

Suppose we are given a $2N$-point 2CHS method of order $2N$ based on the nodes

$\{c_1, \ldots, c_N, -c_N, \ldots, -c_1\}$. We will write this method as

$$y_{n+c_i}^{2N} = (1+c_i)y_n - c_i y_{n-1} + h^2 \sum_{j=1}^{2N} A_{ij}^{2N} f_{n+c_j}^{2N} \quad i = 1, \ldots, 2N \tag{5.87}$$

$$y_{n+1}^{2N} = 2y_n - y_{n-1} + h^2 \sum_{j=1}^{N} A_{2N+1,j}^{2N} \left(f_{n+c_j}^{2N} + f_{n-c_j}^{2N} \right) \tag{5.88}$$

We associate with this method the operators $\mathcal{L}_i^{2N}[y(x)]$ and $\delta_i^{2N}[y(x)]$, for $i = 1, \ldots, 2N+1$, as defined in section 5.3.1. The superscript '2N' has been used in the above definitions to reinforce the fact that these quantities are associated with the $2N$-point method.

We now consider the $2N+1$-point 2CHS method based on the collocation nodes $\{c_1, \ldots, c_N, 0, -c_N, \ldots, -c_1\}$, with $\{c_1, \ldots, c_N\}$ the same as for the above $2N$-step method. Using the same notation as above, we may write the final stage of this method as

$$y_{n+1}^{2N+1} = 2y_n - y_{n-1} + h^2 \sum_{j=1}^{N} A_{2N+2,j}^{2N+1} \left(f_{n+c_j}^{2N+1} + f_{n-c_j}^{2N+1} \right) + h^2 A_{2N+2,N+1}^{2N+1} f_n \tag{5.89}$$

By construction, this method has order at least $2N+2$. Our idea is now to replace the values $f_{n\pm c_i}^{2N+1}$ in (5.89) by the values $f_{n\pm c_i}^{2N}$ computed from the $2N$-point method above. Let

$$\bar{y}_{n+1}^{2N+1} = 2y_n - y_{n-1} + h^2 \sum_{j=1}^{N} A_{2N+2,j}^{2N+1} \left(f_{n+c_j}^{2N} + f_{n-c_j}^{2N} \right) + h^2 A_{2N+2,N+1}^{2N+1} f_n.$$

and define the local truncation error in $\bar{y}_{n+1}^{2N+1}$ to be

$$\bar{\delta}_{2N+1}^{2N+1}[y(x_n)] = y(x_n + h) - \bar{y}_{n+1}^{2N+1}$$

with $y(x)$ a solution to the differential equation under consideration, and where we have assumed that $y(x_n) = y_n$ and $y(x_{n-1}) = y_{n-1}$. Using the operators $\mathcal{L}_i$ with the

appropriate superscripts, we may write $\bar{\delta}_{2N+1}^{2N+1}[y(x_n)]$ as

$$\begin{aligned}\bar{\delta}_{2N+1}^{2N+1}[y(x_n)] &= \mathcal{L}_{2N+2}^{2N+1}[y(x_n)] - h^2\frac{\partial f}{\partial y}(x_n, y(x_n))\sum_{j=1}^{N} A_{2N+2,j}^{2N+1}\left(\mathcal{L}_j^{2N} + \mathcal{L}_{2N+1-j}^{2N}\right) \\ &\quad + O(h^{2N+5})\end{aligned}$$

From our analysis above we know that the off-step approximations y_{n+c_i} generated by $2N$-point method have order at least $2N$, so that in general, $\bar{y}_{n+1}^{2N+1}$ will be an order $2N+2$ approximation for $y(x_{n+1})$. It is possible to express the leading term of this expansion in terms of the A_{ij} coefficients, and then write these as functions of the collocation nodes. It would appear from our numerical experiments that the value of the leading coefficient has a relatively minor effect on the accuracy of $\bar{y}_{n+1}^{2N+1}$, and so there seems to be little point in calculating it. The local truncation error in y_{n+1}^{2N} may now be estimated by looking at the difference

$$|\bar{y}_{n+1}^{2N+1} - y_{n+1}^{2N}|$$

This estimator turns out to be surprisingly accurate, as we will now demonstrate in the following examples.

Example 1 (Harmonic Oscillator)

In this example we consider the application of two 4-point 2CHS methods with corresponding error estimators to the standard test problem

$$y'' = -y, \quad y(0) = 1,\ y'(0) = 0$$

with solution $y(x) = \cos(x)$. Method 1 is found by taking $c_1 = 1$ and $c_2 = \frac{1}{2}$, and is given by

$$\begin{aligned} y_{n+\frac{1}{2}} - \tfrac{3}{2}y_n + \tfrac{1}{2}y_{n-1} &= \frac{h^2}{192}\left(32f_{n+\frac{1}{2}} + 52f_{n-\frac{1}{2}} - 5f_{n-1} - 7f_{n+1}\right) \\ y_{n-\frac{1}{2}} - \tfrac{1}{2}y_n - \tfrac{1}{2}y_{n-1} &= \frac{h^2}{576}\left(-4f_{n+\frac{1}{2}} - 64f_{n-\frac{1}{2}} - 5f_{n-1} + f_{n+1}\right) \end{aligned}$$

$$
\begin{aligned}
y_{n+1} - 2y_n + y_{n-1} &= \frac{h^2}{18}\left(10(f_{n+\frac{1}{2}} + f_{n-\frac{1}{2}}) - (f_{n-1} + f_{n+1})\right) \\
\bar{y}^5_{n+1} - 2y_n + y_{n-1} &= \frac{h^2}{60}\left((f_{n-1} + f_{n+1}) + 16(f_{n-\frac{1}{2}} + f_{n+\frac{1}{2}}) + 26f_n\right)
\end{aligned}
$$

