DOTTORATO DI RICERCA

in

SCIENZE COMPUTAZIONALI ED INFORMATICHE

Ciclo XXII

Consorzio tra Università di Catania, Università di Napoli Federico II,
Seconda Università di Napoli, Università di Palermo, Università di Salerno

SEDE AMMINISTRATIVA: UNIVERSITÀ DI NAPOLI FEDERICO II

Two–step Runge–Kutta Methods for Ordinary and Stochastic Differential Equations

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TESI DI DOTTORATO DI RICERCA

To my Parents, the origin of who I'm

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Introduction

The aim of this research is the derivation and the analysis of high order efficient stable methods, both for Ordinary Differential Equations (ODEs) and Stochastic Differential Equations (SDEs), which are models of many important phenomena in life science. As an example let us consider two possible type of models in tumour growth, in which increasing attention has been devoted, as it is one of the main death causes in our society. Most studies stem out of population growth models mathematically consisting of one or more differential equations. Such models proved to be appropriate to predict the evolution of numerous biological phenomena. Indeed, though simple, they often catch the essence of complicate interaction. Among the proposed models very frequent are those based on Gompertz growth. It models the growth of population consisting of a group of individuals of one or more similar species in the absence of migration and interaction with other species. Gompertz law exhibits an exponential trend around the origin. Such feature is in agreement with observed tumor growth showing that for small tumors growth speed is such that immunitary system is not effective, [43]. However, it should be stressed that quite often discrepancies exist between clinical data and theoretical predictions, due to more or less intense environmental fluctuations. To disregard such fluctuations would lead to incorrect predictions which, in some cases, would suggest inadequate therapies. In order to take into consideration such environmental fluctuations the notion of growth in random environment has been formulated (see, for instance, [84]

and references therein). This growth is accomplished in substituting the intrinsic fertility in the growth equation with a normal delta correlated process whose mean is taken as representative of population fertility. Thus, the growth process can be described by a stochastic process, which is the solution of a stochastic differential equation, [1].

This thesis is mainly divided in two part. The first one is concerned with deterministic ODEs of first and second order, while the second part is devoted to the analysis of numerical approximation of SDEs.

The modeling of continuous time dynamical systems using ordinary differential equations is widely used in many fields of applications, as celestial mechanics, seismology, molecular dynamics (see for instance [82] and [101]) or in the semidiscretisation of partial differential equations. So we deal with high dimensional systems and stiffness. However in some cases more realistic models can be achieved if stochastic effects are taken into account. Many areas of application including microelectronics, signal processing and filtering, epidemiology, finance and insurance and several other fields need to be modeled by continuous time stochastic dynamics. As a result of this, Stochastic Differential Equations, as a generalisation of Ordinary Differential Equations, find application in diverse disciplines.

The first part of this thesis is concerned with the numerical approximation of Ordinary Differential Equations, in particular we consider the classical first order Initial Value Problem

$$\begin{cases} y'(x) = f(x, y(x)), \\ y(x_0) = y_0 \end{cases} \tag{I}$$

and the second order ODEs of special type

$$\begin{cases} y''(x) = f(x, y(x)), \\ y(x_0) = y_0, \\ y'(x_0) = y'_0, \end{cases} \tag{II}$$

having periodic or oscillatory solutions.

Let us consider the problem (I). For this problem there is a broad literature, [25], [52], [53], [56], [65], but the necessity of efficient and fast implementations make this topic still an open research area. We carry on with the derivation of continuous two-step Runge-Kutta methods, by an extension of the collocation technique. Two-step Runge-Kutta methods (TSRK) of the form

$$\begin{aligned} Y_i^{[n]} &= u_i y_{n-1} + (1-u_i) y_n + h \sum_{j=1}^{m} [a_{ij} f(x_{n-1} + c_j h, Y_j^{[n-1]}) \\ &+ b_{ij} f(x_n + c_j h, Y_j^{[n]})], \quad i = 1, ..., m, \qquad \text{(III)} \\ y_{n+1} &= \theta y_{n-1} + (1-\theta) y_n + h \sum_{j=1}^{m} [v_j f(x_{n-1} + c_j h, Y_j^{[n-1]}) \\ &+ w_j f(x_n + c_j h, Y_j^{[n]})], \qquad \text{(IV)} \end{aligned}$$

$n = 1, 2, ..., N-1$, were introduced by Jackiewicz and Tracogna in 1995, [57]; in the last decades they are further investigated by several scientists as Bartoszewski [5], [6], [7], [8], [9], [10], Verner [59], Tracogna [97], Welfert [98]. The interest in TSRK methods is due to the presence of many parameters as well as to the fact that, advancing from x_n to x_{n+1}, we only have to compute $Y^{[n]}$, because $Y^{[n-1]}$ was already evaluated in the previous step. Thus the computational cost of the method depends on the matrix coefficient B, while the matrix A adds extra degrees of freedom, without any need for extra function evaluations.
The collocation technique, introduced by Guillou and Soulé in 1969, [50], provides a continuous methods (having uniform order) on the whole interval of integration and not only at the gridpoints $\{x_n\}$.

As concerning second order differential equations, even if the problem can be solved by transforming it into a system of first order ODEs of double dimension, the development of numerical methods for its direct integration seems more natural and

efficient. The methods we have considered are of the following type

$$Y_i^{[n]} = (1+c_i)y_n - c_i y_{n-1} + h^2 \sum_{j=1}^{s} a_{ij} f(x_n + c_j h, Y_j^{[n]}), \quad i = 1, ..., s \quad \text{(V)}$$

$$y_{n+1} = 2y_n - y_{n-1} + h^2 \sum_{j=1}^{s} b_j f(x_n + c_j h, Y_j^{[n]}). \quad \text{(VI)}$$

introduced by Coleman in [30]. Also in this case we provide a new class of algebraic collocation methods. Classical numerical methods for ODEs relied on polynomials may not be very well-suited to periodic or oscillatory behaviour. In the framework of exponential fitting many numerical methods have been adapted in order to exactly integrate basis of functions other than polynomials, for instance the exponential basis (see [55] and references therein contained), in order to catch the oscillatory behaviour. The parameters of these methods depend on the values of frequencies, which appear in the solution. In order to adapt the collocation technique [52], [63] to an oscillatory behaviour, the collocation function has been chosen as a linear combination of trigonometric functions [78] or of powers and exponential functions [31]. Many modifications of classical methods have been presented in the literature for problem (II): exponentially-fitted Runge-Kutta methods (see for example [46], [99]), or trigonometrically-fitted Numerov methods [45], [100] and many others (for a more extensive bibliography see [55] and references in the already cited papers).

The second part of the present thesis is devoted to the numerical approximation of the solution of stochastic ordinary differential equations (SDEs) in Itô form

$$X(\tau)\Big|_0^t = \int_0^t f(\tau, X(\tau))\,\mathrm{d}\tau + \int_0^t G(\tau, X(\tau))\,\mathrm{d}W(\tau),\ X(0) = X_0,\ t \in [0,T], \quad \text{(VII)}$$

where W denotes an s-dimensional Wiener process given on the probability space $(\Omega, \mathcal{F}, P)$ with a filtration $(\mathcal{F}_t)_{t\geq 0}$. The drift and diffusion functions are given as $f : [0,T]\times\mathbb{R}^d \to \mathbb{R}^d$ and $G = (g_1, \ldots, g_s) : [0,T]\times\mathbb{R}^d \to \mathbb{R}^{d\times s}$ respectively. It is assumed that the initial value X_0 is $\mathcal{F}_0$-measurable, independent of the Wiener process and possesses finite second moments. We assume that there exists a path-wise unique

strong solution $X(\cdot)$ of (VII), see [68]. The aim of this research is to derive a new class of high order efficient methods of Runge-Kutta type, for strong approximation. There is a rich literature on stochastic Runge-Kutta schemes. In one of the first papers on this topic, Rümelin [91] considered the mean-square convergence of explicit Runge-Kutta schemes, where only increments of the Wiener process were used for the approximation of the diffusion term. He proved that the stochastic improved Euler (or Heun) scheme converges in the mean-square sense to the solution of the Stratonovich version of the SDEs (VII). For SDEs with a scalar Wiener process or with commutative noise the order of mean-square convergence of this scheme is 1. He also treated scalar SDEs as well as systems of equations driven by a multi-dimensional Wiener process. In the papers [17], [18], [19], [21], [22] the authors also have studied classes of stochastic Runge-Kutta methods for Stratonovich SDEs and have developed schemes up to order 1.5 in the mean-square sense. To obtain appropriate order conditions in a systematic way they have generalised the theory of Butcher trees to the stochastic setting.

An approach to approximate Itô and Stratonovich SDEs with a scalar Wiener process with convergence of order 1 is presented in [72]. For the Itô case this goal is achieved by including terms into the schemes that involve the square root of the step-size. Additionally using terms that involve mixed classical stochastic integrals, schemes with order 1.5 are developed in [86] for Itô SDEs with scalar noise. Further, strong convergence of stochastic Runge-Kutta methods and Runge-Kutta-type methods have been discussed in [15], [62], [71]. In the context of weak approximations of SDEs stochastic Runge-Kutta methods have been studied, e.g., in [85], [87], [88], [89], [90]. The starting point in the construction of new methods is the derivation of order conditions. In this context there are mainly two way to do this:

- Taylor expansions, widely introduced and used by Kloeden [62].

- Butcher trees, extended in the stochastic framework by Burrage and Burrage

[22]. They expanded the rooted trees theory, well known in the deterministic context, [25], by the use of bi-coloured nodes for the stochastic setting.

We have extended the classical approach introduced by Albrecht in 1987, [2], in the deterministic context. Applying Albrecht's approach to a Stochastic Runge–Kutta method we are able to linearise it and so we can carry out our analysis as done in the context of multistep linear methods, [13], [14], [95]. Moreover we are also able to provide stage order conditions, up to now never considered.

The present thesis is divided into 5 chapters: chapters 1 and 4 are respectively an introduction to the first and the second part, while the main results in chapters 2, 3 and 4 are original.

In *chapter 1* we recall, just for completeness, some preliminary notions on Runge-Kutta methods, Two-step Runge-Kutta methods and General Linear Methods.

In the *second chapter* we introduce a new class of two-step collocation methods for first order ODEs. We derive continuous order conditions, proving that our new methods have uniform order $2m + 1$, where m is the number of stages. We carry out the linear stability analysis, but we did not found A-stable methods within this class. In order to improve the stability properties, we relax the collocation technique and we obtain A-stable and L-stable methods. At the end we give some numerical experiments, in order to confirm the theoretical properties of the new classes of methods, [37], [38], [41].

In the *third chapter* we derive collocation hybrid methods, with constant coefficients, for special second order ordinary differential equations having periodic or oscillatory solutions. As we done for first order ODEs, we derive continuous order conditions and analyse the linear stability properties, [39]. Then we adapt the coefficients of the two-step hybrid method to an oscillatory behaviour, in such a way that it exactly integrates linear combinations of power and trigonometric functions depending on one and two frequencies, which we suppose can be estimated in ad-

vance. Frequency-dependent methods within this class have already been considered in [103], where the coefficients of methods were modified to produce phase-fitted and amplification-fitted methods. We show the constructive technique of methods based on trigonometric and mixed polynomial fitting and consider the linear stability analysis of such methods. Then we carry out some numerical experiments underlining the properties of the derived classes of methods, [40].

The *fourth chapter* is dedicated to an introduction to stochastic ordinary differential equations. Since this is quite a new topic, we will recall the Itô calculus and the properties of multiple stochastic integrals.

The *chapter 5* is concerned to the derivation of order conditions for a new class of Stochastic Runge–Kutta methods, by an extension of Albrecht approach for SDEs. We rewrite our nonlinear Runge–Kutta method as a composition of linear multistep methods. We proceed as done in the linear case in order to derive order conditions also for the internal stages. We also show the advantages in the convergence framework, [12].

Acknowledgments

I would like to thank all those who helped me with scientific suggestions and discussions but also with human encouragements.

I would like to express my sincere gratitude to Dr. Giovanni Capobianco for sharing the enthusiasm he puts in his work.

I am deeply grateful to Prof. Elvira Russo, who followed, during my Ph.D., my research activity.

I would especially like to thank Prof. Beatrice Paternoster for having followed my work; I am very grateful for her suggestions, constructive comments and for her warm support.

During my Ph.D. I spent six months as a guest of the Department of Mathematics (Macs) at Heriot-Watt University in Edinburgh. A special thanks to Dr. Evelyn Buckwar for inviting me, for her stimulating guidance and for providing such a warm weather. I would like to express my gratitude to Macs Department for providing me with all the best facilities of working environment. I also thanks the 'Dottorato in Scienze Computazionali e Informatiche' for giving me the possibility to visit Macs Department.

I would express my sincere thanks to the '*Na-Sa*' research group and to the '*Stochastic*' research group (in HWU): I am very happy to be one of them; the scientific discussions, rich of critical remarks, corrections and hints, as well as the life meetings with them improved a lot my research work during these years.

I am grateful to all the scientists I met during these years: their passion in research activity strengthen the enthusiasm for my work.

Finally I wish to thank all my friends and colleagues of the DMI (Università di Salerno), of the DMA (Università di Napoli Federico II) and of the Heriot-Watt University for having established a very jovial work atmosphere.

Last but not least my special thanks to my family and to Antonietta who patiently supported me!

'Mathematics knows no races or geographic boundaries;
for mathematics, the cultural world is one country',
David Hilbert

ORDINARY DIFFERENTIAL EQUATIONS

Chapter 1

Preliminary notions

In this chapter we recall some known notions concerning Runge–Kutta methods, classic collocation technique, multistep Runge–Kutta methods which we need in the future chapters. Then we discuss about the numerical approximation of second order Initial Value Problems via Runge–Kutta–Nyström methods and collocation methods.

1.1 Introduction

Let us consider the Initial Value Problem

$$\begin{cases} y'(x) = f(x, y(x)), \\ y(x_0) = y_0. \end{cases} \tag{1.1.1}$$

It is assumed that there exists a unique solution $y(x)$ of the equation (1.1.1), on the interval $[x_0, X]$ of x where x_0 and X are finite.
All the classical numerical methods are based on the idea of discretization. The continuous interval $[x_0, X]$ is replaced by the discrete grid point $\{x_n\}$ defined by $x_n = x_0 + nh,\ n = 0, 1, 2, \ldots, N$; the parameter h is called the steplength. We will denote by y_n an approximation of the solution $y(x_n)$ at x_n

$$y(x_n) \approx y(x_n). \tag{1.1.2}$$

A numerical method is a difference equation involving the function f and a certain number of consecutive approximations $y_{n+j},\ j = 1, \ldots, k$, from which it will be possible to compute sequentially the sequence $\{y_n | n = 1, \ldots, N\}$. If $k = 1$ the method is called one-step method, otherwise multistep method.

Of all existent computational methods for the numerical solution of our initial value problem the easiest to implement is Euler's rule

$$y_{n+1} - y_n = hf(x_n, y_n). \tag{1.1.3}$$

It is an explicit one step method, so it requires no additional starting values and it is suitable for variable stepsize implementations. From a practical point of view it is limited because of its low order. In general an higher order can be achieved by sacrificing one-step nature (see *Linear Multistep Methods* (LMMs), [52], [53], [64], [65]) or linearity (see *Runge-Kutta methods* (RK), [25], [52], [53], [65]). The second one is the philosophy behind the methods proposed by Runge (1895), subsequently developed by Kutta (1901) and Heun (1900) and then analysed by Butcher, Burrage,

Hairer, Wanner, Jackiewicz and many other authors . The analysis of Runge–Kutta methods and the development of new ones are still an open research topic.

1.2 An Ordinary Differential Equations based model in tumour growth

If we glance through the past decades, we can outright notice a remarkable increase of interest in the area of mathematical modeling as applied to science, engineering, business and management, generally expressed through functional equations, which are the best way to describe evolution in time and space. In fact, the spread of diseases, the growth of biologic populations, the brain dynamics, elasticity and plasticity, heat conduction, fluid dynamics, scattering theory, seismology, biomechanics, game theory, control, queuing theory, design of electronic filters and many other problems from physics, chemistry, pharmacology, medicine, economics can be modeled through systems of ordinary differential equations. In particular, this kind of models can be found in the context of the following subjects: evolution of biological populations [73], [104], mathematical models in physiology and medicine [11], in particular in the context of oncogenesis [54], [96], spread of infections and diseases [60], economical sciences [44], analysis of signals [74].

We deal with problems whose theoretical investigation has been very wide in terms of existence, uniqueness, asymptotic analysis and stability of the solutions. Sometimes it is not possible to compute the analytic solution of a functional equation: for this reason it gets more and more important to develop numerical methods in order to solve these problems and make some special requirements on these methods, such as high order and strong stability properties.

Oncogenesis generally intends a cancer as the result of several mutations, giving some cells a selective growth advantage. In [96] the tumour growth is reduced to a simple set of rules according to which a normal cell becomes malignant. This point

of view has spread out in the field of cancer research, which is very often treated as a logical science, trying to understand and describe the behaviour of the disease through some underlying principles. This is the reason why the investigation can be done using mathematical tools: in this context, the evolutionary model is expressed through systems of ordinary differential equations that take into account the contribute of different elements to the cancer progression.

Even if many models for oncogenesis are based on stochastic differential equations, ordinary differential equations can also be a very accurate model for the cancer progression. In fact, the introduction of a stochastic component would not produce any change in the rates describing the cancer onset with respect to the ones given by a deterministic model. Moreover, when the aim is not the creation of a model that describes the variability of many different types of cancer all at once, ordinary differential equations are the easiest way to create a generic model to better understand the evolution of the disease.

The evolutionary model considered in [96] is the following

$$\frac{d\mathbf{y}}{dt} = (\text{diag}(\text{diag}(\mathbf{y^T k})^T \mathbf{b})\mathbf{M} + \text{diag}((\mathbf{b}-\mathbf{d})^T \mathbf{y}))\mathbf{S}(1 - a(\mathbf{y})\tfrac{P_{NM}}{10^6}) \times (1 - \tfrac{P_{NM}}{10^{13}}) + \mathbf{m}_m, \tag{1.2.1}$$

where $\mathbf{y} \in \mathbb{R}^{17}$ is a partitioned vector describing the whole cell populations: y_1 is related to normal cells, y_2, y_3 ... y_{15} describes the populations undergoing a mutation, y_{16} is the number of primary tumour cells and y_{17} is the number of metastatic cells. The vector $\mathbf{k}$ describes the mutation rates, i.e. k_i is the mutation rate for the population y_i. The vectors $\mathbf{b}$ and $\mathbf{d}$ respectively describe the birth and death rates, while $\mathbf{m}_m$ is the metastasis rate vector. The upper triangular matrix $\mathbf{M} \in \mathbb{R}^{17\times 17}$ contains the number of genes going from state i to state j, while the matrix $\mathbf{S} \in \mathbb{R}^{17\times 17}$ is related to non-normal, non-metastatic cells, i.e. cells undergoing mutations, which are denoted by P_{NM}, where $P_{NM} = \sum_{i=2}^{16} y_i$. The

logistic term $a(\mathbf{y})$, defined as $a(\mathbf{y}) = \begin{cases} 0, & \frac{P_A}{P_{NM}} > 10\%, \\ 1 & \text{otherwise}, \end{cases}$ expires when more than the 10% of the non-normal, non-metastatic cells are in angiogenesis mutations (the number P_A denotes the amount of cells in this situation).

1.3 An Overview on Classical Runge–Kutta Methods

Classical Runge-Kutta methods are non-linear one-step methods. Therefore there is no difficulty in changing the steplenght, but the structure of the local error is much more complicated and there exists no easy and cheap error estimate comparable with Milne's device, [25], [52], [53], [64], [65]. With Runge–Kutta methods it is hard to tell when to change the stepsize, but easy to change it.

A general m-stage Runge-Kutta method, [25], [52], [53], [65], is defined by

$$y_{n+1} = y_n + h \sum_{j=1}^{m} b_j f(x_n + c_j h, Y_j^{[n]}), \quad n = 0, 1, \ldots, N-1, \tag{1.3.1}$$

where

$$Y_i^{[n]} = y_n + h \sum_{j=1}^{m} a_{ij} f(x_n + c_j h, Y_j^{[n]}), \quad i = 1, 2, \ldots, m. \tag{1.3.2}$$

It is convenient to display the coefficients in the following form, known as a Butcher array

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array} = \begin{array}{c|ccc} c_1 & a_{11} & a_{12} & a_{1m} \\ c_2 & a_{21} & a_{22} & a_{2m} \\ \ldots & \ldots & \ldots & \ldots \\ c_m & a_{m1} & a_{m2} & a_{mm} \\ \hline & b_1 & b_2 & b_m \end{array}$$

with $c = [c_1, \ldots, c_m]^T$, $b = [b_1, \ldots, b_m]^T$, $A = [a_{ij}]$. We can do the following cataloguing:

1. *Explicit method:* $a_{ij} = 0, \quad j \geq i, \quad i, j = 1, 2, \ldots, m \iff A$ is strictly lower triangular. Each stage $Y_i^{[n]}$ is given explicitly in terms of previously computed stages $Y_j^{[n]}$, $j = 1, 2, \ldots, i-1$,

2. *Semi-implicit method:* $a_{ij} = 0, \quad j > i, \quad i, j = 1, 2, \ldots, m \iff A$ is lower triangular,

3. *Implicit method:* $a_{ij} = 0, \quad j = i, \quad i, j = 1, 2, \ldots, m \iff A$ is not lower triangular.

As it is known, the structure of the matrix A influences the computational cost of the method, that is the computational cost of the non linear stage system (1.3.2).

1.3.1 Major Definitions

Here we will list the definitions of the major properties we ask to the numerical methods for the approximation of solutions of ODEs, [65].

Definition 1.3.1

The method (1.3.1) is said to be convergent if, for all initial value problems such that the conditions of existence and uniqness of the solution are satisfied, it holds

$$\max_{0 \leq n \leq N} \|y(x_n) - y_n\| \to 0 \quad as \quad h \to 0. \tag{1.3.3}$$

Note that the starting value, as well as the solution, are required to be convergent. Now we turn to the question of what conditions a numerical method must satisfy if it is to be convergent. We would expect that one such condition would be that it has to be a sufficiently accurate representation of the differential system.

It would be an infinitely accurate representation if the difference equation (1.3.1) were satisfied exactly when we replaced the numerical solution y_{n+1} at x_{n+1} by the

exact solution $y(x_{n+1})$. We therefore take as a measure of the accuracy the value of the residual

$$R_{n+1} := y(x_{n+1}) - y(x_n) - h\sum_{j=1}^{m} b_j f(x_n + c_j h, y(x_n + c_j h)), \tag{1.3.4}$$

called local truncation error.

Definition 1.3.2

The method (1.3.1) is said to be consistent if, for all initial value problems having an unique solution, we have that

$$\lim_{\substack{h\to 0 \\ x=x_0+nh}} \frac{1}{h} R_{n+1} = 0. \tag{1.3.5}$$

Theorem 1.3.1

The necessary and sufficient condition for a general Runge–Kutta method to be consistent is

$$\sum_{i=1}^{m} b_i = 1 \tag{1.3.6}$$

Definition 1.3.3

If p is the largest integer such that $R_{n+1} = O(h^{p+1})$, we say that the method has order p.

Remark 1.3.1

Observe that if the method is consistent, it follows that it has at least order 1.

Although, it is known that convergence implies consistency, the converse is not true. It can happen that the method suffers an in-built instability which persists even in the limit as $h \to 0$ and prevents convergence. The form of stability concerned with the stability of the difference system in the limit as h goes to 0 is the zero-stability.

Definition 1.3.4

Let $\{\delta_n,\ n = 0, 1, ..., N\}$ and $\{\delta_n^*,\ n = 0, 1, ..., N\}$ be any two perturbations of the method (1.3.1), and let $\{z_n,\ n = 0, 1, ..., N\}$ and $\{z_n^*,\ n = 0, 1, ..., N\}$ be the

resulting perturbed solutions. Then if there exist constants S and h_0 such that, for all $h \in (0, h_0]$, whenever

$$\|z_n - z_n^*\| \leq S\epsilon, 0 \leq n \leq N, \tag{1.3.7}$$

$$\|\delta_n - \delta_n^*\| \leq S\epsilon, 0 \leq n \leq N, \tag{1.3.8}$$

we say that the method is zero-stable.

Zero-stability is concerned with the roots of the characteristic polynomial of the difference equation.

Definition 1.3.5

The methods is said to satisfy the root condition if all the roots of the characteristic polynomial have modulus less than or equal to unity, and those of modulus unity are simple.

Theorem 1.3.2

The necessary and sufficient condition for the method given by (1.3.1) to be zero-stable is that it satisfies the root condition.

It is obvious that a Runge–Kutta method always satisfies the root condition.

1.3.2 Linear Stability Theory

For some problems (as stiff problems) it can happen that for all fixed positive values of h, the errors produced by a convergent method increase step by step. In such situations, it is clear that the local errors are accumulating in an adverse fashion: we are dealing with a stability phenomenon. We need a stability theory which applies when h takes a fixed non-zero value. We can choose as test system $y' = Fy$, where $F \in \mathbb{R}^{d\times d}$ has distinct eigenvalues $\{\lambda_t, t = 1, 2, ..., d\}$ lying strictly in the negative half-plane, a condition which ensures that all solutions of the test system tend to zero as x tends to infinity. Since the eigenvalues of F are distinct there exists a non-singular matrix Q such that $Q^{-1}FQ = \Lambda = diag[\lambda_1, \lambda_2, ..., \lambda_d]$,

and by using a transformation $y = Qz$ we can show that it was enough to consider only the scalar test equation $y' = \lambda y$, where $\lambda \in \mathbb{C}$ and $\Re(\lambda) < 0$.

Linear stability was concerned with the question of whether or not the numerical solution of this scalar test equation tended to zero as n tended to infinity. If we apply the classical Runge–Kutta method (1.3.1) to the scalar test equation we obtain a one-step difference equation of the form

$$y_{n+1} = R(z)y_n, \tag{1.3.9}$$

where $z = h\lambda$. We call $R(z)$ the *stability function* of the method. It is clear that $y_n \to 0$ as $n \to \infty$ if and only if

$$|R(z)| < 1 \tag{1.3.10}$$

and the method is absolutely stable for whose values of z for which this condition holds. The region of the complex z-plane for which (1.3.10) holds is the region of absolute stability of the method.

Definition 1.3.6

A method is said to be A-stable if $R_A \supseteq \{z : R(z) < 0\}$.

Definition 1.3.7

A method is said to be $A(\alpha)$*-stable,* $\alpha \in (0, \pi/2)$ *if* $R_{A(\alpha)} \supseteq \{z : -\alpha < \pi - \arg z < \alpha\}$*; it is said to be* $A(0)$*-stable if it is* $A(\alpha)$*-stable for some* $\alpha \in (0, \pi/2)$.

Definition 1.3.8

A method is said to be L-stable if it is A−stable and, in addition, when applied to the scalar test equation $y' = \lambda y$*,* λ *a complex constant with* $\Re(\lambda) < 0$*, it yields* $y_{n+1} = R(h\lambda)y_n$*, where* $|R(h\lambda)| \to 0$ *as* $\Re(h\lambda) \to -\infty$.

For a complete theory on Runge–Kutta methods see [25], [52], [53], [65].

1.4 Order Conditions: Albrecht's approach

It is usual to derive order conditions for Runge–Kutta methods by using the well-established Butcher trees theory, [24], [25], [27]. A quite different approach has been proposed by Albrecht in 1987, [2]. An interesting feature of Albrecht's work is that it applies to Runge–Kutta methods the ideas already developed for linear multistep methods.
Here we give only the idea of Albrecht approach, full details can be found in [2]. Albrecht defined a general class of methods, the $\mathcal{A}$-methods, by

$$Z_{n+1} = \mathcal{A}Z_n + h\phi_f(x_n, Z_n, Z_{n+1}; h), \tag{1.4.1}$$

where

- $Z_{n+1} \in \mathbb{R}^{\sigma d}$, where d is the dimension of the system of differential equations;
- $\mathcal{A}$ is a $\sigma d \times \sigma d$ matrix;
- $\phi_f \in \mathbb{R}^{\sigma d}$ satisfies a Lipschitz condition with respect to its second and third arguments.

Observe that the class of $\mathcal{A}$-methods is very broad and encompasses. One of the features of this approach is that analysis in the case of scalar initial value problem yield all the order conditions for the system case. Thus we consider only the scalar initial value problem $y' = f(x, y),\ y_{x_0} = y_0$. Define Z_{n+1} and $F(x_n, Z_{n+1}; h) \in R^{m+1}$ by

$$\begin{aligned} Z_{n+1} &:= [Y_1^{[n]}, Y_2^{[n]}, \ldots, Y_m^{[n]}, y_{n+1}]^T \\ F(x_n, Z_{n+1}; h) &:= [f(x_n + c_1 h, Y_1^{[n]}), \ldots, f(x_n + c_m h, Y_m^{[n]}), f(x_{n+1}, y_{n+1}]^T \end{aligned} \tag{1.4.2}$$

and define $\mathcal{A}$ and $\mathcal{B}$ by

$$\mathcal{A} = \begin{pmatrix} 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & \cdots & 0 & 1 \\ & & \cdots & & \\ 0 & 0 & \cdots & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0_{mm} & e \\ 0_m & 1 \end{pmatrix}, \tag{1.4.3}$$

$$\mathcal{B} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1m} & 0 \\ a_{21} & a_{22} & \cdots & a_{2m} & 0 \\ & & \cdots & & \\ a_{m1} & a_{m2} & \cdots & a_{mm} & 0 \\ b_1 & b_2 & \cdots & b_m & 0 \end{pmatrix} = \begin{pmatrix} A & 0_m \\ b^T & 0 \end{pmatrix}, \tag{1.4.4}$$

where 0_{mm} is the $m \times m$ null matrix, 0_m is the null vector (column or row) in $\mathbb{R}^m$ and $e = [1, 1, \cdots, 1]^T \in \mathbb{R}^m$.

Thus the Runge–Kutta method can be written as an $\mathcal{A}$-method

$$Z_{n+1} = \mathcal{A}Z_n + h\mathcal{B}F(x_n, Z_n; h). \tag{1.4.5}$$

The essence of Albrecht approach is to observe that each of the m internal stages and the final stage of a Runge–Kutta method are linear, in the sense that all the stages can be seen as a linear multistep methods. We can regard each of the $m + 1$ stages as being a generalized linear multistep method and associate with it a linear difference operator, in the same way we did for a linear multistep method. Let $z(x)$ be a sufficiently differentiable arbitrary function and define L_i, $i = 1, 2, ..., m$ and $\hat{L}$ by

$$L_i[z(x); h] := z(x + c_i h) - z(x) - h \sum_{j=1}^{m} a_{ij} z'(x + c_j h), \tag{1.4.6}$$

$$\hat{L}[z(x); h] := z(x + h) - z(x) - h \sum_{j=1}^{m} b_j z'(x + c_j h). \tag{1.4.7}$$

Proceeding as it is usual for linear multistep methods, we expand $z(x+c_ih),\ z(x+h)$ and $z'(x+c_ih)$ around x and collect powers in h to obtain

$$\begin{aligned} L_i[z(x);h] &:= C_{i1}hz^{(1)}(x) + C_{i2}h^2z^{(2)}(x) + \cdots \\ \hat{L}[z(x);h] &:= \hat{C}_1hz^{(1)}(x) + \hat{C}_2h^2z^{(2)}(x) + \cdots \end{aligned} \tag{1.4.8}$$

with

$$C_{iq} = \frac{c_i^q}{q!} - \frac{1}{(q-1)!}\sum_{j=1} a_{ij}c_j^{q-1}, \quad i = 1,\ldots,m,\ q = 1,2,... \tag{1.4.9}$$

$$\hat{C}_q = \frac{1}{q!} - \frac{1}{(q-1)!}\sum_{j=1} b_jc_j^{q-1}, \quad q = 1,2,.... \tag{1.4.10}$$

We could define order in the same way as we did for a linear multistep method and say that the i-th internal stage, Y_i, has order p_i if $C_{i1} = C_{i2} = ... = C_{ip_i} = 0,\ C_{ip_{i+1}} = 0$ and the final stage has order p if $\hat{C}_1 = \hat{C}_2 = ... = \hat{C}_p = 0,\ \hat{C}_{p+1} = 0$. Note that the row-sum condition implies that $C_{i1} = 0,\ i = 1,2,...,m$, so that each internal stage has order at least 1, that is consistent.

1.5 Classical Collocation Methods

The idea of collocation is old and well known in Numerical Analysis [33], [52], [53], [65]. In order to advance from x_n to x_{n+1}, it is constructed an algebraic polynomial $P(x)$, which interpolates the numerical solution in the step point x_n, and satisfies the ODEs in the points $x_n + c_ih$, where $\{c_1, c_2, ..., c_m\}$ are m real numbers (typically between 0 and 1), that is

$$\begin{cases} P(x_n) = y_n, \\ P'(x_n + c_ih) = f(x_n + c_ih, P(x_n + c_ih)), \quad i = 1,2,...,m. \end{cases} \tag{1.5.1}$$

The solution in x_{n+1} is given by

$$y_{n+1} = P(x_{n+1}). \tag{1.5.2}$$

Conditions (1.5.1) define $P(x)$ uniquely.

Theorem 1.5.1 (Wright, 1970)

One–step collocation methods are a subset of implicit Runge-Kutta methods where

$$a_{ij} = \int_0^{c_i} L_j(t)dt, \qquad b_j = \int_0^1 L_j(t)dt, \qquad i,j = 1,2,...,m \tag{1.5.3}$$

and $L_j(t)$, $j = 1,...,m$, *are fundamental Lagrange polynomials*

$$L_j(t) = \prod_{i=j} \frac{t - c_i}{c_j - c_i}. \tag{1.5.4}$$

Proof:

To prove the thesis observe that $P'(x)$ is a polynomial of degree $m-1$, which interpolate the m data point $x_n + c_i h, P(x_n + c_i h),\ i = 1,2,...,m$. Define $Y_i^{[n]} = P(x_n + c_i h),\ i = 1,\dots,m$, on writing $x = x_n + th$, we have

$$P'(x_n + c_i h) = \sum_{j=1}^{m} L_j(t) f(x_n + c_i h, Y_i^{[n]}). \tag{1.5.5}$$

Now integrate with respect to x, from $x = x_n$ to $x = x_n + c_i h$, $i = 1,\dots,m$, and from $x = x_n$ to $x = x_{n+1}$, to get

$$P(x_n + c_i h) - P(x_n) = h \sum_{j=1}^{m} \int_0^{c_i} L_j(t)dt f(x_n + c_j h, Y_j^{[n]}), \quad i = 1,\dots,m,$$

and

$$P(x_{n+1}) - P(x_n) = h \sum_{j=1}^{m} \int_0^{1} L_j(t)dt f(x_n + c_j h, Y_j^{[n]}).$$

For $j = 1,\dots,m$, define

$$a_{ij} = \int_0^{c_i} L_j(t)dt, \quad b_j = \int_0^1 L_j(t)dt, \tag{1.5.6}$$

from (1.5.6) and (1.5.6) we derive

$$\begin{aligned} Y_i^{[n]} &= n_n + h \sum_{j=1}^{s} a_{ij} f(x_n + c_i h, Y_j^{[n]}), \\ y_{n+1} &= y_n + h \sum_{j=1}^{s} b_j f(x_n + c_i h, Y_j^{[n]}). \end{aligned} \tag{1.5.7}$$

Thus we have an implicit Runge–Kutta method, with the elements of c being the collocation points. ♢

Remark 1.5.1

Only some implicit Runge–Kutta methods are collocation methods.