This method has order 4, and is periodic for $\nu^2 \in (0,12) \cup (16,\infty)$. For method 2 we take $c_1 = 1/4$ and $c_2 = 3/4$ to get

$$
\begin{aligned}
y_{n-\frac{1}{4}} - \tfrac{3}{4}y_n - \tfrac{1}{4}y_{n-1} &= \frac{h^2}{1536}\left(9f_{n+\frac{1}{4}} - 108f_{n-\frac{1}{4}} - 2f_{n+\frac{3}{4}} - 43f_{n-\frac{3}{4}}\right) \\
y_{n+\frac{1}{4}} - \tfrac{5}{4}y_n + \tfrac{1}{4}y_{n-1} &= \frac{h^2}{1536}\left(44f_{n+\frac{1}{4}} + 161f_{n-\frac{1}{4}} - 3f_{n+\frac{3}{4}} + 38f_{n-\frac{3}{4}}\right) \\
y_{n-\frac{3}{4}} - \tfrac{1}{4}y_n - \tfrac{3}{4}y_{n-1} &= \frac{h^2}{1536}\left(6f_{n+\frac{1}{4}} - 57f_{n-\frac{1}{4}} - f_{n+\frac{3}{4}} - 92f_{n-\frac{3}{4}}\right) \\
y_{n+\frac{3}{4}} - \tfrac{7}{4}y_n + \tfrac{3}{4}y_{n-1} &= \frac{h^2}{1536}\left(399f_{n+\frac{1}{4}} + 462f_{n-\frac{1}{4}} + 28f_{n+\frac{3}{4}} + 119f_{n-\frac{3}{4}}\right) \\
y_{n+1} - 2y_n + y_{n-1} &= \frac{h^2}{48}\left(19(f_{n-\frac{1}{4}} + f_{n+\frac{1}{4}}) + 5(f_{n-\frac{3}{4}} + f_{n+\frac{3}{4}})\right) \\
\bar{y}^5_{n+1} - 2y_n + y_{n-1} &= \frac{h^2}{30}\left(13(f_{n-\frac{1}{4}} + f_{n+\frac{1}{4}}) + 3(f_{n-\frac{3}{4}} + f_{n+\frac{3}{4}}) - 2f_n\right)
\end{aligned}
$$

This method is also of order 4, and is periodic for $\nu^2 \in (0, 8.2196) \cup (13.1138, 32.0000)$ (to 4 d.p.). Note that for brevity we have suppressed the superscripts on all but the y^{2N+1}_{n+1} values.

The tables below show the results of applying these methods to the test problem above. The second and fourth columns of each table show the estimated LTE obtained from our estimator, while the third and fifth columns show the value of $\delta_5[y]$ with $y(x) = \cos(x)$. These tables show that the local truncation errors in method 2 are approximately 50 times smaller than those of method 1 at the output points. From our Taylor analysis above we find that the leading coefficients for these methods also differ by a factor of approximately 50. This is yet another example of the apparent conflict between the conditions required for higher accuracy, and those for improving the stability properties of a method.

There were two main factors that influenced our choice of stepsize for tables 5.1 and 5.2. We expect our error estimator to perform well when the stepsize is small, since

	Method 1		Method 2	
X	Est. LTE	LTE	Est. LTE	LTE
1.000	-2.8030×10^{-09}	-2.7991×10^{-09}	6.0672×10^{-11}	6.0840×10^{-11}
2.000	1.4578×10^{-09}	1.4557×10^{-09}	-3.1555×10^{-11}	-3.1642×10^{-11}
3.000	4.3782×10^{-09}	4.3721×10^{-09}	-9.4771×10^{-11}	-9.5032×10^{-11}
4.000	3.2734×10^{-09}	3.2688×10^{-09}	-7.0855×10^{-11}	-7.1051×10^{-11}
5.000	-8.4101×10^{-09}	-8.3985×10^{-09}	1.8205×10^{-11}	1.8255×10^{-11}
6.000	-4.1822×10^{-09}	-4.1764×10^{-09}	9.0527×10^{-11}	9.0777×10^{-11}
7.000	-3.6783×10^{-09}	-3.6731×10^{-09}	7.9619×10^{-11}	7.9839×10^{-11}
8.000	2.0742×10^{-09}	2.0714×10^{-09}	-4.4901×10^{-12}	-4.5025×10^{-12}
9.000	3.9024×10^{-09}	3.8970×10^{-09}	-8.4471×10^{-11}	-8.4705×10^{-11}
10.000	4.0095×10^{-09}	4.0040×10^{-09}	-8.6790×10^{-11}	-8.7030×10^{-11}

Table 5.1: Error estimator performance for $y'' = -y$ over a short integration interval, with $h = 0.1$.