Theorem 1.5.2

An implicit Runge–Kutta method, with distinct c_i and of order at least m is a collocation method iff

$$C(s): \quad \sum_{i=1}^{m} a_{ij} c_j^{q-1} = \frac{c_i^q}{q}, \quad i = 1, \ldots, m \quad q = 1, \ldots, s, \tag{1.5.8}$$

is true.

Proof:

$C(s)$ determines the a_{ij} uniquely. We write it as

$$\sum_{i=1}^{m} a_{ij} p(c_j) = \int_0^{c_i} p(t)dt \tag{1.5.9}$$

for all polynomials p of degree $\leq m-1$. $a_{ij} = \int_0^{c_i} L_j(t)dt$ satisfies the relation (1.5.9), because with this coefficients it is the Lagrange interpolation formula. $\diamondsuit$
Moreover the maximum attainable order is at most $2m$, and it is obtained by using Gaussian collocation points [52], [65].

1.6 Two-step Runge–Kutta Methods

Jackiewicz and Tracogna in 1995, in [57], introduced the Two–Step Runge–Kutta (TSRK) formulas that depend on stage values at two consecutive step points. These methods have the form

$$\begin{aligned} Y_i^{[n]} &= u_i y_{n-1} + (1-u_i) y_n + h \sum_{j=1}^{m} [a_{ij} f(x_{n-1} + c_j h, Y_j^{[n-1]}) \\ &\quad + b_{ij} f(x_n + c_j h, Y_j^{[n]})], \quad i = 1, ..., m, \end{aligned} \tag{1.6.1}$$

$$\begin{aligned} y_{n+1} &= \theta y_{n-1} + (1-\theta) y_n + h \sum_{j=1}^{m} [v_j f(x_{n-1} + c_j h, Y_j^{[n-1]}) \\ &\quad + w_j f(x_n + c_j h, Y_j^{[n]})], \end{aligned} \tag{1.6.2}$$

$n = 1, 2, ..., N-1$. The presence of extra parameters in the formula as compared to classical Runge-Kutta methods (1.3.1) makes it possible to construct high-order methods with relatively few stages. This big gain in efficiency makes them attractive for the solution of large systems of ODEs. To start this method we need in addition to y_0 the approximation y_1 at x_1 and stage values $Y_j^{[0]},\ j = 1, 2, ..., m$ on the first step $[x_0, x_1]$. These values could be computed, for example, by Runge–Kutta methods of appropriate orders. As usual it is convenient to represent the method (1.6.2) by the table of coefficients

$$\begin{array}{c|cc} u & A & B \\ \hline \theta & v^T & w^T \end{array} = \begin{array}{c|cccc|cccc} u_1 & a_{11} & a_{12} & \dots & a_{1m} & b_{11} & b_{12} & \dots & b_{1m} \\ u_2 & a_{21} & a_{22} & \dots & a_{2m} & b_{21} & b_{22} & \dots & b_{2m} \\ & & & \dots & & & & \dots & \\ & & & \dots & & & & \dots & \\ & & & \dots & & & & \dots & \\ u_m & a_{m1} & a_{m2} & \dots & a_{mm} & b_{m1} & b_{m2} & \dots & b_{mm} \\ \hline \theta & v_1 & v_2 & \dots & v_m & w_1 & w_2 & \dots & w_m \end{array}$$

with $c = (A + B)e - u,\ e = [1, ..., 1]^T \in R^m$. Observe that in advancing from x_n to x_{n+1} we need only compute $Y_j^{[n]}$ since $Y_j^{[n-1]}$ were already evaluated in the previous step. Only the matrix B determines the implementation costs of the TSRK method. Thus we gain extra degrees of freedom associated with a two-step scheme without the need of extra function evaluations.

In [57] general order conditions are derived using the approach proposed by Albrecht, there are also some examples of methods up to the order 5. This general class of TSRK methods was investigated in [5], [7], [28], [29], [35], [51], [59], [97], and [98]. These methods belong to the class of General Linear Methods, §1.7, introduced by Butcher [25], with the aim to provide an unifying approach to analyse the classical subjects of consistency, convergence and stability of numerical methods for Ordinary Differential Equations, which represents an active and increasing area of investigation [27], [56].

1.7 General Linear Methods

"Following the advice of Aristotle, we look for the greatest good as a mean between extremes. Of the various methods devised as generalizations of the classical method of Euler, two extreme approaches are usually followed. One is to generalize the Euler method through the use of multistep methods; the other is to increase the complexity of one-step methods as in the Runge–Kutta methods. General linear methods are introduced as a middle ground between these type of generalization", Butcher [23].

General linear methods (GLMs) for the numerical solution of ordinary differential equations are defined by

$$Y_i^{[n]} = h\sum_{j=1}^{s} a_{ij} f(x_n + c_j h, Y_j^{[n]}) + \sum_{j=1}^{r} u_{ij} y_j^{[n-1]}, \quad i = 1, 2, \ldots, s, \tag{1.7.1}$$

$$y_i^{[n]} = h\sum_{j=1}^{s} b_{ij} f(x_n + c_j h, Y_j^{[n]}) + \sum_{j=1}^{r} v_{ij} y_j^{[n-1]}, \quad i = 1, 2, \ldots, r, \tag{1.7.2}$$

$n = 0, 1, \ldots, N$. These methods were introduced by Burrage and Butcher in 1980, [20] (see also [24], [25], [27], [52], [56]). We also refer to a recent article by Butcher, [26] and to the monography by Jackiewicz, [56], for an extensive review of many aspects of GLMs such as motivation for these formulas, order conditions, linear and non-linear stability, special families of methods, and order and stability barriers. GLMs include as special cases Runge-Kutta methods, linear multistep methods, e.g. BDF methods, and predictor-corrector methods. As discussed in [26] both RK methods LMMs have limitations and the class of GLMs offers new possibilities of constructing new formulas which attempt to combine the advantages of RK methods (large regions of stability) and LMMs (high stage order) at the same time avoiding the disadvantages of these methods (low stage order for RK formulas, small regions of stability for LMMs).

1.8 Runge–Kutta Nyström methods

Many differential equations which appear in applications are systems of second order

$$\begin{cases} y''(x) = f(x, y(x), y'(x)), \\ y(x_0) = y_0,\ y'(x_0) = y'_0. \end{cases} \tag{1.8.1}$$

The general m-stage Runge-Kutta-Nyström, [52], [102], is defined by

$$\begin{aligned} y_{n+1} &= y_n + hy'_n + h^2 \sum_{j=1}^{m} b_j f(x_n + c_j h, Y_j^{[n]}) \\ y'_{n+1} &= y'_n + h^2 \sum_{j=1}^{m} d_j f(x_n + c_j h, Y_j^{[n]}) \\ Y_i^{[n]} &= y_n + c_i h y'_n + h^2 \sum_{j=1}^{m} a_{ij} f(x_n + c_j h, Y_j^{[n]}),\ i = 1, \ldots, m \end{aligned} \tag{1.8.2}$$

where $y_{n+1},\ y'_{n+1}$ denote the numerical approximation to $y(x_{n+1}),\ y'(x_{n+1})$.

Definition 1.8.1

Let $Y(x_{n+\mathbf{c}})$ denote the vector with the components $y(x_n + c_j h)$, where y is the exact solution of (1.8.1), and let be $Y^{[n]} = [Y_1^{[n]}, \ldots, Y_m^{[n]}]^T$; let suppose that the local errors are given by

$$\begin{aligned} y(x_{n+1}) - y_{n+1} &= O(h^{p_1+1}), \\ y'(x_{n+1}) - y'_{n+1} &= O(h^{p_2+1}), \\ Y(x_{n+\mathbf{c}}) - Y^{[n]} &= O(h^{p_3+1}). \end{aligned} \tag{1.8.3}$$

then the order of accuracy p and the stage order r are respectively defined by

$$p = \min\{p_1, p_2\}, \quad r = \min\{p_1, p_2, p_3\}. \tag{1.8.4}$$

For stiff first order ODEs the accuracy reducing effect of order reduction for methods with low stage orders is well known; collocation methods (which automatically possess high stage order) are rather accurate integration methods for stiff problems. A similar phenomenon occurs in the case of stiff second order equations.

The linear stability of RKN methods is investigated by applying them to the test equation $y'' = -\lambda^2 y$, [101], [102]. This leads to recursions of the form

$$\begin{bmatrix} y_n \\ hy'_n \end{bmatrix} = M(\nu) = \begin{bmatrix} y_{n-1} \\ hy'_{n-1} \end{bmatrix}, \tag{1.8.5}$$

where $\nu = -\lambda^2 h^2$, and the matrix $M(\nu)$ is the amplification matrix. The eigenvalues $\mu(\nu)$ of the amplification matrix are the roots of the equation

$$\mu^2 - S(\nu)\mu + P(\nu) = 0,\ S(\nu) := \mathrm{trace} M(\nu),\ P(\nu) := \det M(\nu). \tag{1.8.6}$$

1.9 Collocation methods for $y''(x) = f(x, y(x), y'(x))$

In the case of second order systems we can distinguish direct and indirect collocation methods, [102].

1.9.1 Indirect collocation methods

The second order system (1.8.1) can be transformed into a first order differential equation of doubled dimension by considering the vector (y, y') as the new variable:

$$\begin{pmatrix} y \\ y' \end{pmatrix}' = \begin{pmatrix} y' \\ f(x, y, y') \end{pmatrix} \tag{1.9.1}$$

with $y(x_0) = y_0,\ y'(x_0) = y'_0$. Indirect collocation methods are generated by applying a collocation method to the first order representation (1.9.1). Thus applying the Runge–Kutta method derived by collocation technique defined by the Butcher array

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array}$$

we obtain the RKN method

$$\begin{array}{c|c} c & A^2 \\ \hline & b^T A \\ & b^T \end{array}.$$

Notice that the RKN method has the same order of the original RK method. Now, let the RK method be a collocation method based on the m collocation points $x_n + c_j h,\ j = 1, \ldots, m$, then

$$A = (a_{ij}) := \alpha_j(c_i),\ b = b_j = \alpha_j(1), \tag{1.9.2}$$

$$\alpha_j(x) := \int_0^x L_j(s)ds,\ L_j(s) := \prod_{i=1, i=j}^{m} \cdot \frac{x - c_i}{c_j - c_i},\ i, j = \ldots, m. \tag{1.9.3}$$

$L_j(x)$ is the $j-$th Lagrange polynomial associated with the m collocation parameters c_i. The family of indirect collocation methods has order $p = r = m$ for all collocation nodes c_j. By a special choice of the collocation points, it is possible to increase the order p beyond m.

1.9.2 Direct collocation methods

Direct collocation methods for second order equations approximate the exact solution of (1.8.1) by polynomials, which satisfy, at the collocation points, the differential equation and its differentiated form. Let S be the space of real, piecewise continuously differentiable polynomials of degree not exceeding $m + 1$ associated with the set of intervals $[x_n, x_{n+1}]$. Thus if P is in S, $P(t)$ is a polynomial of degree $\leq m + 1$ on each interval $[x_n, x_{n+1}],\ n = 0, \ldots, N - 1$. For such functions, P'' is a polynomial of degree not exceeding $m - 1$, so that we may write

$$P''(x_n + th) = \sum_{j=1}^{m} L_j(t) P''(x_n + c_j h). \tag{1.9.4}$$

By integrating we derive

$$P'(x_n + th) = P'(x_n) + h \sum_{j=1}^{m} \alpha_j(t) P''(x_n + c_j h), \tag{1.9.5}$$

$$P(x_n + th) = P(x_n) + thP'(x_n) + h^2 \sum_{j=1}^{m} \beta_j(t) P''(x_n + c_j h) \tag{1.9.6}$$

where $\alpha_j(x) = \int_0^x L_j(\tau)d\tau,\ \beta_j(x) = \int_0^x \int_0^\mu L_j(\tau)d\tau d\mu$.
Next we require that the function P satisfies the (1.8.1) at the collocation points

$$P''(x_n + c_j h) = f(x_n + c_j h, P(x_n + c_j h)),\ j = 1, ..., m. \tag{1.9.7}$$

Conditions (1.9.5) and (1.9.6) lead to

$$P(x_n + c_i h) = P(x_n) + c_i h P'(x_n) + c_i^2 \sum_{j=1}^{m} \beta_j(c_i) P''(x_n + c_j h), \tag{1.9.8}$$

$$P'(x_n + c_i h) = P'(x_n) + h \sum_{j=1}^{m} \alpha_j(c_i) P''(x_n + c_j h). \tag{1.9.9}$$

Furthermore we derive

$$P(x_n + h) = P(x_n) + h P'(x_n) + h^2 \sum_{j=1}^{m} \beta_j(1) P''(x_n + c_j h), \tag{1.9.10}$$

$$P'(x_n + h) = P'(x_n) + h \sum_{j=1}^{m} \alpha_j(1) P''(x_n + c_j h). \tag{1.9.11}$$

The method (1.9.8), (1.9.10) is recognized as an m stage RKN method by introducing the quantities

$$y_n := P(x_n),\ y'(x_n) := P'(x_n),\ Y_i^{[n]} := P(x_n + c_i h), \tag{1.9.12}$$

$$b_i := \beta_i(1),\ d_i := \alpha_i(1),\ a_{ij} := \beta_j(c_i). \tag{1.9.13}$$

Theorem 1.9.1 ([102])

The direct RKN collocation method defined above has global step point order and global stage order $p = r = m$ for all sets of distinct collocation parameters c_i.

Chapter 2

Collocation–based two–step Runge–Kutta methods for $y'(x) = f(x, y(x))$

It is the purpose of this chapter to discuss the construction and the analysis of highly stable two-step continuous methods for the numerical solution of initial value problem for the system of Ordinary Differential Equations, which turn out to be the heart of many modern applications of Mathematics to natural phenomena and are used more and more for the description of complex system.

2.1 Introduction

In this chapter we introduce a general family of continuous two–step Runge–Kutta methods for the numerical integration of Ordinary Differential Equations depending on the stage values at two consecutive step points. This new extension falls into the class of Two–Step Runge–Kutta methods, Section 1.6. This method requires the starting procedure to compute the approximate solution on the initial interval $[x_0, x_1]$. For this purpose we can use, for example, the continuous Runge-Kutta methods constructed by Owren and Zennaro [75], [76], [77]. The special case of collocation methods provide a continuous approximation to the solution $y(x)$ on the whole interval of integration, and not only at the gridpoints x_n as is the case for the methods defined in [57]. Different approach to the construction of continuous two-step Runge-Kutta methods is presented in [8], [10] and [58]. Continuous two-step Runge-Kutta methods for delay differential equations are considered in [6], [9] and for Volterra integral equations in [36]. The reason of interest in these methods lies in the fact that, advancing from x_n to x_{n+1}, we only have to compute $Y^{[n]}$, because $Y^{[n-1]}$ was already evaluated in the previous step. Therefore it is of interest to investigate the class of collocation based methods within the class of TSRK methods, in order to derive continuous methods with higher order of convergence, in comparison with classical collocation methods. We extend the idea of multistep collocation methods using two different constructive techniques, [53], [67], considering the two–step case. By adding some extra collocation conditions, the resulting methods depend on the stage values at two consecutive step points. We derive the order conditions so that the method has uniform order p and stage order $q = p$. We derive the recurrence relation which are needed to analyse linear stability properties of these methods. In particular we give the analysis of methods with $m = 1$ and $m = 2$, then we try to achieve stability properties relaxing the collocation technique. In the end we give examples of A-stable and L-stable methods, [34], [37], [38], [41].

2.2 Multistep Collocation Methods

The idea behind multistep collocation, introduced by Guillou and Soulé [50], is to let the collocation polynomial use informations from previous points in the integration, so that the collocation polynomial is defined by

$$\begin{cases} P(x_{n-i}) = y_{n-i} \quad i = 0, 1, ..., k-1, \\ P'(x_n + c_j h) = f(x_n + c_j h, P(x_n + c_j h)) \quad j = 1, ..., m. \end{cases} \tag{2.2.1}$$

The numerical solution is given by

$$y_{n+1} = P(x_{n+1}). \tag{2.2.2}$$

Hairer and Wanner, in [53], proved that this method is equivalent to a multistep Runge–Kutta method, [16], and the points which guarantee superconvergence are called Radau points. Lie and Norsett derived the same methods in a different way and analysed the order of convergence [67].