	Method 1		Method 2	
X	Est. LTE	LTE	Est. LTE	LTE
1000	-2.8962×10^{-09}	-2.8914×10^{-09}	6.2674×10^{-11}	6.2847×10^{-11}
2000	1.2280×10^{-09}	1.2283×10^{-09}	-2.6625×10^{-11}	-2.6698×10^{-11}
3000	4.2779×10^{-09}	4.2729×10^{-09}	-9.2621×10^{-11}	-9.2876×10^{-11}
4000	3.5852×10^{-09}	3.5777×10^{-09}	-7.7550×10^{-11}	-7.7765×10^{-11}
5000	-2.4412×10^{-10}	-2.4885×10^{-10}	5.3964×10^{-12}	5.4089×10^{-12}
6000	-3.8598×10^{-09}	-3.8576×10^{-09}	8.3619×10^{-11}	8.3849×10^{-11}
7000	-4.0987×10^{-09}	-4.0900×10^{-09}	8.8655×10^{-11}	8.8901×10^{-11}
8000	-7.5175×10^{-10}	-7.4269×10^{-10}	1.6095×10^{-11}	1.6143×10^{-11}
9000	3.2529×10^{-09}	3.2547×10^{-09}	-7.0552×10^{-11}	-7.0744×10^{-11}
10000	4.4117×10^{-09}	4.4034×10^{-09}	-9.5448×10^{-11}	-9.5713×10^{-11}

Table 5.2: Error estimator performance for $y'' = -y$ over an extended integration interval, with $h = 0.1$.

it approximates only the leading term of the LTE. Before drawing any conclusions as to the usefulness of this estimator, we need to know how well it performs for "large" steplengths. Unfortunately, due to the low order of these methods, we must impose fairly tight bounds on the range of permitted stepsizes in order to keep the global truncation errors sufficiently small. As a compromise between these two conflicting requirements, we chose a steplength of 1/10. This steplength guarantees that the maximum global truncation errors over the interval $x \in [0, 10000]$ are bounded above by 2.25×10^{-3} in the case of Method 1, and 4.9×10^{-5} in the case of Method 2.

The results shown in these two tables are very encouraging. For this problem, our error estimator agrees to 2, or in some cases 3 significant digits with the actual local truncation errors.

Example 2 (Two Body Problem)

In this example we repeat the experiments of the previous example, but this time we will use as our test problem Kepler's Two-Body problem:

$$\begin{aligned} y'' + \frac{y}{r^3} &= 0 \qquad y(0) = 1 - e, \quad y'(0) = 0 \\ z'' + \frac{z}{r^3} &= 0 \qquad z(0) = 0, \qquad z'(0) = \sqrt{\left(\frac{1+e}{1-e}\right)} \end{aligned}$$

with $r^2 = y^2 + z^2$. This problem has exact solution

$$y(x) = \cos(E) - e, \qquad z(x) = \sqrt{1 - e^2}\sin(E)$$

where E is defined implicitly by

$$x = E - e\sin(E).$$

and e is taken to be 0.1. The results of our experiments are shown in the table below. The format of this table is the same as that used in Example 1, except that here we quote that component of the LTE which has largest absolute value at the output

points. For these experiments we chose our steplength to be 0.05. This was sufficient to guarantee that the maximum global truncation errors over the integration interval $x \in [0, 10000]$ were bounded above by 6.65×10^{-3} in the case of the first method, and 1.44×10^{-4} in the case of the second. Once again our error estimator performs surprisingly well.

	Method 1		Method 2	
X	Est. LTE	LTE	Est. LTE	LTE
1000	2.6942×10^{-10}	2.6943×10^{-10}	-5.8364×10^{-12}	-5.8433×10^{-12}
2000	9.4463×10^{-11}	9.4329×10^{-11}	-2.0406×10^{-12}	-2.0397×10^{-12}
3000	-3.0050×10^{-11}	-3.0073×10^{-11}	6.5015×10^{-13}	6.4945×10^{-13}
4000	-4.7849×10^{-11}	-4.8158×10^{-11}	1.0418×10^{-12}	1.0414×10^{-12}
5000	1.7515×10^{-10}	1.7671×10^{-10}	-3.8255×10^{-12}	-3.8276×10^{-12}
6000	5.1886×10^{-10}	5.1938×10^{-10}	-1.1240×10^{-11}	-1.1236×10^{-11}
7000	-5.1928×10^{-10}	-5.1927×10^{-10}	1.1236×10^{-11}	1.1234×10^{-11}
8000	1.8317×10^{-10}	1.8049×10^{-10}	-3.9053×10^{-12}	-3.9095×10^{-12}
9000	4.9741×10^{-11}	4.9053×10^{-11}	-1.0607×10^{-12}	-1.0608×10^{-12}
10000	-3.0172×10^{-11}	-3.0172×10^{-11}	6.5237×10^{-13}	6.5159×10^{-13}

Table 5.3: Error estimator performance for the two body problem over an extended integration interval, with $h = 0.05$.

These examples demonstrate the effectiveness of our error estimator for a non-linear problem as well as for the usual linear test problem. Without a full theoretical analysis, we are not in a position to make claims regarding the effectiveness of this estimator when applied to an arbitrary non-linear problem; however these results, and the relatively insignificant implementation costs, justify its inclusion in any code based on the 2CHS methods. Observe that good performance on a range of test problems is the only justification for the inclusion of several error estimators in modern ODE solvers.

5.4 Some two-step symmetric MCH methods

In this section we analyse in detail the order and stability properties of the 2-step MCH methods with 1, 2, 3 and 4 collocation nodes. Some of these methods have

already been analysed in the examples at the end of sections 5.1.2, 5.2.1 and 5.2.2; in these cases we give a summary of the results obtained.

The 2-step 1-point symmetric MCH method

The only method of this type is the linear multistep method

$$y_{n+1} - 2y_n + y_{n-1} = h^2 f_n$$

which has order two and is periodic for $\nu^2 \in (0,4)$. Observe that this method is equivalent to Euler's method applied to the first order system

$$y' = z, \qquad z' = f(x,y).$$

The 2-step 2-point symmetric MCH methods

The general method from this family is given in example 2 of section 5.1.2. The value $c_1 = 1/\sqrt{6}$ (0.4082 to 4d.p.) produces a method of order four which is periodic for $\nu^2 \in (0,6)$, all other methods from this family have order two. P-stable methods may be derived by taking $c_1 \in [1/\sqrt{2}, 1]$.

The 2-step 3-point symmetric MCH methods

The general method from this family takes the form

$$\begin{aligned} y_{n+1} - 2y_n + y_{n-1} &= \frac{h^2}{12c_1^2}(f_{n+c_1} + 2(6c_1^2 - 1)f_n + f_{n-c_1}) \\ y_{n\pm c_1} - (1 \pm c_1)y_n \pm c_1 y_{n-1} &= \frac{h^2(1 \pm c_1)}{\pm 24c_1}((3c_1^2 \mp 3c_1 + 1)f_{n\pm c_1} \\ &\quad +(5c_1^2 \pm c_1 - 1)f_n + (c_1^2 \mp c_1 - 1)f_{n\mp c_1}) \end{aligned}$$

In particular, notice that when $c_1 = 1$ this reduces to Numerov's method. Expanding the quantities $\mathcal{L}_i[y(x_n)]$, for $i = 1, \ldots, m+1$ as Taylor series, we obtain

$$\begin{aligned}
\mathcal{L}_4[y(x_n)] &= \frac{(2-5c_1^2)h^6 y^{(6)}(x_n)}{720} + O(h^8), \\
\mathcal{L}_1[y(x_n)] &= \frac{c_1(c_1^2-1)(7c_1^2-3)h^5 y^{(5)}(x_n)}{360} + O(h^6), \\
\mathcal{L}_3[y(x_n)] &= -\mathcal{L}_1[y(x_n)] + O(h^6).
\end{aligned}$$

Thus a method from this family will have order four, unless $c_1^2 = 2/5$, in which case it will have order six. The stability properties of methods from this family were investigated in example 2 of section 5.2.2. From that analysis we find that the sixth order method mentioned above is periodic for $\nu^2 \in (0, 20)$

The 2-step 4-point MCH methods

In view of the length and complexity of the coefficients involved, we will not give the general method from this family. Expanding the quantities $\mathcal{L}_i[y(x_n)]$, for $i = 1, \ldots, m+1$ as Taylor series, we obtain

$$\begin{aligned}
\mathcal{L}_5[y(x_n)] &= \frac{(30c_1^2c_2^2 - 5(c_1^2+c_2^2)+2)h^6 y^{(6)}}{720} \\
&\quad + O(h^8), \\
\mathcal{L}_1[y(x_n)] &= \frac{c_1(1+c_1)(5c_2^2(5c_1^2+5c_1-1) - 3c_1^4 + 3c_1^3 - 3c_1^2 - 2c_1 + 2)h^6 y^{(6)}}{1440} \\
&\quad + O(h^7), \\
\mathcal{L}_4[y(x_n)] &= \frac{c_1(c_1-1)(5c_2^2(5c_1^2-5c_1-1) - 3c_1^4 - 3c_1^3 - 3c_1^2 + 2c_1 + 2)h^6 y^{(6)}}{1440} \\
&\quad + O(h^7), \\
\mathcal{L}_2[y(x_n)] &= \frac{c_2(1+c_2)(5c_1^2(5c_2^2+5c_2-1) - 3c_2^4 + 3c_2^3 - 3c_2^2 - 2c_2 + 2)h^6 y^{(6)}}{1440} \\
&\quad + O(h^7), \\
\mathcal{L}_3[y(x_n)] &= \frac{c_2(c_2-1)(5c_1^2(5c_2^2-5c_2-1) - 3c_2^4 - 3c_2^3 - 3c_2^2 + 2c_2 + 2)h^6 y^{(6)}}{1440} \\
&\quad + O(h^7).
\end{aligned}$$

By construction, these methods have order at least four. Sixth order methods may be derived by requiring that the nodes satisfy

$$c_2^2 = \frac{2 - 5c_1^2}{5 - 30c_1^2}.$$

It is not possible to obtain a method of order eight from this family, instead we seek methods with order of dispersion eight. With the collocation nodes satisfying the above condition, we apply our method to the scalar test problem, and expand the quantity $\delta_{m+1}[y(x_n)]$ as a Taylor series to obtain

$$\delta_5[y(x_n)] = \frac{(630c_1^4 - 330c_1^2 + 13)\nu^8 \cos(\omega x_n)}{302400(6c_1^2 - 1)} + O(h^{10}).$$

Thus the method will have order of dispersion eight if $c_1^2 = (55 - 3\sqrt{235})/210$ and $c_2^2 = (55 + 3\sqrt{235})/210$.