2.3 Construction of General TSRK

We carry on the idea of multistep collocation methods, by considering the case of two–step methods, and by adding some extra collocation conditions, so that the resulting methods depend on the stage values at two consecutive step points. The collocation polynomial is defined by the following conditions:

$$\begin{cases} P(x_{n-1}) = y_{n-1}, \\ P(x_n) = y_n, \\ P'(x_{n-1} + c_j h) = f(x_{n-1} + c_j h, P(x_{n-1} + c_j h)), \quad j = 1, 2, ..., m, \\ P'(x_n + c_j h) = f(x_n + c_j h, P(x_n + c_j h)), \quad j = 1, 2, ..., m. \end{cases}$$

The previous problem constitutes a Hermite interpolation problem with incomplete data, because the function values $P(x_{n-1} + c_j h),\ P(x_n + c_j h),\ j = 1, \ldots, m$, are

missing. We introduce the generalised Lagrange basis

$$\{\overline{\varphi}_i(x), \overline{\chi}_j(x), \overline{\psi}_j(x), \quad i = 0, 1, \quad j = 1, 2, ..., m\}$$

in such a way that the collocation polynomial is expressed as follows

$$\begin{aligned} P(x) &= \overline{\varphi}_0(x) y_{n-1} + \overline{\varphi}_1(x) y_n + \\ &+ h \sum_{j=1}^{m} \left[\overline{\chi}_j(x) P'(x_{n-1} + c_j h) + \overline{\psi}_j(x) P'(x_n + c_j h) \right]. \end{aligned} \tag{2.3.1}$$

Introducing the dimensionless coordinate $t = \frac{x - x_n}{h}$, the collocation polynomial takes the form

$$\begin{aligned} P(x_n + th) &= \varphi_0(t) y_{n-1} + \varphi_1(t) y_n + \\ &+ h \sum_{j=1}^{m} \left[\chi_j(t) P'(x_{n-1} + c_j h) + \psi_j(t) P'(x_n + c_j h) \right]. \end{aligned} \tag{2.3.2}$$

To determine the methods we must exhibit the expression of the basis functions $\varphi_i(t)$, $i = 0, 1$, $\psi_j(t)$ and $\chi_j(t)$, $j = 1, 2, ...m$. They are obtained by applying the interpolation conditions

$$\begin{aligned} &\varphi_0(t_0) = 1, \ \varphi_0(t_1) = 0, \ \varphi_1(t_0) = 0, \ \varphi_1(t_1) = 1, \\ &\chi_i(t_0) = 0, \ \chi_i(t_1) = 0, \ \psi_i(t_0) = 0, \ \psi_i(t_1) = 0, \end{aligned} \tag{2.3.3}$$

and the collocation ones

$$\begin{aligned} &\varphi_0'(c_i - 1) = 0, \quad \varphi_0'(c_i) = 0, \quad \varphi_1'(c_i - 1) = 0, \quad \varphi_1'(c_i) = 0, \\ &\chi_j'(c_i - 1) = \delta_{ij}, \quad \chi_j'(c_i) = 0, \quad \psi_j'(c_i - 1) = 0, \quad \psi_j'(c_i) = \delta_{ij}, \end{aligned} \tag{2.3.4}$$

where $t_0 = -1$, $t_1 = 0$, $l = 0, 1$, $i, j = 1, 2, \ldots, m$.

In order to compute the polynomials $\varphi_i(t)$, $\chi_j(t)$, $\psi_j(t)$ we extend the technique used by Hairer and Wanner in [53].

Theorem 2.3.1

The method defined by (2.3.1) is equivalent to a two–step Runge–Kutta method,

$$\begin{aligned} Y_i^{[n]} &= u_i y_{n-1} + (1-u_i) y_n + h \sum_{j=1}^{m} [a_{ij} f(x_{n-1} + c_j h, Y_j^{[n-1]}) \\ &+ b_{ij} f(x_n + c_j h, Y_j^{[n]})], \quad i = 1, ..., m, \qquad (2.3.5) \\ y_{n+1} &= \theta y_{n-1} + (1-\theta) y_n + h \sum_{j=1}^{m} [v_j f(x_{n-1} + c_j h, Y_j^{[n-1]}) \\ &+ w_j f(x_n + c_j h, Y_j^{[n]})], \qquad (2.3.6) \end{aligned}$$

where

$$\begin{aligned} &\theta = \varphi_0(1), \qquad v_j = \chi_j(1), \qquad w_j = \psi_j(1), \\ &u_j = \varphi_0(c_j), \quad a_{js} = \chi_j(c_s), \quad b_{js} = \psi_j(c_s), \quad j, s = 1, ..., m. \end{aligned}$$

Proof:

We express the basis polynomials in the following way:

$$\begin{aligned} \varphi_i(t) &= \sum_{l=0}^{2m+1} d_l^{(i)} t^l, \qquad i = 1, 2 \qquad (2.3.7) \\ \chi_j(t) &= \sum_{l=0}^{2m+1} p_l^{(j)} t^l, \qquad \psi_j(t) = \sum_{l=0}^{2m+1} q_l^{(j)} t^l \qquad j = 1, ..., m \qquad (2.3.8) \end{aligned}$$

Imposing the interpolation and collocation conditions (2.3.3), (2.3.4) to the polynomials (2.3.7), (2.3.8) we obtain the following $2m + 2$ linear systems:

$$\begin{aligned} H d^{(i)} &= N_1, \quad i = 1, 2, \qquad (2.3.9) \\ H p^{(i)} &= N_2, \quad H q^{(i)} = N_3 \quad i = 1, ..., m, \qquad (2.3.10) \end{aligned}$$

where H is the coefficient matrix

$$H = \begin{pmatrix} 1 & t_0 & t_0^2 & \cdots & \cdots & t_0^{2m+1} \\ 1 & t_1 & t_1^2 & \cdots & \cdots & t_1^{2m+1} \\ 0 & 1 & 2(c_1-1) & 3(c_1-1)^2 & \cdots & (2m+1)(c_1-1)^{2m} \\ & & & \cdots & & \\ & & & \cdots & & \\ 0 & 1 & 2(c_m-1) & 3(c_m-1)^2 & \cdots & (2m+1)(c_m-1)^{2m} \\ 0 & 1 & 2c_1 & 3c_1^2 & \cdots & (2m+1)c_1^{2m} \\ & & & \cdots & & \\ & & & \cdots & & \\ 0 & 1 & 2c_m & 3c_m^2 & \cdots & (2m+1)c_m^{2m} \end{pmatrix}.$$

N_1, N_2, N_3 are the following vectors

$$\begin{aligned} N_1 &= [\delta_{i1}, \delta_{i2}, 0, ..., 0]^T, \quad N_2 = [0, 0, \delta_{i1}, ..., \delta_{im}, 0, ..., 0]^T \\ N_3 &= [0, ..., 0, \delta_{i1}, ..., \delta_{im}]^T \end{aligned}$$

and $d^{(i)}, p^{(i)}$, $q^{(i)}$ are the unknowns vectors. Each linear system arising in the construction of these methods is nonsingular, because its coefficient matrix is of Vandermonde type. We omit the details of the proof, simply because it uses the well-known technique applied in computing the determinant of the Vandermonde matrix [69]. These linear systems can be solved (apart from some exceptional values of the collocation abscissa), giving the expressions of the collocation polynomial $P(x)$. $\diamondsuit$

Remark 2.3.1

The linear systems (2.3.9), (2.3.10) must be solved exactly. If the stage number m is big, these systems are not easily solved, because they are ill conditioned.

For this reason, even if the Theorem (2.3.1) it is useful to prove the uniqueness of the solution, we extend the technique used by Lie and Norsett in [67] in order to derive general two–step Runge–Kutta methods of collocation type.

Theorem 2.3.2

The method defined by (2.3.1) is equivalent to a two–step Runge–Kutta method having the following form:

$$\begin{aligned} Y_i^{[n]} &= u_i y_{n-1} + (1-u_i) y_n + h \sum_{j=1}^{m} [a_{ij} f(x_{n-1} + c_j h, Y_j^{[n-1]}) \\ &+ b_{ij} f(x_n + c_j h, Y_j^{[n]})], \quad i = 1, ..., m, \end{aligned} \tag{2.3.11}$$

$$\begin{aligned} y_{n+1} &= \theta y_{n-1} + (1-\theta) y_n + h \sum_{j=1}^{m} [v_j f(x_{n-1} + c_j h, Y_j^{[n-1]}) \\ &+ w_j f(x_n + c_j h, Y_j^{[n]})], \end{aligned} \tag{2.3.12}$$

where

$$\psi_j(t) = \int_0^t l_j(\tau) d\tau - \frac{\int_{-1}^0 l_j(\tau) d\tau}{\int_{-1}^0 M(\tau) d\tau} \int_0^t M(\tau) d\tau, \quad j = 1, \ldots, m, \tag{2.3.13}$$

$$\chi_j(t) = \int_0^t \tilde{l}_j(\tau) d\tau - \frac{\int_{-1}^0 \tilde{l}_j(\tau) d\tau}{\int_{-1}^0 M(\tau) d\tau} \int_0^t M(\tau) d\tau, \quad j = 1, \ldots, m, \tag{2.3.14}$$

$$\varphi_0(t) = -\frac{\int_0^t M(\tau) d\tau}{\int_{-1}^0 M(\tau) d\tau}, \tag{2.3.15}$$

$$\varphi_1(t) = 1 + \frac{\int_0^t M(\tau) d\tau}{\int_{-1}^0 M(\tau) d\tau}. \tag{2.3.16}$$

with

$$l_i(t) = \prod_{j=1, j=i}^{2m} \frac{t - d_j}{d_i - d_j}, \quad M(t) = \prod_{j=1}^{2m} (t - d_j), \quad \begin{cases} d_i = c_i \\ d_{m+i} = c_i - 1, \\ \qquad i = 1, 2, ..., m \end{cases} \tag{2.3.17}$$

$$\tilde{l}_i(t) = \prod_{j=1, j=i}^{2m} \frac{t - e_j}{e_i - e_j}, \qquad \begin{cases} e_i = c_i - 1 \\ e_{m+i} = c_i, \qquad i = 1, 2, ..., m \end{cases}$$

Proof:

To prove that the general two–step collocation method defined by (2.3.1) is equivalent to the TSRK method (2.3.11), (2.3.12), again we must exhibit the form of the basis polynomials $\varphi_i(x)$, $i = 0, 1$, $\psi_j(x)$ and $\chi_j(x)$, $j = 1, 2, ...m$. As before, we use the scaled time variable t.

We first consider $\psi_j(t)$, $j = 1, 2, ...m$. The interpolation and collocation conditions on $\psi_j,\ j = 1, \ldots, m$, are

$$\begin{aligned} \psi_j(-r) &= 0, \qquad r = 0, 1 \\ \psi_j'(c_s - 1) &= 0, \qquad s = 1, ..., m \\ \psi_j'(c_s) &= \delta_{js}, \qquad s = 1, ..., m. \end{aligned}$$

We denote the collocation knots in the following way:

$$\begin{cases} d_i = c_i \\ d_{m+i} = c_i - 1, \qquad i = 1, 2, ..., m. \end{cases}$$

Therefore the previous conditions on ψ_j are

$$\psi_j(-r) = 0, \qquad r = 0, 1, \tag{2.3.18}$$

$$\psi_j'(d_s) = \Delta_{js}, \qquad s = 1, ..., 2m. \tag{2.3.19}$$

where

$$\Delta_{js} = \begin{cases} \delta_{js}, & \text{if } 1 \le s \le m \\ 0, & \text{else.} \end{cases} \tag{2.3.20}$$

Following [67], the collocation conditions can be satisfied by a polynomial of the form

$$\psi_j'(t) = l_j(t) + \frac{\alpha_0}{a_j} M(t),\ j = 1, \ldots, m, \tag{2.3.21}$$

where $l_j(t)$ are the Lagrange basis polynomials,

$$\begin{aligned} l_j(t) &= \prod_{i=1, i=j}^{2m} \frac{t - d_i}{d_j - d_i}, \\ M(t) &= \prod_{j=1}^{2m} (t - d_j) \qquad a_j = \prod_{s=1, s=j}^{2m} (d_j - d_s), \qquad \alpha_0 \in \mathbb{R}. \end{aligned}$$

Setting $\bar{\alpha}_0 = \frac{\alpha_0}{a_j}$, equation (2.3.21) becomes

$$\psi_j'(t) = l_j(t) + \bar{\alpha}_0 M(t), \ j = 1, \ldots, m. \tag{2.3.22}$$

Integrating the last equation, we find

$$\psi_j(t) = \int_0^t l_j(\tau) d\tau + \bar{\alpha}_0 \int_0^t M(\tau) d\tau. \tag{2.3.23}$$

We impose the interpolation conditions (2.3.18) and we compute $\bar{\alpha}_0$ by solving the linear equation

$$\bar{\alpha}_0 \int_{-1}^0 M(\tau) d\tau = -\int_{-1}^0 l_j(\tau) d\tau. \tag{2.3.24}$$

For $\psi_j(t)$ we have

$$\psi_j(t) = \int_0^t l_j(\tau) d\tau - \frac{\int_{-1}^0 l_j(\tau) d\tau}{\int_{-1}^0 M(\tau) d\tau} \int_0^t M(\tau) d\tau. \tag{2.3.25}$$

We then consider $\chi_j(t)$, $j = 1, 2, ...m$. The proof is the same as above, putting

$$\begin{cases} e_i = c_i - 1 \\ e_{m+i} = c_i, \qquad = 1, 2, ..., m \end{cases}$$

instead of d_i, $i = 1, ..., 2m$.

We now consider $\varphi_i(t), i = 0, 1$. Using collocation knots d_j, for φ_i we have:

$$\varphi_i(-r) = 1 - \delta_{ir} \qquad r = 0, 1, \tag{2.3.26}$$

$$\varphi_i'(d_j) = 0 \qquad j = 1, ..., m. \tag{2.3.27}$$

The previous conditions are then verified by

$$\varphi_i(t) = \gamma_0^{(i)} + \gamma_1^{(i)} \int_0^t M(\tau)d\tau,$$

where $M(t) = \prod_{j=1}^{2m}(t - d_j)$ and $\gamma_j^{(i)} \in \mathbb{R}$. First of all we consider $\varphi_0(t)$:

$$\varphi_0(t) = \gamma_0^{(0)} + \gamma_1^{(0)} \int_0^t M(\tau)d\tau.$$

We know that

$$0 = \varphi_0(0) = \gamma_0^{(0)} + \gamma_1^{(0)} \int_0^0 M(\tau)d\tau$$

so we have $\gamma_0^{(0)} = 0$. Moreover, it is

$$1 = \varphi_0(-1) = \gamma_1^{(0)} \int_0^{-1} M(\tau)d\tau = -\gamma_1^{(0)} \int_{-1}^0 M(\tau)d\tau \tag{2.3.28}$$

therefore we obtain

$$\gamma_1^{(0)} = -\frac{1}{\int_{-1}^0 M(\tau)d\tau}. \tag{2.3.29}$$

To conclude the proof we must exhibit the form of the basis polynomial $\varphi_1(t)$. As for $\varphi_0(t)$, we impose the interpolation conditions (2.3.26), obtaining

$$1 = \varphi_1(0) = \gamma_0^{(1)}$$

while, applying the collocation ones (2.3.27), it is

$$0 = \varphi_1(-1) = \gamma_0^{(1)} + \gamma_1^{(1)} \int_0^{-1} M(\tau)d\tau = 1 - \gamma_1^{(1)} \int_{-1}^0 M(\tau)d\tau. \tag{2.3.30}$$

So, we arrive to the following expression of the coefficients of $\varphi_1(t)$

$$\gamma_0^{(1)} = 1, \qquad \gamma_1^{(1)} = \frac{1}{\int_{-1}^0 M(\tau)d\tau}. \tag{2.3.31}$$

$\diamondsuit$

2.4 Order conditions

In this section we want to derive order conditions for the method determined by (2.3.1). As it is a continuous method, it seems advantageous to derive continuous order conditions for a general continuous methods, defined by

$$\begin{cases} P(x_n + sh) = \varphi_0(s)y_{n-1} + \varphi_1(s)y_n + \\ \qquad +h\sum_{j=1}^{m}\left[\chi_j(s)P'(x_{n-1} + c_jh) + \psi_j(s)P'(x_n + c_jh)\right], \\ y_{n+1} = P(x_{n+1}). \end{cases} \tag{2.4.1}$$

We can observe that if the polynomials $\varphi_0(s), \varphi_1(s), \chi_j(s), \psi_j(s)$ satisfy the interpolation and the collocation conditions (2.3.3), (2.3.4) then the method is the collocation one derived in §2.3. We assume that $P(x_n + sh)$ is a uniform approximation to $y(x_n + sh)$, $s \in [0, 1]$, of order p. As the result the stage values $P(x_n + c_jh)$ have stage order $q = p$. We investigate the local discretisation error $\xi(x_n + sh)$, which is defined as the residuum obtained by replacing $P(x_n+sh)$ by $y(x_n+sh)$, $P(x_n+c_jh)$ by $y(x_n + c_jh)$, $j = 1, 2, \ldots, m$, y_{n-1} by $y(x_{n-1})$ and y_n by $y(x_n)$, where $y(x)$ is the true solution. This leads to

$$\begin{aligned} \xi(x_n + sh) &= y(x_n + sh) - \varphi_0(s)y(x_n - h) - \varphi_1(s)y(x_n) \\ &- h\sum_{j=1}^{m}\Big(\chi_j(s)y'(x_n + (c_j - 1)h) + \psi_j(s)y'(x_n + c_jh)\Big), \end{aligned} \tag{2.4.2}$$

$s \in [0, 1]$, $n = 1, 2, \ldots, N - 1$. We have the following theorem.