The Routh-Hurwitz polynomial for methods from this family takes the form

$$R(\zeta) = a_2\zeta^2 + a_0$$

with a_2 and a_0 given by

$$\begin{aligned} a_0 &= 2\nu^4(2c_1^2c_2^2 - (c_1^2 + c_2^2) + 1) + 8\nu^2(c_1^2 + c_2^2 - 3) + 96 \\ a_2 &= 2\nu^4(c_1^2 + c_2^2 - 1) + 24\nu^2 \end{aligned}$$

We know from theorem 5.4 that every method from this family possesses a non-empty interval of periodicity, so we look for methods which are P-stable. From theorem 5 of Coleman [21], a fourth order method from this family will be P-stable if and only if

$$c_1^2 + c_2^2 \geq 3 \qquad \text{and} \qquad 2c_1^2c_2^2 - (c_1^2 + c_2^2) + 1 \geq 0$$

or

$$1 \leq c_1^2 + c_2^2 < 3 \qquad \text{and} \qquad c_1^4 - 22c_1^2c_2^2 + c_2^4 - 6(c_1^2 + c_2^2) - 3 < 0$$

Observe that since the nodes $\{c_1, c_2\}$ are required to lie in $[0,1]$, only the second of these conditions is relevant here. We have so far been unable to determine whether there are any P-stable sixth order methods from this family. The sixth order method with order of dispersion eight is periodic for $\nu^2 \in (0, 126/5)$.

If we require that $c_1 = 1$ then, from lemma 5.5 we know that all the resulting methods must be almost P-stable, and from theorem 5 of Coleman [21] the necessary and sufficient condition under which a fourth order method of this type is P-stable is

$$4 - 16c_2^2 + c_2^4 < 0$$

i.e. $c_2^2 \in (2(4-\sqrt{15}), 1]$, or $c_2 \in (0.5040, 1)$ (4 d.p.). The sixth order method of this type is periodic for $\nu^2 \in (0, 7.2133) \cup (55.4534, \infty)$.

5.5 Numerical results

In this section we present the results of a number of numerical experiments in which symmetric two-step MCH methods with 2,3 and 4 collocation nodes were applied to both linear and non-linear test problems, these results are then compared with those from the Panovsky-Richardson methods with comparable computational costs. All results given here were computed using FORTRAN double precision programs running on a Sun workstation.

Methods tested

The following methods are tested in this section:

M24: The 2-point 2CHS method of order four. This method is periodic for $\nu^2 \in (0, 6)$.

M34: A 3-point 2CHS method of order four. This method is periodic for $\nu^2 \in (0, 9.4641) \cup (0, 4641, 22.3924)$, (4d.p.).

M36: The sixth order 3-point 2CHS method. This method is periodic for

$\nu^2 \in (0, 20)$.

M44: A P-stable fourth order 4-point 2CHS method which nearly minimises the leading efficient in the local truncation error expansion.

M46: The sixth order, almost P-stable, 4-point 2CHS method with $c_1 = 1$. This method is periodic for $\nu^2 \in (0, 7.2133) \cup (55.4532, \infty)$, (4d.p.).

M468: The sixth order 4-point 2CHS method with order of dispersion eight. This method is periodic for $\nu^2 \in (0, 25.2)$.

The following Panovsky-Richardson methods, formulated as RKN methods, are also used:

RKN24: The degree 2 Panovsky-Richardson method. This method has order four and is periodic for $\nu^2 \in (0, 9.6) \cup (12, 48)$.

RKN34: The degree 3 Panovsky-Richardson method. This method has order four and is periodic for $\nu^2 \in (0, 9.8515) \cup (9.9868, 19.4629) \cup (25.0293, 33.1935)$.

RKN46: The degree 4 Panovsky-Richardson method. This method has order six and is periodic for $\nu^2 \in (0, 9.8673) \cup (9.8805, 19.5616) \cup (20.7558, 29.7766) \cup (43.7717, 54.1644)$, (4d.p.).

The harmonic oscillator

The results of applying all the methods mentioned above to the harmonic oscillator problem,

$$y'' = -y; \quad y(0) = 1, \; y'(0) = 0, \tag{5.90}$$

with the fixed steplength $h = 0.1$ are shown in table 5.4. As expected, method M468 is the most accurate for this problem. Also, since the error constants for the Panovsky-Richardson methods are somewhat smaller than those for the 2CHS methods used here, they are more accurate than the remaining 2CHS methods. Observe that, for this problem, method M36 is both more accurate and more efficient than the almost P-stable method M46. Though method M46 is almost P-stable, the gap between its primary and secondary intervals of periodicity is rather large, and its primary interval

is approximately a third of the length of that for method M36.

x	M24	M34	M44	RKN24	RKN34
1	1.58 E-07	4.86 E-08	1.77 E-07	4.38 E-08	3.65 E-09
2	3.60 E-07	1.11 E-07	4.05 E-07	9.47 E-08	7.90 E-09
5	9.83 E-07	3.03 E-07	1.10 E-06	2.51 E-07	2.09 E-08
10	1.63 E-06	5.02 E-07	1.83 E-06	4.12 E-07	3.44 E-08
20	3.79 E-06	1.17 E-06	4.26 E-06	9.50 E-07	7.93 E-08
50	1.01 E-05	3.12 E-06	1.14 E-05	2.54 E-06	2.11 E-07
100	2.06 E-05	6.34 E-06	2.31 E-05	5.15 E-06	4.29 E-07

x	M36	M46	M468	RKN46
1	1.63 E-11	7.84 E-11	2.66 E-15	4.35 E-13
2	3.72 E-11	1.79 E-10	7.05 E-15	9.39 E-13
5	1.01 E-10	4.88 E-10	1.95 E-14	2.49 E-12
10	1.68 E-10	8.09 E-10	3.23 E-14	4.09 E-12
20	3.91 E-10	1.88 E-09	6.97 E-14	9.43 E-12
50	1.05 E-09	5.03 E-09	1.89 E-13	2.52 E-11
100	2.13 E-09	1.02 E-08	3.78 E-13	5.11 E-11

Table 5.4: Maximum absolute errors on intervals $[0, x]$ for problem (5.90) with steplength $h = 0.1$.

The Stiefel-Bettis problem

As our second test problem we take the Stiefel-Bettis problem

$$z'' + z = 0.001e^{ix}; \quad z(0) = 1, \; z'(0) = 0.9995i, \tag{5.91}$$

which has solution

$$z = (1 + 0.0005ix)e^{ix}.$$

Table 5.5 shows the results obtained by applying the methods mentioned above, and two methods, T4 and T6, due to Thomas [60]. In each case the number tabulated is the error in approximating $|z(40\pi)| = (1 + 0.0004\pi^2)^{1/2}$. Method T4 is a fourth order method with order of dispersion six, and method T6 is sixth order with order of dispersion eight. The results for methods RKN24, RKN34, RKN46, T4 and T6 are taken from table 3.4 from section 3.6. Once again, Thomas' method T4, with

h	M24	M34	M44	RKN24	RKN34	T4
$\pi/2$	5.19 E-02	-2.53 E-02	-3.61 E-02	-1.17 E-02	-1.11 E-03	
$\pi/4$	3.15 E-03	-1.06 E-03	-3.39 E-03	-7.53 E-04	-6.58 E-05	-7.15 E-05
$\pi/8$	1.96 E-04	-6.11 E-05	-2.16 E-04	-4.81 E-05	-4.06 E-07	-7.94 E-07
$\pi/16$	1.22 E-05	-3.75 E-06	-1.36 E-05	-3.03 E-06	-2.53 E-07	-1.35 E-08

h	M36	M46	M468	RKN46	T6
$\pi/2$	-1.76 E-03	6.24 E-03	-7.44 E-05	-2.95E-05	
$\pi/4$	-2.12 E-05	9.69 E-05	-2.39 E-07	-4.71E-07	-5.61 E-06
$\pi/8$	-3.14 E-07	1.49 E-06	-9.58 E-10	-7.40E-09	-1.45 E-08
$\pi/16$	-4.85 E-09	2.33 E-08	-4.70 E-12	-1.16E-10	7.60 E-09

Table 5.5: Errors in approximating $|z(40\pi)|$ for problem (5.91).

its advantage of higher order of dispersion, is the most accurate of the fourth order methods. For the sixth order 2CHS methods, only method M468, which, like T6, has order of dispersion eight, is more accurate than method T6. In fact, for the smaller steplengths, the accuracy, for this problem, of method M468 is comparable to that of the degree 5 Panovsky-Richardson method.

The two-body problem

For our non-linear test-problem we take Kepler's two-body problem

$$y'' + y/r^3 = 0, \qquad y(0) = 1 - e, \qquad y'(0) = 0 \tag{5.92}$$

$$z'' + z/r^3 = 0, \qquad z(0) = 0, \qquad z'(0) = \sqrt{(1+e)/(1-e)} \tag{5.93}$$

with $r^2 = y^2 + z^2$.

Table 5.6 shows the results obtained by applying our 2CHS methods and the Panovsky-Richardson methods to this problem with the fixed steplength $h = 0.1$. Of the fourth order 2CHS methods, method M34 is once again the most accurate, having errors approximately equal to those of RKN24, though both of these are larger than those for RKN34. Method M46 is once again the poorest of the sixth order methods, and it seems that, for this problem and this steplength, the higher order of dispersion of method M468 is less beneficial than the low error constant for method RKN46.

x	M24	M34	M44	RKN24	RKN34
1	1.82 E-06	3.74 E-07	1.36 E-06	2.47 E-07	2.67 E-08
2	7.57 E-06	2.12 E-06	7.73 E-06	3.87 E-07	1.52 E-07
5	2.50 E-05	1.44 E-05	5.26 E-05	9.77 E-07	9.85 E-07
10	5.18 E-05	1.89 E-05	6.91 E-05	2.83 E-06	1.29 E-06
20	8.67 E-05	5.65 E-05	2.07 E-04	8.39 E-06	3.86 E-06
50	2.61 E-04	1.44 E-04	5.27 E-04	2.11 E-05	9.81 E-06
100	5.42 E-04	2.83 E-04	1.04 E-03	4.18 E-05	1.93 E-05

x	M36	M46	M468	RKN46
1	3.32 E-10	2.50 E-09	1.63 E-10	1.17 E-11
2	1.38 E-09	6.58 E-09	7.80 E-10	1.17 E-11
5	9.12 E-09	1.14 E-08	3.93 E-09	1.79 E-10
10	1.21 E-08	3.69 E-08	5.61 E-09	3.02 E-10
20	3.61 E-08	6.25 E-08	1.39 E-08	9.05 E-10
50	9.19 E-08	1.90 E-07	3.55 E-08	2.29 E-09
100	1.81 E-07	3.95 E-07	6.97 E-08	4.52 E-09

Table 5.6: Maximum absolute errors on intervals $[0, x]$ for problem (5.92)-(5.93) with steplength $h = 0.1$.