Theorem 2.4.1

Assume that the function $f(y)$ is sufficiently smooth. Then the method (2.4.1) has uniform order p if the following conditions are satisfied

$$\begin{cases} \varphi_0(s) + \varphi_1(s) = 1, \\ \dfrac{(-1)^k}{k!}\varphi_0(s) + \displaystyle\sum_{j=1}^{m}\left(\chi_j(s)\frac{(c_j - 1)^{k-1}}{(k-1)!} + \psi_j(s)\frac{c_j^{k-1}}{(k-1)!}\right) = \frac{s^k}{k!}, \end{cases} \tag{2.4.3}$$

$s \in [0,1]$, $k = 1, 2, \ldots, p$.

Moreover, the local discretisation error (2.4.2) takes the form

$$\xi(x_n + sh) = h^{p+1} C_p(s) y^{(p+1)}(x_n) + O(h^{p+2}), \tag{2.4.4}$$

as $h \to 0$, where the error function $C_p(s)$ is defined by

$$C_p(s) = \frac{s^{p+1}}{(p+1)!} - \frac{(-1)^{p+1}}{(p+1)!}\varphi_0(s) - \sum_{j=1}^{m} \left(\chi_j(s) \frac{(c_j - 1)^p}{p!} + \psi_j(s) \frac{c_j^p}{p!} \right). \tag{2.4.5}$$

Proof:

Expanding $y(x_n + sh)$, $y(x_n - h)$, $y'(x_n + (c_j - 1)h)$ and $y(x_n + c_j h)$ into Taylor series around the point x_n and collecting terms with the same powers of h we obtain

$$\begin{aligned} \xi(x_n + sh) &= \big(1 - \varphi_0(s) - \varphi_1(s)\big) y(x_n) \\ &+ \sum_{k=1}^{p+1} \left(\frac{s^k}{k!} - \frac{(-1)^k}{k!}\varphi_0(s) \right) h^k y^{(k)}(x_n) \\ &- \sum_{k=1}^{p+1} \sum_{j=1}^{m} \left(\chi_j(s) \frac{(c_j - 1)^{k-1}}{(k-1)!} + \psi_j(s) \frac{c_j^{k-1}}{(k-1)!} \right) h^k y^{(k)}(x_n) \\ &+ O(h^{p+2}). \end{aligned}$$

Equating to zero the terms of order k, $k = 0, 1, \ldots, p$, we obtain order conditions (2.4.3). Comparing the terms of order $p+1$ we obtain (2.4.4) with error function $C_p(s)$ defined by (2.4.5). ♢

Let observe that the condition $\varphi_0(s) + \varphi_1(s) = 1, \quad s \in [0,1]$, is the generalisation of preconsistency conditions for TSRK methods (1.6), compare [56].

The next result shows that the polynomials $\varphi_0(s)$, $\varphi_1(s)$, $\chi_j(s)$, and $\psi_j(s)$, $j = 1, 2, \ldots, m$, corresponding to the methods of order $p = 2m + 1$, derived as the unique solution of the system of order conditions (2.4.3) satisfy the interpolation and collocation conditions (2.3.3), (2.3.4).

Theorem 2.4.2

Assume that $\varphi_0(s)$, $\varphi_1(s)$, $\chi_j(s)$, and $\psi_j(s)$, $j = 1, 2, \ldots, m$, satisfy (2.4.3) for $p = 2m + 1$. Then these polynomials satisfy the interpolation conditions (2.3.3) and the collocation ones (2.3.4).

Proof:

The conditions (2.3.3) follow immediately by substituting $s = 0$ and $s = -1$ into (2.4.3) corresponding to $p = 2m + 1$. To show (2.3.4) we differentiate (2.4.3) to get

$$\begin{cases} \varphi_0'(s) + \varphi_1'(s) = 0, \\ \dfrac{(-1)^k}{k!}\varphi_0'(s) + \displaystyle\sum_{j=1}^{m}\left(\chi_j'(s)\frac{(c_j-1)^{k-1}}{(k-1)!} + \psi_j'(s)\frac{c_j^{k-1}}{(k-1)!}\right) = \frac{s^{k-1}}{(k-1)!}, \end{cases} \tag{2.4.6}$$

$k = 1, 2, \ldots, 2m + 1$. substituting $s = c_i$ and $s = c_i - 1$, $i = 1, 2, \ldots, m$, into (2.4.6) we obtain (2.3.4). ♢

It follows from (2.3.3) that the methods described in Theorem 2.4.2 satisfy the conditions $C_p(-1) = 0$ and $C_p(0) = 0$.

2.5 Linear stability analysis

To analyse the stability properties of the methods (2.3.5), (2.3.6) we will use the standard test equation

$$y' = \lambda y, \quad t \geq 0, \tag{2.5.1}$$

where λ is a complex parameter. Applying (2.3.5), (2.3.6) to (2.5.1) and computing the resulting expression at the points $s = c_i$, $i = 1, 2, \ldots, m$, and $s = 1$ we obtain

$$Y_i^{[n]} = \varphi_0(c_i)y_{n-1} + \varphi_1(c_i)y_n + h\lambda\sum_{j=1}^{m}\left(\chi_j(c_i)Y_j^{[n-1]} + \psi_j(c_i)Y_j^{[n]}\right), \tag{2.5.2}$$

$$y_{n+1} = \varphi_0(1)y_{n-1} + \varphi_1(1)y_n + h\lambda\sum_{j=1}^{m}\left(\chi_j(1)Y_j^{[n-1]} + \psi_j(1)Y_j^{[n]}\right), \tag{2.5.3}$$

$i = 1, 2, \ldots, m$, $n = 1, 2, \ldots, N - 1$. Introducing the notation $z = h\lambda$,

$$Y^{[n]} = \begin{bmatrix} Y_1^{[n]} \\ \vdots \\ Y_m^{[n]} \end{bmatrix}, \quad \varphi_0(c) = \begin{bmatrix} \varphi_0(c_1) \\ \vdots \\ \varphi_0(c_m) \end{bmatrix}, \quad \varphi_1(c) = \begin{bmatrix} \varphi_1(c_1) \\ \vdots \\ \varphi_1(c_m) \end{bmatrix},$$

$$v^T = \begin{bmatrix} \chi_1(1) & \cdots & \chi_m(1) \end{bmatrix}^T, \quad w^T = \begin{bmatrix} \psi_1(1) & \cdots & \psi_m(1) \end{bmatrix}^T,$$

and

$$A = [\chi_j(c_i)]_{i,j=1}^{m}\,, \quad B = [\psi_j(c_i)]_{i,j=1}^{m}\,,$$

the relations (2.5.2), (2.5.3) can be written in a vector form

$$\begin{cases} Y^{[n]} = \varphi_0(c)y_{n-1} + \varphi_1(c)y_n + z\Big(AY^{[n-1]} + BY^{[n]}\Big), \\ y_{n+1} = \varphi_0(1)y_{n-1} + \varphi_1(1)y_n + z\Big(v^TY^{[n-1]} + w^TY^{[n]}\Big), \end{cases} \tag{2.5.4}$$

$n = 1, 2, \ldots, N-1$. Hence,

$$Y^{[n]} = \big(I - zB\big)^{-1}\Big(\varphi_0(c)y_{n-1} + \varphi_1(c)y_n + zAY^{[n-1]}\Big) \tag{2.5.5}$$

and substituting this relation into the equation for y_{n+1} leads to

$$\begin{aligned} y_{n+1} &= \Big[\varphi_0(1) + zw^T(I - zB)^{-1}\varphi_0(c)\Big]y_{n-1} \\ &+ \Big[\varphi_1(1) + zw^T(I - zB)^{-1}\varphi_1(c)\Big]y_n \\ &+ z\Big[v^T + zw^T(I - zB)^{-1}A\Big]Y^{[n-1]}. \end{aligned} \tag{2.5.6}$$

The relations (2.5.5) and (2.5.6) are equivalent to

$$\begin{bmatrix} y_{n+1} \\ y_n \\ Y^{[n]} \end{bmatrix} = \begin{bmatrix} M_{11}(z) & M_{12}(z) & M_{13}(z) \\ 1 & 0 & 0 \\ Q\varphi_1(c) & Q\varphi_0(c) & zQA \end{bmatrix} \begin{bmatrix} y_n \\ y_{n-1} \\ Y^{[n-1]} \end{bmatrix}, \tag{2.5.7}$$

where

$$M_{11}(z) = \varphi_1(1) + zw^TQ\varphi_1(c), \tag{2.5.8}$$

$$M_{12}(z) = \varphi_0(1) + zw^TQ\varphi_0(c), \tag{2.5.9}$$

$$M_{13}(z) = z(v^T + zw^TQA), \tag{2.5.10}$$

and

$$Q = (I - zB)^{-1} \in C^{m\times m}. \tag{2.5.11}$$

The matrix appearing in (2.5.7) is called *stability*, or *amplification*, *matrix* of the method (2.3.5), (2.3.6), and as usual will be denoted by $M(z) \in C^{(m+2)\times(m+2)}$. We

can also define the stability function of the method (2.3.5), (2.3.6) as

$$p(w, z) = \det\Big(wI - M(z)\Big). \tag{2.5.12}$$

We will be mainly interested in methods which are A-stable. This means that all the roots $w_1, w_2, \ldots, w_{m+2}$ of the polynomial $p(w, z)$ defined by (2.5.12) are in the unit circle for all $z \in C$ such that $\Re(z) \leq 0$. By the maximum principle this will be the case if the denominator of $p(w, z)$ does not have poles in the negative half plane C_- and if the roots of $p(w, iy)$ are in the unit circle for all $y \in \mathbb{R}$. This last condition will be investigated using the Schur theorem [94] (see also [64]). This criterion for a polynomial of any degree k can be formulated as follows. Consider the polynomial

$$\phi(w) = c_k w^k + c_{k-1} w^{k-1} + \cdots + c_1 w + c_0, \tag{2.5.13}$$

where c_i are complex coefficients, $c_k = 0$ and $c_0 = 0$.
$\phi(w)$ is said to be a Schur polynomial if all its roots w_i, $i = 1, 2, \ldots, k$, are inside of the unit circle. Define

$$\hat{\phi}(w) = \overline{c}_0 w^k + \overline{c}_1 w^{k-1} + \cdots + \overline{c}_{k-1} w + \overline{c}_k, \tag{2.5.14}$$

where $\overline{c}_i$ is the complex conjugate of c_i. Define also the polynomial

$$\phi_1(w) = \frac{1}{w}\Big(\hat{\phi}(0)\phi(w) - \phi(0)\hat{\phi}(w)\Big) \tag{2.5.15}$$

of degree at most $k - 1$. We have the following theorem.

Theorem 2.5.1 (Schur [94])
$\phi(w)$ is a Schur polynomial if and only if

$$|\hat{\phi}(0)| > |\phi(0)| \tag{2.5.16}$$

and $\phi_1(w)$ is a Schur polynomial.

We will be also interested in methods which are L-stable, i.e., methods which are A-stable and all the roots of the stability function $p(w, z)$ given by (2.5.12) are equal to zero as $z \to -\infty$. Now we will analyse more in detail one and two stage methods.

2.5.1 Analysis of methods with $m = 1$

Consider firstly the collocation methods of order $p = 2m+1 = 3$. We can derive this family of methods by using Theorem 2.3.1, Theorem 2.3.2 or order conditions with p=3. We obtain a one parameter family of two-step methods depending on the abscissa c. The coefficients of these methods are

$$\begin{aligned}
\varphi_0(s) &= \frac{s[6c(c-1)+3(1-2c)s+2s^2]}{1-6c^2},\\
\varphi_1(s) &= \frac{(1+s)[6c^2-1+(1-6c)s+2s^2]}{1-6c^2},\\
\chi(s) &= \frac{s(1+s)[2c+3c^2-(1+2c)s]}{1-6c^2},\\
\psi(s) &= \frac{s(1+s)[1-4c+3c^2+(1-2c)s]}{1-6c^2},
\end{aligned}$$

and the error constant $C_3(1)$ is given by

$$C_3(1) = \frac{1-3c-3c^2+12c^3-6c^4}{6(1-6c^2)}.$$

To investigate stability properties of the resulting class of methods it is more convenient to work with the polynomial obtained by multiplying the stability function (2.5.12) by its denominator. The resulting polynomial, which will be denoted by the same symbol $p(w, z)$, for this family of methods takes the form

$$p(w,z) = p_3(z)w^3 + p_2(z)w^2 + p_1(z)w + p_0(z), \tag{2.5.17}$$

where the polynomials $p_i(z)$, $i = 0, 1, 2, 3$, assume the form

$$\begin{aligned}
p_0(z) &= -(c-1)^2c^2z,\\
p_1(z) &= 5-12c+6c^2+(2-5c+6c^2-6c^3+3c^4)z,\\
p_2(z) &= -4+12c-12c^2+(4-8c-3c^2+6c^3-3c^4)z,\\
p_3(z) &= -1+6c^2+(1-2c-2c^2+c^3)cz.
\end{aligned}$$

We will look for A-stable methods in this class of two-step formulas. Let

$$\tilde{p}(w,y) := \overline{p}(w,iy),$$

where $\bar{p}(w, z)$ is the stability polynomial (2.5.17). We compute the constant polynomial with respect to w, which will be denoted by $\tilde{p}_0(y)$, using the recursive procedure described above. This polynomial takes the form

$$\tilde{p}_0(y) = \alpha(c)y^4 + \beta(c)y^6 + \gamma(c)y^8,$$

where $\alpha(c)$, $\beta(c)$ and $\gamma(c)$ are polynomials with respect to the abscissa c. It follows from the Schur criterion in Theorem 2.5.1 that the condition

$$\tilde{p}_0(y) \geq 0, \quad \text{for all} \quad y \geq 0,$$

is the necessary condition for A-stability. However, it can be verified that the polynomials $\alpha(c)$, $\beta(c)$ and $\gamma(c)$ are not simultaneously greater or equal to zero for any c. This proves that A-stable methods do not exist in this class of methods of order $p = 3$. In fact the region of stability of such methods is bounded. In Fig. 2.1 we show an example of stability region. In Fig. 2.2, for $m = 1$ and $p = 2m + 1 = 3$, we

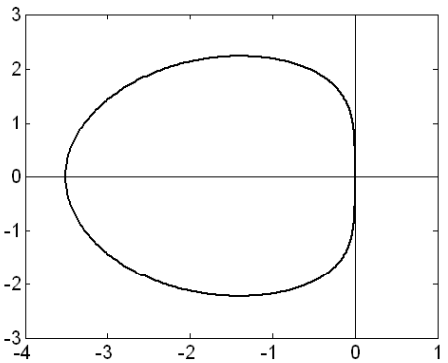

Figure 2.1: Stability region of one-stage method for $c = 1$.

have plotted, in the (c, z)-plane, the stability interval of the methods corresponding to each value of c, considering $c \geq \frac{1}{2}$ in order to satisfy the condition $-1 \leq \theta < 1$ required for zero-stability.

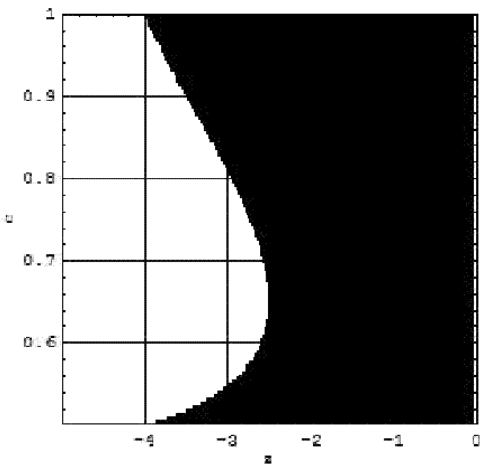

Figure 2.2: Interval of absolute stability in the (c, z)-plane for the two-step collocation methods with $m = 1$ and $p = 3$.

2.5.2 Analysis of methods with $m = 2$

We consider the methods (2.3.5), (2.3.6) of order $p = 2m + 1 = 5$. Solving the order conditions (2.4.3) corresponding to $m = 2$ and $p = 5$ we obtain a family of methods depending on the components of the abscissa vector c_1 and c_2. We have plotted in Fig. 3.1 the contour plots of error constant $C_5(1)$ of these formulas for $0 \leq c_1 \leq 1$ and $0 \leq c_2 \leq 1$. Choosing, for example, $c_1 = \frac{1}{2}$ and $c_2 = 1$ we obtain two-step formula of uniform order $p = 5$ with coefficients given by

$$\begin{aligned}
\varphi_0(s) &= -\frac{[15 - 10s - 30s^2 + 24s^3]s^2}{29}, \\
\varphi_1(s) &= \frac{(1+s)[29 - 29s + 44s^2 - 54s^3 + 24s^4]}{29}, \\
\chi_1(s) &= -\frac{s^2(1+s)[89 - 187s + 96s^2]}{87},
\end{aligned}$$

$$\begin{aligned}
\chi_2(s) &= \frac{s(1+s)[29-31s-16s^2+20s^3]}{29}, \\
\psi_1(s) &= \frac{s^2(1+s)[19+7s-16s^2]}{29}, \\
\psi_2(s) &= -\frac{s^2(1+s)[7-2s-12s^2]}{87}.
\end{aligned}$$

The error constant of this method is $C_5(1) = \frac{113}{83520}$. The stability polynomial of two

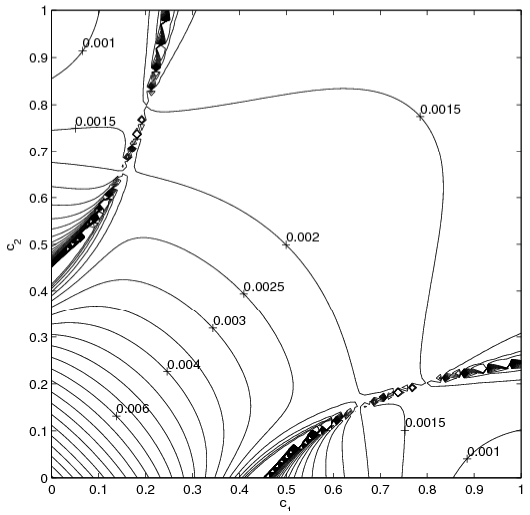

Figure 2.3: Contour plots of error constant $C_5(1)$ for two-step collocation methods od order $2m + 1 = 5$.

parameter family of methods takes the form

$$p(w, z) = p_4(z)w^4 + p_3(z)w^3 + p_2(z)w^2 + p_1(z)w + p_0(z),$$

where $p_i(z)$, $i = 0, 1, 2, 3, 4$ are quadratic polynomials with respect to z. These polynomials depend also on c_1 and c_2. We have performed an extensive computer search based on Schur criterion in the two dimensional space (c_1, c_2) looking for methods with good stability properties but so far we were not able to find methods which are A-stable. We suspect that such methods do not exist in this class of formulas with $m = 2$ and $p = 5$.