In chapter 3 we observed that the global errors in the Panovsky-Richardson methods appeared to exhibit a near-linear dependence on the length of integration interval. To see if this is the case for any of our 2CHS methods we repeated our computations with much larger integration intervals. The results from these computations are shown in figure 5.1, for the fourth order methods, and figure 5.2 for the sixth order methods. From these figures we see that the long-term global error for these methods, as in the case of the Panovsky-Richardson methods, does exhibit a near linear dependence on the length of the integration interval. We still have no explanation as to why this is the case.

Of the MCH methods considered in this section, the P-stable method M44 is the least accurate and most inefficient method for these problems. The most accurate method is, as expected the sixth order method M468 with order of dispersion eight. The other method which stands out is method M36. This method has a sizeable interval of periodicity, requires only two new function evaluations per iteration, and is more accurate, for the problems considered here, than both the remaining MCH methods and the Panovsky-Richardson methods of degrees 2 and 3.

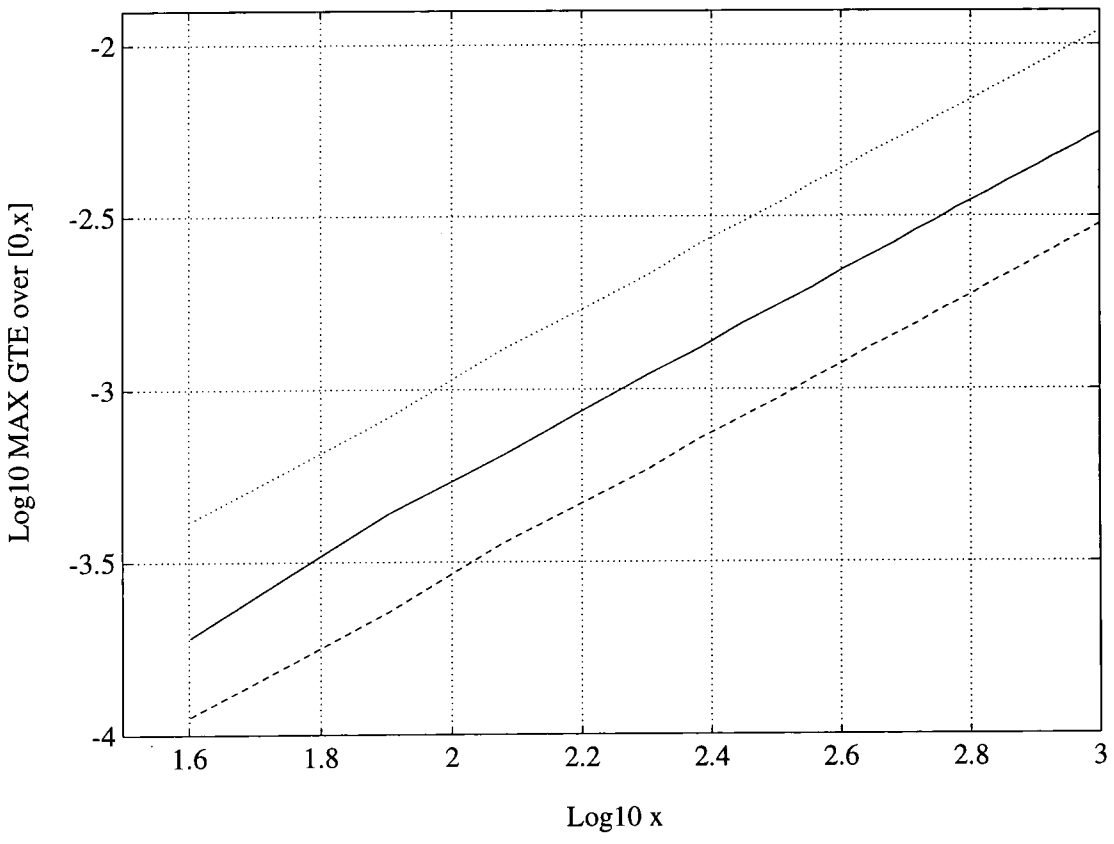

Figure 5.1: Long-term propagation of the maximum global errors in the methods M24, M34 and M44 when applied to problem (5.92)-(5.93) with steplength $h = 0.1$. Solid line = M24, dashed line = M34, dotted line = M44.