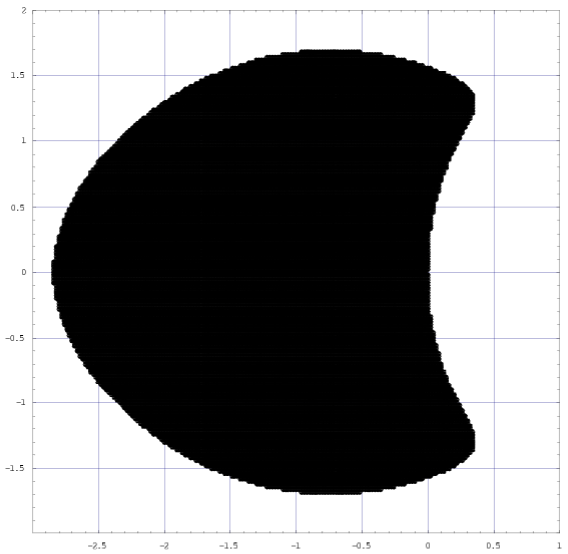

Figure 2.4: Stability region of two–stage collocation method with $c_1 = \frac{1}{2}$ and $c_2 = 1$.

2.6 Almost collocation methods

The aim of our research is the derivation of methods having high order as well as strong stability properties. By using collocation technique we found a class of methods of order $p = 2m + 1$, without acceptable stability properties: *there are not A-stable methods within this family, surely for m=1 and almost surely for m=2.* We are still interested in continuous methods of the form (2.3.5), (2.3.6), so we relax the interpolation or collocation conditions, in order to have some free parameters which we can use to improve stability properties. In this way we obtain continuous methods within the TSRK class, but of course the order is less than $2m+1$. We are mainly interested in methods corresponding to $p = m+r$, where $r = 1, 2, \ldots, m+1$. The advantage of these methods as compared, for example, with methods of low stage order, consists of the fact that they provide an uniform approximation $P(t)$ of order p to the solution $y(t)$ over the entire interval of integration. As a result these

methods do not suffer from the order reduction phenomenon [24]. This is in contrast to implicit Runge-Kutta methods with m stages of order $p = 2m$, $p = 2m - 1$, or $p = 2m - 2$ for which the continuous approximation to $y(t)$ is only of stage order m. This leads to the reduction of order for stiff systems of ODEs for which the effective order is equal only to the stage order m.

In general, for the methods of order $p = m + r$, $r = 1, 2, \ldots, m$, we will choose $\varphi_0(s)$ and $\chi_j(s)$, $j = 1, 2, \ldots, m - r$, as polynomials of degree $\leq m + r$ which satisfy the interpolation conditions

$$\varphi_0(0) = 0, \quad \chi_j(0) = 0, \quad j = 1, 2, \ldots, m - r, \tag{2.6.1}$$

and the collocation conditions

$$\varphi_0'(c_i) = 0, \quad \chi_j'(c_i) = 0, \quad j = 1, 2, \ldots, m - r. \tag{2.6.2}$$

This leads to the polynomials $\varphi_0(s)$ and $\chi_j(s)$, $j = 1, 2, \ldots, m - r$, of the form

$$\varphi_0(s) = s\big(q_0 + q_1 s + \cdots + q_{m+r-1} s^{m+r-1}\big), \tag{2.6.3}$$

$$\chi_j(s) = s\big(r_{j,0} + r_{j,1} s + \cdots + r_{j,m+r-1} s^{m+r-1}\big), \tag{2.6.4}$$

$j = 1, 2, \ldots, m - r$, where

$$q_0 + 2q_1 c_i + \cdots + (m + r) q_{m+r-1} c_i^{m+r-1} = 0,$$
$$r_{j,0} + 2r_{j,1} c_i + \cdots + (m + r) r_{j,m+r-1} c_i^{m+r-1} = 0,$$

$j = 1, 2, \ldots, m - r$, $i = 1, 2, \ldots, m$. The methods obtained in this way satisfy some of the interpolation and collocation conditions (2.3.3) and (2.3.4). We have the following theorem.

Theorem 2.6.1

Assume that $\varphi_0(s)$ *and* $\chi_j(s)$, $j = 1, 2, \ldots, m - r$, *satisfy (2.6.1) and (2.6.2). Then the solution* $\varphi_1(s)$, $\chi_j(s)$, $j = m - r + 1, m - r + 2, \ldots, m$, *and* $\psi_j(s)$, $j = 1, 2, \ldots, m$,

satisfy the interpolation conditions

$$\varphi_1(0) = 1, \quad \chi_j(0) = 0, \quad j = m - r + 1, m - r + 2, \ldots, m, \tag{2.6.5}$$

$$\psi_j(0) = 0, \quad j = 1, 2, \ldots, m, \tag{2.6.6}$$

and the collocation conditions

$$\varphi_1'(c_i) = 0, \quad \chi_j'(c_i) = 0, \quad j = m - r + 1, m - r + 2, \ldots, m, \tag{2.6.7}$$

$$\psi_j'(c_i) = \delta_{ij}, \quad j = 1, 2, \ldots, m, \tag{2.6.8}$$

$i = 1, 2, \ldots, m$.

Proof:

Substituting $s = 0$ into (2.4.3) corresponding to $p = m + r$, $r = 1, 2, \ldots, m$, and taking into account that the solution to (2.4.3) is unique the condition (2.6.5) follows. Differentiating (2.4.3) with respect to s and substituting $s = c_i$, $i = 1, 2, \ldots, m$, into the resulting relations for $k = 1, 2, \ldots, m + r$, we obtain (2.6.7). This completes the proof. ♢

The formulas obtained by imposing the conditions (2.6.1) and (2.6.2) will be then called ***almost two-step collocation methods***. It follows from Theorem 2.6.1 that the polynomial $P(t)$ defined by the method (2.4.1) of order $p = m+r$, $r = 1, 2, \ldots, m$, satisfies the interpolation condition

$$P(t_n) = y_n \tag{2.6.9}$$

and the collocation conditions at the points c_i, i.e.,

$$P'(t_n + c_i h) = f(P(t_n + c_i h)), \quad i = 1, 2, \ldots, m. \tag{2.6.10}$$

However, in general, these methods do not satisfy the interpolation condition

$$P(t_{n-1}) = y_{n-1} \tag{2.6.11}$$

and the collocation conditions

$$P'(t_{n-1} + c_i h) = f(P(t_{n-1} + c_i h)), \quad i = 1, 2, \ldots, m. \tag{2.6.12}$$

In our search for highly stable methods (i.e. A-stability, L-stability) we will be mainly concerned with methods of order $p = 2m$ and $p = 2m - 1$.

2.6.1 One stage almost collocation methods

Let us consider the methods (2.4.1) of order $p = 2m = 2$. We choose the polynomial $\varphi_0(s)$ of degree less than or equal to two which satisfies the interpolation condition (2.6.1) and collocation condition (2.6.2), i.e., the conditions

$$\varphi_0(0) = 0 \quad \text{and} \quad \varphi_0'(c) = 0.$$

This leads to the polynomial $\varphi_0(s)$ of the form

$$\varphi_0(s) = q_0 s\left(1 - \frac{1}{2c}s\right), \tag{2.6.13}$$

where q_0 is a real parameter and $c = 0$. Solving the order conditions (2.4.3) corresponding to $m = 1$ and $p = 2$, where $\varphi_0(s)$ is given by (2.6.13), we obtain a two-parameter family of two-step methods depending on the parameter q_0 and the abscissa c. The coefficients of these formulas are given by

$$\varphi_1(s) = 1 - q_0 s + \frac{q_0}{2c}s^2, \tag{2.6.14}$$

$$\chi(s) = \left(c + \frac{q_0}{2} + cq_0\right)s - \left(\frac{1}{2} + \frac{q_0}{2} + \frac{q_0}{4c}\right)s^2, \tag{2.6.15}$$

$$\psi(s) = \left(1 - c + \frac{q_0}{2} - q_0 c\right)s + \left(\frac{1}{2} + \frac{q_0}{2} - \frac{q_0}{4c}\right)s^2, \tag{2.6.16}$$

and the error constant $C_2(1)$ takes the form

$$C_2(1) = \frac{10c - 24c^2 + 12c^3 + q_0 - 2q_0 c - 6q_0 c^2 + 12q_0 c^3}{24c}, \tag{2.6.17}$$

$c = 0$. The stability polynomial of this family of methods is

$$p(w, z) = w\big[p_2(z)w^2 + p_1(z)w + p_0(z)\big], \tag{2.6.18}$$

where the polynomials $p_0(z)$, $p_1(z)$ and $p_2(z)$ are now given by

$$p_0(z) = 2q_0 - 4q_0c + [2c - 4c^2 + 2c^3 + q_0 - 2q_0c - q_0c^2 + 2q_0c^3]z,$$

$$p_1(z) = -4c - 2q_0 + 4q_0c - [6c - 8c^2 + 4c^3 - q_0 + 2q_0c - 2q_0c^2 + 4q_0c^3]z,$$

and

$$p_2(z) = 4c - c^2(4 - 2c + q_0 - 2q_0c)z.$$

We have performed a computer search based on the Schur criterion using the poly-

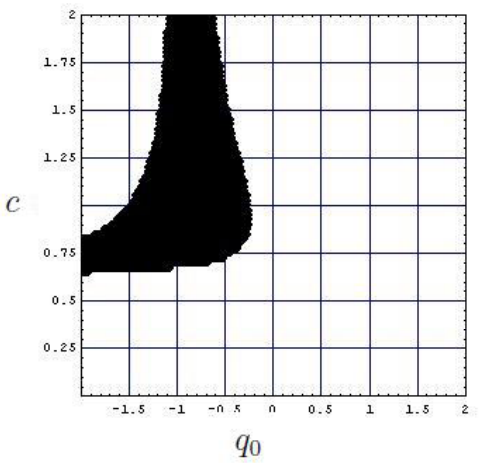

Figure 2.5: Region of A-stability in the (q_0, c)-plane for the two-step methods (2.3.5), (2.3.6) with $m = 1$ and $p = 2$.

nomial $p(w, z)$ given by (2.6.18) with $p_0(z)$, $p_1(z)$ and $p_2(z)$ defined above. This search was performed in the parameter space (q_0, c) and the results are presented in Fig. 2.5 for $-3 \leq q_0 \leq 1$ and $0 \leq c \leq 2$, where the shaded region corresponds

to the A-stable formulas. Choosing, for example, $q_0 = -1$ and $c = \frac{3}{4}$ we obtain the A-stable two-step method with coefficients given by

$$\varphi_0(s) = \frac{(2s-3)s}{3}, \quad \varphi_1(s) = \frac{3+3s-2s^2}{3}, \tag{2.6.19}$$

$$\chi(s) = \frac{(2s-3)s}{6}, \quad \psi(s) = \frac{(2s+3)s}{6}. \tag{2.6.20}$$

For this method the stability polynomial $p(w, z)$ is given by

$$p(w,z) = w\left(\left(3 - \frac{27}{16}z\right)w^2 - \left(4 + \frac{5}{8}z\right)w + \left(1 + \frac{5}{16}z\right)\right), \tag{2.6.21}$$

the error constant $C_2(1) = -\frac{17}{144}$.

We will look next for L-stable methods, i.e., methods for which all roots of the polynomial $p(w, z)/p_2(z))$, where $p(w, z)$ is given by (2.6.18), are equal to zero as $z \to -\infty$. Such methods correspond to the solutions of the nonlinear system of equations

$$\lim_{z->-\infty} \frac{p_0(z)}{p_2(z)} = 0, \quad \lim_{z->-\infty} \frac{p_1(z)}{p_2(z)} = 0. \tag{2.6.22}$$

It can be verified that this system takes the form

$$\begin{cases} (c-1)(2c - 2c^2 + q_0 - q_0 c - 2q_0 c^2) = 0, \\ c - 8c^2 + 4c^3 - q_0 + 2q_0 c - 2q_0 c^2 + 4q_0 c^3 = 0, \end{cases}$$

and has solutions

$$q_0 = -\frac{2}{3}, \quad c = 1 \qquad \text{and} \qquad q_0 = -\frac{4}{9}, \quad c = 2. \tag{2.6.23}$$

The coefficients of the method corresponding to the first set of the above parameters are

$$\varphi_0(s) = \frac{(s-2)s}{3}, \quad \varphi_1(s) = \frac{3+2s-s^2}{3}, \quad \chi(s) = 0, \quad \psi(s) = \frac{(s+1)s}{3}. \tag{2.6.24}$$

The coefficients of the method corresponding to the second set of the parameters q_0 and c are

$$\varphi_0(s) = \frac{s(s-4)}{9}, \ \varphi_1(s) = \frac{9+4s-s^2}{9}, \ \chi(s) = \frac{2(s-4)s}{9}, \ \psi(s) = \frac{(s-1)s}{9}. \tag{2.6.25}$$

It can be verified that for $s = 1$ both of the above methods reduce to backward differentiation method of order $p = 2$, compare [25], [64].

2.6.2 Two stages almost collocation methods

We consider next the methods of order $p = 2m = 4$. We choose the polynomial $\varphi_0(s)$ which satisfies the conditions of the form

$$\varphi_0(0) = 0 \quad \text{and} \quad \varphi_0'(c_i) = 0, \quad i = 1, 2.$$

This leads to the polynomial of the form

$$\varphi_0(s) = s[q_0 + q_1 s + q_2 s^2 + q_3 s^3],$$

where q_2 and q_3 are given by

$$q_2 = -\frac{7q_0 + 6q_1}{3}, \quad q_3 = \frac{3q_0 + 2q_1}{2}.$$

Choosing, for example, $c_1 = \frac{3}{4}$, $c_2 = 1$, $q_0 = q_1 = -1$, we obtain the method with coefficients given by

$$\varphi_0(s) = -\frac{s[27 + 27s - 79s^2 + 39s^3]}{27}, \tag{2.6.26}$$

$$\varphi_1(s) = \frac{27 + 27s + 27s^2 - 79s^3 + 39s^4}{27}, \tag{2.6.27}$$

$$\chi_1(s) = -\frac{2s[783 + 1026s - 2669s^2 + 1293s^3]}{405}, \tag{2.6.28}$$

$$\chi_2(s) = \frac{s[783 + 756s - 2249s^2 + 1113s^3]}{162}, \tag{2.6.29}$$

$$\psi_1(s) = -\frac{2s[27 + 18s - 97s^2 + 57s^3]}{27}, \tag{2.6.30}$$

$$\psi_2(s) = \frac{s[837 + 594s - 2881s^2 + 1857s^3]}{810}. \tag{2.6.31}$$

The error constant of this method is $C_4(1) = \frac{1085}{248832}$. The stability polynomial of the four parameter family of methods of order $p = 4$ takes the form

$$p(w, z) = w[p_3(z)w^3 + p_2(z)w^2 + p_1(z)w + p_0(z)], \tag{2.6.32}$$

where $p_i(z)$, $i = 0, 1, 2, 3$ are quadratic polynomials with respect to z. These polynomials depend also on the parameters q_0, q_1, c_1, and c_2. We have performed an extensive computer search based on the Schur criterion in the four dimensional space (q_0, q_1, c_1, c_2) but so far we were not able to find methods which are A-stable. We suspect again that such methods do not exist in this class of formulas with $m = 2$ and $p = 4$.

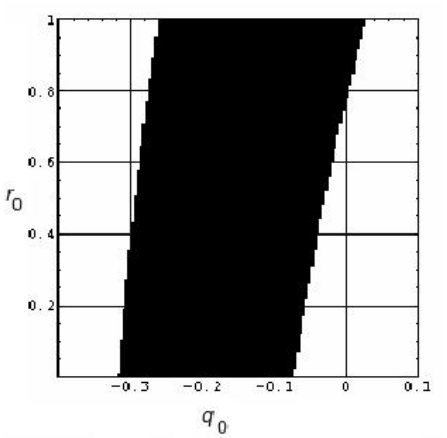

Figure 2.6: Region of A-stability in the (q_0, r_0)-plane for the two-step methods (2.3.5), (2.3.6), with $m = 2$ and $p = 3$.