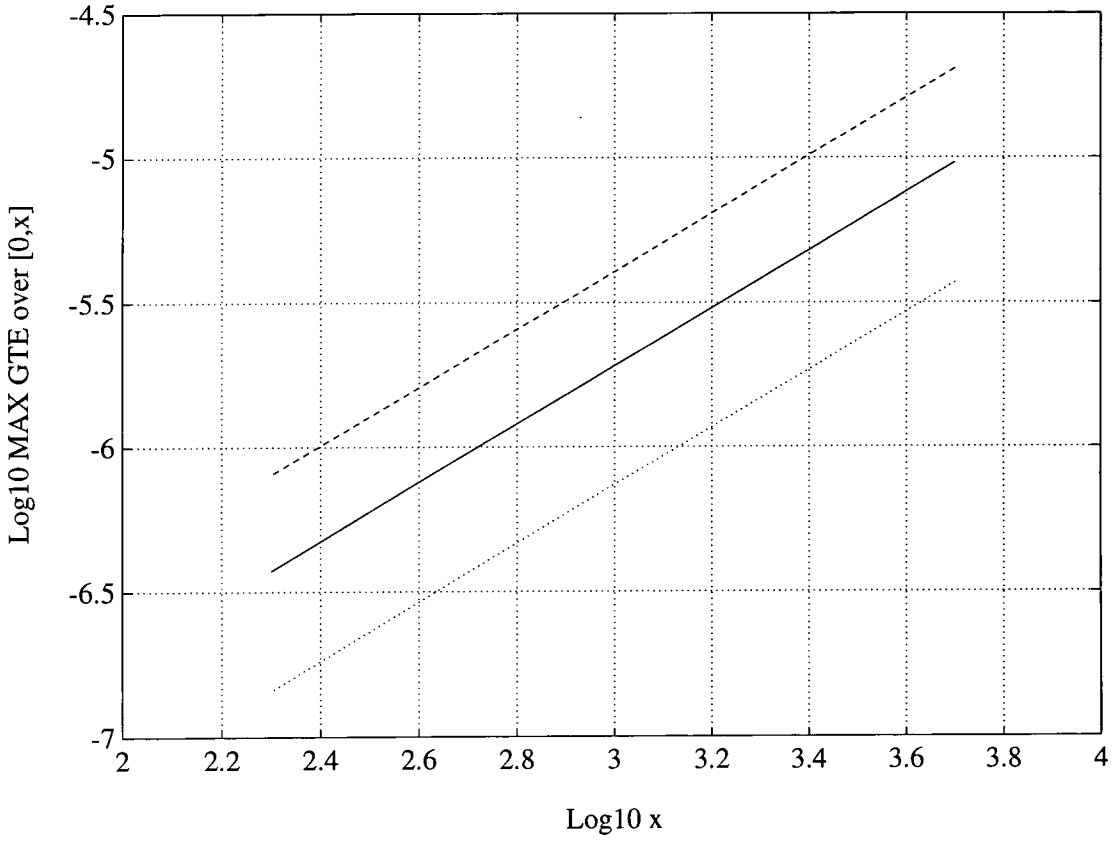

Figure 5.2: Long-term propagation of the maximum global errors in the methods M36, M46 and M468 when applied to problem (5.92)-(5.93) with steplength $h = 0.1$. Solid line = M36, dashed line = M46, dotted line = M468.

5.6 Conclusion

We have shown how to construct multistep collocation-based hybrid methods with arbitrary stepnumber k and number of collocation nodes m, and have given expressions for the coefficients of these methods.

Conditions have been derived for a two-step $2N$-point or $2N+1$-point symmetric MCH method to have order $2N+4$, and we have used these conditions to derive superconvergent methods with 2,3 and 4 collocation nodes. We have also given a simple and inexpensive local truncation error estimator for the $2N$-point methods of order $2N$ and demonstrated its effectiveness using a number of test problems.

The stability properties of the two-step symmetric MCH methods have been investigated and, in particular, we have given conditions under which a method with an even number of collocation nodes is almost P-stable. We have also succeeded in deriving P-stable methods with 2 and 4 collocation nodes. The two-step symmetric MCH methods considered require the same computational effort as the methods of Panovsky & Richardson of degree m, but in chapter 3 we showed that none of the Panovsky-Richardson methods are P-stable.

Numerical results have demonstrated an apparent conflict between the requirements of high accuracy and P-stability for these methods. These results suggest that the P-stable MCH methods are reserved for problems which are known to be stiff, and that the superconvergent methods which are not required to be stable at infinity, but which possess sizable intervals of periodicity, are used for non-stiff problems.

The results in this chapter are very encouraging and, in our opinion, certainly justify further investigation of these methods.

Chapter 6

Conclusion and areas for further research

The work of Panovsky & Richardson has given us an interesting family of methods for the initial value problems with which we are concerned here. In chapter 3 we investigated their order and stability properties, and also showed that they are equivalent to collocation-based Runge-Kutta-Nyström methods. In our numerical tests these methods performed very well, and were shown to be more accurate than some established methods. Of particular interest was the near-linear dependence of the global error upon the length of integration interval which these methods exhibited. This same near-linear dependence was also observed for the two-step symmetric MCH methods of chapter 5, but not for the explicit Runge-Kutta-Nyström methods used in chapter 3. The identification of the properties of a method which distinguishes between linear and quadratic error growth we leave as a problem for further research.

In chapters 4 and 5 we derived and analysed two families of multistep collocation methods. The stability polynomial for these methods was found, and we also went some way to investigating their order. The multistep Runge-Kutta-Nyström methods of chapter 4 were the most difficult to analyse, and the specific methods considered were inferior to the Panovsky-Richardson methods of chapter 3 in the areas of both accuracy and stability. The derivation of order conditions for MCRKN methods for

arbitrary k and m, and an answer to the question of whether the poor performance observed is common to all methods of this type we leave as challenges for future work.

The multistep hybrid methods of chapter 5, on the other hand, were seen to possess extremely good stability properties. We saw that, for the specific methods analysed, the conditions under which these methods were almost P-stable were considerably less restrictive than the conditions for the corresponding MCRKN methods to possess a non-vanishing interval of periodicity. The lack of derivative information did present a few problems in the analysis of the order of these methods, but the results that were obtained were sufficient for a complete investigation of the two-step symmetric MCH methods with 1,2,3 and 4 collocation nodes. Numerical experiments showed that it is possible to derive efficient and useful methods from this family. As for the MCRKN methods above, we suggest the derivation of order conditions and the investigation of methods with higher stepnumber and number of collocation points as areas for further research.

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