Finally, consider the methods of order $p = m+1 = 3$. We choose the polynomials $\varphi_0(s)$ and $\chi_1(s)$ of degree less than or equal to three which satisfy the following conditions

$$\varphi_0(0) = 0, \quad \chi_1(0) = 0, \quad \varphi_0'(c_i) = 0, \quad \chi_1'(c_i) = 0, \quad i = 1, 2.$$

These polynomials take the form

$$\varphi_0(s) = s[q_0 + q_1 s + q_2 s^2], \quad \chi_1(s) = s[r_0 + r_1 s + r_2 s^2],$$

where

$$q_1 = r_1 = -\frac{(c_1 + c_2)q_0}{2c_1c_2}, \quad q_2 = r_2 = \frac{q_0}{3c_1c_2}.$$

Solving the order conditions (2.4.3) corresponding to $m = 2$ and $p = 3$ we obtain a four parameter family of methods depending on q_0, r_0, c_1 and c_2. The stability polynomial of this family of methods is given by

$$p(w, z) = w^2[p_2(z)w^2 + p_1(z)w + p_0(z)],$$

where $p_i(z)$, $i = 0, 1, 2$, are polynomials of degree less than or equal to two with respect to z. These polynomials depend also on q_0, r_0, c_1 and c_2. We have performed again an extensive computer search looking for methods which are A-stable. We have found such methods only if both components of the abscissa vector are outside of the interval $[0, 1]$. The results of this search for $c_1 = \frac{5}{2}$ and $c_2 = \frac{9}{2}$ are presented in Fig. 2.6 for $-0.4 \le q_0 \le 0.1$ and $0 \le r_0 \le 1$, where the shaded region corresponds to A-stable methods. The coefficients of the resulting methods with $m = 2$ and $p = 3$ are given by $c = [\frac{5}{2}, \frac{9}{2}]$,

$$\varphi_0(s) = \frac{q_0 s[135 - 42s + 4s^2]}{135}, \quad \varphi_1(s) = \frac{135 - 135q_0 s + 42q_0 s^2 - 4q_0 s^3}{135}, \tag{2.6.33}$$

$$\chi_1(s) = \frac{r_0 s[135 - 42s + 4s^2]}{135}, \tag{2.6.34}$$

$$\chi_2(s) = -\frac{[135 + 181q_0 - 36r_0][135 - 42s + 4s^2]s}{1620}, \tag{2.6.35}$$

$$\psi_1(s) = \left(\frac{63}{8} + \frac{241}{24}q_0 - 3r_0\right)s - \left(2 + \frac{1687}{540}q_0 - \frac{14}{15}r_0\right)s^2 + \left(\frac{1}{6} + \frac{241}{810}q_0 - \frac{4}{45}r_0\right)s^3. \tag{2.6.36}$$

$$\psi_2(s) = \left(\frac{35}{8} + \frac{145}{24}q_0 - r_0\right)s - \left(\frac{3}{2} + \frac{203}{108}q_0 - \frac{14}{45}r_0\right)s^2 + \left(\frac{1}{6} + \frac{29}{162}q_0 - \frac{4}{135}r_0\right)s^3. \tag{2.6.37}$$

The error constant $C_3(1)$ is

$$C_3(1) = \frac{4494825 + 6019723q_0 - 1229184r_0}{77760}. \tag{2.6.38}$$

We have also found methods in this class which are L-stable. Such methods correspond to solutions of the nonlinear system

$$\lim_{z\to-\infty} \frac{p_0(z)}{p_2(z)} = 0, \quad \lim_{z\to-\infty} \frac{p_1(z)}{p_2(z)} = 0. \tag{2.6.39}$$

One such solution is

$$q_0 \approx -\frac{21225899}{77647080} \approx -0.273364, \quad r_0 \approx \frac{113887980}{163068619} \approx 0.698405, \tag{2.6.40}$$

and the resulting method is A-stable and L-stable. A faster damping of errors can be possibly achieved by the stronger property of stiff accuracy, considered in H. Podhaisky, B.A. Schmitt and R. Weiner [83].

2.7 Numerical Experiments

We present below a selection of results of numerical tests, on many non-stiff and stiff problems, designed to compare our methods with respect to classical one step collocation Runge–Kutta methods. The numerical experiments are carried over with a fixed stepsize, without the usage of strategies to save function evaluations. Even if our collocation methods have no unbounded stability regions, they can be suitable to integrate also stiff problems, just by adapting the choice of the step size to the amplitude of the interval of stability. Indeed, methods having unbounded stability regions, for example A-stable methods, can integrate stiff problems also with larger step size, but this kind of integration could highten the error committed too much.

Test 1. We first consider the following linear problem, [65],

$$\begin{cases} y_1'(x) = -2y_1(x) + y_2(x) + 2\sin x \\ y_2'(x) = y_1(x) - 2y_2(x) + 2(\cos x - \sin x) \end{cases} \tag{2.7.1}$$

with $x \in [0, 10]$, with the initial condition $y(0) = [2, 3]^T$, whose exact solution is

$$\begin{cases} y_1(x) = 2e^{-x} + \sin x \\ y_2(x) = 2e^{-x} + \cos x \end{cases} \tag{2.7.2}$$

We solve this problem using the two–step collocation method with $m = 1$ and $c = 1$ (GTSCOLL) and we compare it with the one step Gauss method with one stage

(of order 2) and the Radau IIA with 2 stages (of order 3), in order to have a comparison between methods having the same number of stages (Gauss) and the same order (Radau IIA) and also with BDF method of order 3 (BDF), which is usually considered a standard method for stiff problems [63]. The result of the implementation is shown in the following tables, where h is the step size used, fe is the number of function evaluations, cd is the number of correct digits, ge is the global error committed at the end of the integration interval.

GTSCOLL method, m=1, p=3				**Gauss method, m=1, p=2**			
h	fe	cd	ge	h	fe	cd	ge
0.1	2242	4.9435	1.1387e-005	0.1	297	3.0565	8.7792e-004
0.05	3522	5.8438	1.4328e-006	0.05	597	3.6588	2.1936e-004
0.025	5866	6.7454	1.7968e-007	0.025	1197	4.2609	5.4835e-005
0.0125	9580	7.6491	2.2430e-008	0.0125	2397	4.8630	1.3708e-005
0.00625	18144	8.5507	2.8133e-009	0.00625	4797	5.4650	3.4270e-006
0.003125	31984	9.4569	3.4917e-010	0.003125	9597	6.0671	8.5676e-007
Radau IIA method, m=2, p=3				**BDF method, k=3, p=3**			
h	fe	cd	ge	h	fe	cd	ge
0.1	2966	4.7535	1.7637e-005	0.1	198	4.0413	9.0920e-005
0.05	4750	5.6481	2.2484e-006	0.05	398	4.9149	1.2163e-005
0.025	7904	6.5468	2.8386e-007	0.025	798	5.8036	1.5716e-006
0.0125	12972	7.4478	3.5660e-008	0.0125	1598	6.6996	1.9968e-007
0.00625	25036	8.3497	4.4689e-009	0.00625	3190	7.5992	2.5163e-008
0.003125	44684	9.2523	5.5928e-010	0.003125	3708	8.5006	3.1579e-009

As shown in fig. 2.7, the method GTSCOLL gives the best accuracy. If we compare the results obtained by our method and the Gauss one, we can see that the GTSCOLL method, using the same number of stages, gives a higher order of accuracy. If compared with the Radau IIA method with same order, but with two stages, our method gives a better accuracy as well. BDF method gives less accurate results, by using less function evaluations.

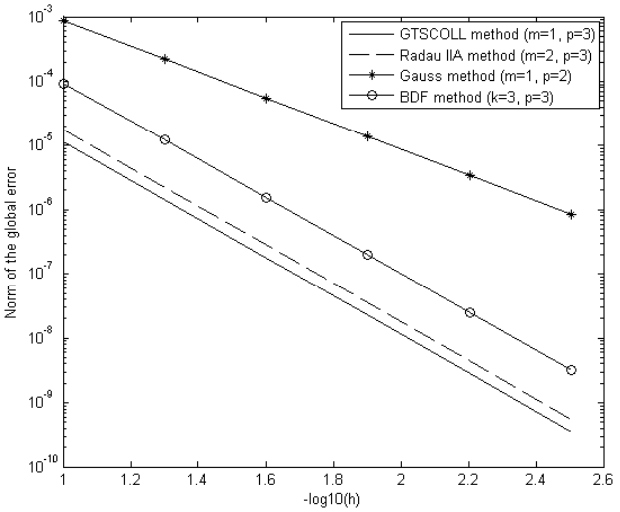

Figure 2.7: Comparison between three solvers for the problem (2.7.1).

Test 2. We next consider the well known Van der Pol's equation [53]. We reduce this second order ODE to the following first order system of two equations

$$\begin{cases} y_1' = y_2 \\ y_2' = \mu(1 - y_1^2)y_2 - y_1 \end{cases} \tag{2.7.3}$$

with $x \in [0, 100]$ and with the initial condition $y(0) = [2, 0]^T$. In particular, we consider the case $\mu = 1000$. The parameter $\mu > 0$ hightens the importance of the nonlinear part of the equation. This problem exhibits a particular phenomenon: the problem switches from stiff to nonstiff with a very sharp changing solution. This makes the equation quite challenging for ODEs solvers.

The GTSCOLL method, having a bounded stability region, is able to integrate this nonlinear stiff problem using a stepsize adapted to the amplitude of the stability region: in particular, it shows the same behaviour of the Gauss method and it is

better than the Radau and BDF methods.

GTSCOLL method			
h	fe	cd	ge
0.1	1889	6.8483	1.4180e-007
0.05	3098	6.8870	1.2971e-007

Gauss method			
h	fe	cd	ge
0.1	2996	6.9023	1.2520e-007
0.05	5996	6.9023	1.2520e-007

Radau IIa method			
h	fe	cd	ge
0.1	13010	4.1495	7.0869e-005
0.05	24010	4.4498	3.5496e-005

BDF method			
h	fe	cd	ge
0.1	1554	6.9013	1.2509e-007
0.05	3108	6.9029	1.2510e-007

In many cases, it is possible to give an upper bound for the stepsize, in order to integrate a stiff system also with methods having a bounded stability interval. We show an example in which we obtain such an estimation of the stepsize.

Test 3. The following problem is Kramarz's system [63], which is often used in numerical experiments on periodic stiffness, [82], on second order ODEs:

$$y''(x) = Ay(x) = \begin{pmatrix} 2498 & 4998 \\ -2499 & -4999 \end{pmatrix} y(x), \tag{2.7.4}$$

where A is the matrix of coefficients in (2.7.4), $y(x) = [y_1(x), y_2(x)]^T$, with $y(0) = [2, -1]^T$ and $x \in [0, 2\pi]$. The exact solution of this problem is

$$y(x) = \begin{pmatrix} 2\cos x \\ -\cos x. \end{pmatrix} \tag{2.7.5}$$

The eigenvalues of A are $\lambda_1 = -2500$, $\lambda_2 = -1$; then the analytical solution of the system exhibits the two frequencies 1 and $\sqrt{2500}$, but the high frequency component is eliminated by the initial conditions. Notwithstanding this, its presence in the general solution of the system dictates restrictions on the choice of the stepsize, so that the system is stiff.

We transform this problem in a system of 4 ordinary differential equations of the first order and we integrate it by using the GTSCOLL method, whose stability interval is $[-\frac{79}{20}, 0]$. In order to get stable results, the product $h\lambda$ must be in $[-\frac{79}{20}, 0]$, so $h \leq \frac{79}{50000} = 0.00158$. If we use a stepsize $h \leq 0.00158$, the GTSCOLL method integrates the above problem with a bounded error. The following table shows that this actually happens. Then we compare these results with the one obtained by the Gauss method.

GTSCOLL method			
h	fe	cd	ge
0.00158	19883	2.6095	2.4575e-3
0.00079	39768	3.1539	7.0154e-4
0.000395	79533	3.1523	7.0418e-4
0.0001975	159068	3.5797	2.6320e-4
0.00009875	318138	4.3710	4.2559e-5
0.000049375	636273	4.3706	4.2600e-5

Gauss method			
h	fe	cd	ge
0.00158	19873	2.6065	2.4745e-3
0.00079	39726	3.1513	7.0579e-4
0.000395	79237	3.1517	7.0523e-4
0.0001975	156735	3.5793	2.6347e-4
0.00009875	298833	4.3703	4.2624e-5
0.000049375	509014	4.3704	4.2616e-5

BDF method			
h	fe	cd	ge
0.00158	6543	2.6070	2.4715e-3
0.00079	9694	3.1517	7.0504e-4
0.000395	15906	3.1517	7.0504e-4
0.0001975	31813	3.5793	2.6342e-4
0.00009875	63627	4.3704	4.2613e-5
0.000049375	127254	4.3706	4.2607e-5

Actually our collocation method shows the same behaviour of the Gauss method and BDF method, despite of its bounded stability region.

Test 4. Now we test our almost collocation method (ACOLL) on the so-called ROBER problem. This problem describes the kinetics of an autocatalytic reaction given by Robertson (1966). Under some idealised conditions and the assumption that the mass action law is applied for the rate functions, the following mathematical

model consisting of a set of three ODEs can be set up

$$\begin{cases} y_1' = -k_1 y_1 + k_3 y_2 y_3 \\ y_2' = k_1 y_1 - k_2 y_2^2 - k_3 y_2 y_3 \\ y_3' = k_2 y_2^2 \end{cases} \tag{2.7.6}$$

with $(y_{01}, y_{02}, y_{03})^T = (y_1(0), y_2(0), y_3(0))^T = (1, 0, 0)^T$, where $y_1,\ y_2,\ y_3$ denote the concentrations of the chemical species involved.

The ROBER problem is very popular in numerical studies and it is often used as a test problem in the stiff integrators comparisons. The numerical values of the rate constants used in the test problem are $k_1 = 0.04,\ k_2 = 3 \cdot 10^7,\ k_3 = 10^4$.

The large difference among the reaction rate constants is the reason for stiffness. As is typical for the problems arising in chemical kinetics this special system has a small very quick initial transient. This phase is followed by a very smooth variation of the components where a large stepsize would be appropriate for a numerical method. We solve this problem using our one-stage ACOLL method, with $c = \frac{3}{4}$ and $q_0 = -1$, and with the one-stage one-step Gauss method. In this way we compare methods having the same order. In the following tables, where $h,\ cd$ and ge are the same as before, we can notice that the ACOLL method gives more accurate results.

ACOLL method			**Gauss method**		
h	cd	ge	h	cd	ge
0.1	4.8156	1.5287e-5	0.1	4.3859	4.1121e-5
0.05	5.3856	4.1161e-6	0.05	4.6268	2.3612e-5
0.025	5.8994	1.2606e-6	0.025	5.5454	2.8482e-6
0.0125	6.2856	5.1806e-7	0.0125	6.4036	3.9479e-7
0.00625	6.4654	3.4242e-7	0.00625	6.5002	3.1602e-7
0.0003125	6.5004	3.1591e-7	0.0003125	6.5273	2.9692e-7

Chapter 3

Two–step Hybrid Methods for $y''(x) = f(x, y(x))$

The purpose of this chapter is to derive two-step hybrid methods for special second order ordinary differential equations with oscillatory or periodic solutions. Firstly we consider a new class of two–step collocation methods, discuss the order of the resulting methods and analyse their stability properties. Then we show the constructive technique of methods based on trigonometric and mixed polynomial fitting and consider the linear stability analysis of such methods. We carry out some numerical experiments underlining the properties of the derived classes of methods.

3.1 Introduction

It is the purpose of this chapter to construct a new class of two–step hybrid methods for the numerical integration of second order Initial Value Problems

$$\begin{cases} y''(x) = f(x, y(x)), \\ y(x_0) = y_0, \\ y'(x_0) = y'_0, \end{cases} \tag{3.1.1}$$

having periodic or oscillatory solutions. We suppose f smooth enough in order to ensure the existence and uniqueness of the solution. Even if (3.1.1) can be transformed into a first order system of double dimension, the development of numerical methods for its direct integration seems more natural and efficient. This problem, having periodic or oscillatory solutions, often appears in many applications: celestial mechanics, seismology, molecular dynamics, and so on (see for instance [82], [101] and references therein contained). In the construction of two–step methods for this type of problems, different possibilities can be taken into account. First we have to choose if we want to approximate, in addition to the solution in the step points, also the derivative of the solution, as for instance Runge–Kutta–Nyström methods do in the one step case. Then we can use also stage values which are associated to the previous step points, in order to highten the order of the resulting method, without heightening the computational cost too much, as done for instance in [57]. The methods we have considered belong to the class of two–step hybrid methods introduced by Coleman in [30]

$$Y_i^{[n]} = u_i y_{n-1} + (1 - u_i) y_n + h^2 \sum_{j=1}^{m} a_{ij} f(x_n + c_j h, Y_j^{[n]}), \tag{3.1.2}$$

$$y_{n+1} = \theta y_{n-1} + (1 - \theta) y_n + h^2 \sum_{j=1}^{m} w_j f(x_n + c_j h, Y_j^{[n]}), \tag{3.1.3}$$

in which $y_{n-1},\ y_n$ and y_{n+1} are approximations for $y(x_n - h),\ y(x_n)$ and $y(x_n + h)$, respectively. There methods are characterised by two s-dimensional vectors, **b** and

c, with elements b_i and c_i, and an $m \times m$ matrix A with elements a_{ij}.

Many other methods, though not normally written like this, can be expressed in the same way by simple rearrangement. Order conditions are relationship between coefficients of a method which cause successive terms in a Taylor expansion of the local truncation error to vanish. Coleman expressed the Taylor series as B2-series. In [30], the methods are formulated as one-step methods, and the local truncation error is expressed in terms of a set of coefficient functions. There are also tabulated some order conditions, and the coefficients of some particular classes of methods.

3.2 Two–Step Collocation Hybrid Methods

We derive the parameters of the methods by using a collocation technique based on algebraic polynomials, then we handle the study of order and stability properties of the resulting methods, [39]. The development of classical collocation methods (i.e. methods based on algebraic polynomials) is the first necessary step in order to construct collocation methods whose collocation function is expressed as linear combination of different functions, e.g. trigonometric polynomials, mixed or exponential basis (see, for instance, [31], [55]).

3.2.1 Derivation of methods

We compute the parameters of the methods extending the technique introduced by Hairer and Wanner in [53] in the first order case. In order to derive two–step collocation methods of the form (3.1.2), (3.1.3), we compute the collocation polynomial, which satisfies the following $m + 2$ conditions

$$P(x_{n-1}) = y_{n-1}, \qquad P(x_n) = y_n, \tag{3.2.1}$$

$$P''(x_n + c_j h) = f(x_n + ch, P(x_n + c_j h)), \qquad j = 1, \ldots, m. \tag{3.2.2}$$

which allow us to derive a polynomial of degree at most $m+1$. We express the collocation polynomial as linear combination of polynomials of degree at most $m+1$:

$$P(x_n+th)=\varphi_1(t)y_{n-1}+\varphi_2(t)y_n+h^2\sum_{j=1}^{m}\chi_j(t)P''(x_n+c_jh), \tag{3.2.3}$$

where $t=\frac{x-x_n}{h}$. In order to satisfy (3.2.1), (3.2.2), we impose the following set of conditions on the basis functions:

$$\begin{array}{llllll}\varphi_1(-1)=1, & \varphi_2(-1)=0, & \chi_j(-1)=0, & \varphi_1(0)=0, & \varphi_2(0)=1,\\ \chi_j(0)=0, & \varphi_1''(c_i)=0, & \varphi_2''(c_i)=0, & \chi_j''(c_i)=\delta_{ij}, & \end{array} \tag{3.2.4}$$

for $i,j=1,\ldots,m$. The coefficients of the unknown basis functions

$$\{\varphi_1(t),\ \varphi_2(t),\ \chi_j(t),\ j=1,\ 2,\ ...,\ m\}$$

are given by the solutions of $m+2$ linear systems having the following coefficient matrix

$$H=\begin{pmatrix}1 & -1 & 1 & \ldots & (-1)^i & \ldots & (-1)^{m+1}\\ 1 & 0 & 0 & \ldots & 0 & \ldots & 0\\ 0 & 0 & 2 & \ldots & i(i-1)c_1^{i-2} & \ldots & m(m+1)c_1^{m-1}\\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\ 0 & 0 & 2 & \ldots & i(i-1)c_m^{i-2} & \ldots & m(m+1)c_m^{m-1}\end{pmatrix},$$

which is a nonsingular matrix (apart for some exceptional values of the collocation abscissa) because of Vandermonde type (see [69]). After computing the basis functions, the class of methods takes the following form

$$Y_i^{[n]} = \varphi_1(c_i)y_{n-1}+\varphi_2(c_i)y_n+h^2\sum_{j=1}^{m}\chi_j(c_i)f(x_n+c_jh,Y_j^{[n]}), \tag{3.2.5}$$

$$y_{n+1} = \varphi_1(1)y_{n-1}+\varphi_2(1)y_n+h^2\sum_{j=1}^{m}\chi_j(1)f(x_n+c_jh,Y_j^{[n]}). \tag{3.2.6}$$

We list the coefficient functions of the methods:

- one stage $\varphi_1(t)=-t,\ \chi_1(t)=\frac{1}{2}t(1+t)$;

- two-stages

$$\begin{aligned}
\varphi_1(t) &= -t,\\
\chi_1(t) &= -\frac{1+3c_2}{6(c_1-c_2)}t - \frac{c_2}{2(c_1-c_2)}t^2 + \frac{1}{6(c_1-c_2)}t^3,\\
\chi_2(t) &= \frac{1+3c_1}{6(c_1-c_2)}t + \frac{c_1}{2(c_1-c_2)}t^2 - \frac{1}{6(c_1-c_2)}t^3;
\end{aligned}$$

- three stages

$$\begin{aligned}
\varphi_1(t) &= -t,\\
\chi_1(t) &= -\frac{-1-2c^2-2c^3-6c^2c^3}{12(c^1-c^2)(c^1-c^3)}t + \frac{c^2c^3}{2(c^1-c^2)(c^1-c^3)}t^2\\
&\quad -\frac{c^2+c^3}{6(c^1-c^2)(c^1-c^3)}t^3 + \frac{1}{12(c^1-c^2)(c^1-c^3)}t^4,\\
\chi_2(t) &= -\frac{1+2c^1+2c^3+6c^1c^3}{12(c^1-c^2)(c^2-c^3)}t - \frac{c^1c^3}{2(c^1-c^2)(c^2-c^3)}t^2\\
&\quad -\frac{-c^1-c^3}{6(c^1-c^2)(c^2-c^3)}t^3 + \frac{1}{12(c^1-c^2)(-c^2+c^3)}t^4,\\
\chi_3(t) &= -\frac{1+2c^1+2c^2+6c^1c^2}{12(c^1-c^3)(-c^2+c^3)}t - \frac{c^1c^2}{2(c^1-c^3)(-c^2+c^3)}t^2\\
&\quad -\frac{c^1+c^2}{6(c^1-c^3)(c^2-c^3)}t^3 + \frac{1}{12(c^1-c^3)(c^2-c^3)}t^4,
\end{aligned}$$

3.2.2 Order conditions

We now derive order conditions, by considering $P(x_n + th)$ as an uniform approximation of $y(x_n + th)$ on the whole integration interval.

Theorem 3.2.1

Assume that the function f is sufficiently smooth. Then the method (3.2.5), (3.2.6) has uniform order p if the following conditions are satisfied:

$$\begin{cases}
1 - \varphi_1(t) - \varphi_2(t) = 0,\\
t + \varphi_1(t) = 0,\\
\frac{t^k}{k!} - \varphi_1(t)\frac{(-1)^k}{k!} - \sum_{j=1}^{m} \chi_j(t)\frac{(c_j)^{k-2}}{(k-2)!} = 0.
\end{cases} \tag{3.2.1}$$

$k = 2, \ldots, p, \quad t \in [0, 1]$.

Proof:

We consider the local discretisation error

$$\xi(x_n + th) = y(x_n + th) - \varphi_1(t)y(x_n - h) - \varphi_2(t)y(x_n) - h^2 \sum_{j=1}^{m} \chi_j(t) y''(x_n + c_j h),$$

and expand $y(x_n + th), \quad y(x_n - h), \quad y''(x_n + c_j h)$ in Taylor series around the point x_n, obtaining

$$\begin{aligned} \xi(x_n + th) &= y(x_n) + thy'(x_n) + \cdots + \frac{(th)^p}{p!} y^{(p)}(x_n) + \\ &- \varphi_1(t)[y(x_n) - hy'(x_n) + \cdots + \frac{(-1)^p h^p}{p!} y^{(p)}(x_n)] - \varphi_2(t)y(x_n) \\ &- h^2 \sum_{j=1}^{m} \chi_j(t)[y''_n + c_j h y'''(x_n) + \cdots + \frac{(c_j h)^{p-2}}{(p-2)!} y^{(p)}(x_n)] + O(h^{p+1}). \end{aligned}$$

We then compare the coefficients of the same power of h, achieving the thesis. $\diamondsuit$

Theorem 3.2.1 allows us to prove that every two–step collocation method of the type (3.2.5), (3.2.6) has order $p = m$ on the whole integration interval, and this result is in keeping with [30]. In the context of General Linear Methods [25], [56], the first condition of (3.2.1) is the so-called *preconsistency condition*, while the second one is the *consistency condition*.

In order to be the method preconsistent and consistent, it must be $\varphi_1(t) = -t$ and $\varphi_2(t) = 1 + t$, i.e. the methods (3.1.2), (3.1.3) exactly fall in the class of Coleman hybrid methods [30], as $\theta = -1$ and $u_i = c_i$, $i = 1, ..., m$.

3.2.3 Linear Stability Analysis

We handle the linear stability analysis, [82], [101], [102], of the obtained methods. We apply the class of methods (3.1.2), (3.1.3), to the test problem

$$y'' = -\lambda^2 y, \qquad \lambda \in \mathbf{R}$$

obtaining

$$Y_i^{[n]} = u_i y_{n-1} + (1 - u_i) y_n - \nu^2 \sum_{j=1}^{m} a_{ij} Y_j^{[n]}, \tag{3.2.2}$$

$$y_{n+1} = \theta y_{n-1} + (1 - \theta) y_n - \nu^2 \sum_{j=1}^{m} w_j Y_j^{[n]}, \tag{3.2.3}$$

where $\nu^2 = \lambda^2 h^2$. In tensor notation,

$$Y^{[n]} = u y_{n-1} + \tilde{u} y_n - \nu^2 A Y^{[n]}, \tag{3.2.4}$$

$$y_{n+1} = \theta y_{n-1} + (1 - \theta) y_n - \nu^2 w^T Y^{[n]}, \tag{3.2.5}$$

where $Y^{[n]} = (Y_i^{[n]})_{i=1}^m$, $u = (u_i)_{i=1}^m$, $\tilde{u} = (1 - u_i)_{i=1}^m$, $w = (w_i)_{i=1}^m$, $A = (a_{ij})_{i,j=1}^m$. The following expression for the stage values holds:

$$Y^{[n]} = Q[u y_{n-1} + \tilde{u} y_n], \tag{3.2.6}$$

where $Q = [I + \nu^2 A]^{-1}$ and I is the identity matrix of dimension m. If we substitute this expression in (3.2.5), the following recurrence relation arises:

$$y_{n+1} = [\theta - \nu^2 w^T Q u] y_{n-1} + [1 - \theta - \nu^2 w^T Q \tilde{u}] y_n, \tag{3.2.7}$$

that is

$$\begin{bmatrix} y_{n+1} \\ y_n \end{bmatrix} = \begin{bmatrix} M_{11} & M_{12} \\ 1 & 0 \end{bmatrix} \begin{bmatrix} y_n \\ y_{n-1} \end{bmatrix}, \tag{3.2.8}$$

where

$$M_{11} = 1 - \theta - \nu^2 w^T Q \tilde{u}, \qquad M_{12} = \theta - \nu^2 w^T Q u.$$

The stability matrix takes the form

$$M(z^2) = \begin{bmatrix} M_{11} & M_{12} \\ 1 & 0 \end{bmatrix}. \tag{3.2.9}$$

From [101], [102], we consider the following definitions.

Definition 3.2.1

$(0, \beta^2)$ is a stability interval for the method (3.1.2), (3.1.3) if $\forall \nu^2 \in (0, \beta^2)$ the spectral radius of $M(\nu^2)$ is such that

$$\rho(M(\nu^2)) < 1.$$

Definition 3.2.2

*The method (3.1.2), (3.1.3) is **A**–stable if $(0, \beta^2) = (0, +\infty)$.*

In order to reach A–stability, it must be $\rho(M(\nu^2, c)) < 1$ where $\rho(M(\nu^2, c))$ is the spectral radius of the stability matrix, i.e. both the eigenvalues μ_1, μ_2 of $M(\nu^2, c)$ must satisty the condition $|\mu_1| < 1$, $|\mu_2| < 1$, for any value of ν^2. For $m = 1$, through an analytical study of the stability matrix (3.2.9), it is possible to prove the following result which characterises A–stable methods. If the eigenvalues of the stability matrix (3.2.9) (or in equivalent way, the roots of the stability polynomial) are on the unit circle, then the interval of stability becomes an interval of periodicity, according to the following definition.

Definition 3.2.3

$(0, H_0^2)$ is a periodicity interval if $\forall \nu^2 \in (0, H_0^2)$ the roots r_1, r_2 of the stability polynomial $\pi(\mu) = \det[M(\nu^2) - \mu I]$ satisfy

$$r_1 = e^{i\phi(\nu)}, \quad r_2 = e^{-i\phi(\nu)}.$$

Definition 3.2.4

*The method (3.1.2), (3.1.3) is **P**–stable if its periodicity interval is $(0, +\infty)$.*

Theorem 3.2.2

For $m = 1$, the method (3.2.5), (3.2.6) is A–stable if and only if $c \in (\frac{1}{\sqrt{2}}, 1]$

Through a numerical search, it is possible to find nonempty periodicity intervals. For instance, in the case $m = 1$, for any $c \in [0, \frac{1}{50})$, the periodicity interval of the resulting methods is $[0, 4]$.

3.3 Hybrid methods with frequency dependent parameters

Classical numerical methods for ODEs relied on polynomials may not be very well-suited to periodic or oscillatory behaviour. In the framework of exponential fitting many numerical methods have been adapted in order to exactly integrate basis of functions other than polynomials, for instance the exponential basis (see [55] and references therein contained), in order to catch the oscillatory behaviour. The parameters of these methods depend on the values of frequencies, which appear in the solution. In order to adapt the collocation technique [52], [63] to an oscillatory behaviour, the collocation function has been chosen as a linear combination of trigonometric functions [78] or of powers and exponential functions [31]. Many modifications of classical methods have been presented in the literature for problem (3.1.1): exponentially-fitted Runge-Kutta methods (see for example [46], [99]), or trigonometrically-fitted Numerov methods [45], [100] and many others (for a more extensive bibliography see [55] and references in the already cited papers).

Our aim is to adapt the coefficients of methods (3.1.2), (3.1.3) to an oscillatory behaviour, in such a way that it exactly integrates linear combinations of power and trigonometric functions depending on one and two frequencies, which we suppose can be estimated in advance. Frequency-dependent methods within the class (3.1.2), (3.1.3) have already been considered in [103], where the coefficients of methods were modified to produce phase-fitted and amplification-fitted methods.

We rewrite the hybrid method (3.1.2), (3.1.3) as an $\mathcal{A}$-method, following the idea in [2], [65], in order to regard it as a generalized linear multistep method and consider linear operators associated to it, which will play a crucial rule in the development of the new methods. Then we derive the methods, by imposing that the internal and external stages exactly integrate linear combinations of mixed basis functions. In particular, we construct methods with constant coefficients and methods with

parameters depending on one or two frequencies. Finally we analyse linear stability properties of the derived methods, [40].

3.3.1 Two-step hybrid methods as $\mathcal{A}$-methods: order conditions

We show some preliminary and helpful results we will use in the remainder of this section in order to carry out the construction of numerical methods belonging to the class of two-step hybrid methods (3.1.2), (3.1.3). In particular, following the approach introduced by Albrecht, we rewrite the class of two-step hybrid methods as $\mathcal{A}$-methods. We first define the following vectors in $\mathbb{R}^{m+2}$

$$\begin{aligned} Z_{n+1} &= [Y_1^{[n]}, ..., Y_m^{[n]}, y_n, y_{n+1}]^T, \\ F(x_n, Z_{n+1}; h) &= [f(x_n + c_1 h, Y_1^{[n]}), ..., f(x_n + c_m h, Y_m^{[n]}), f(x_n, y_n), f(x_n, y_{n+1})]^T. \end{aligned}$$

In this way, a two-step hybrid method (3.1.2), (3.1.3) can be expressed as an $\mathcal{A}$–method of the form

$$Z_{n+1} = \mathcal{A} Z_n + h^2 \mathcal{B} F(x_n, Z_{n+1}; h), \tag{3.3.1}$$

with

$$\mathcal{A} = \begin{bmatrix} 0 & -c & \mathbf{e}+c \\ 0 & -1 & 2 \\ 0 & 0 & 1 \end{bmatrix}, \ \mathcal{B} = \begin{bmatrix} A & 0 & 0 \\ b^T & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \in \mathbb{R}^{(m+2)\times(m+2)}. \tag{3.3.2}$$

$\mathbf{e}$ is the unitary vector of $\mathbb{R}^m$. This representation is very useful, because it constitutes an $m+2$ linear stages representation, in the sense that each of the m internal stages and the external stages are linear, so we can look at them as a generalized linear multistep formula on a non-equidistant grid. For this reason, we can consider the following $m+1$ linear operators

$$\begin{aligned} L_i[z(x); h] &= z(x + c_i h) - (1 + c_i) z(x) + c_i z(x - h) \\ &- h^2 \sum_{j=1}^{m} a_{ij} z''(x + c_j h), \quad i = 1, ..., m \end{aligned} \tag{3.3.3}$$

$$\hat{L}[z(x); h] = z(x + h) - 2z(x) + z(x - h) - h^2 \sum_{i=1}^{m} b_i z''(x + c_i h) \tag{3.3.4}$$

where $z(x)$ is a smooth enough function. Expanding in power series of h around x we obtain

$$\begin{aligned} L_i[z(x);h] &= C_{i2}h^2 z^{(2)}(x) + C_{i3}h^3 z^{(3)}(x) + ..., \quad i = 1, ..., m \\ \hat{L}[z(x);h] &= \hat{C}_2 h^2 z^{(2)}(x) + \hat{C}_3 h^3 z^{(3)}(x) + ... \end{aligned}$$

where

$$\begin{aligned} C_{iq} &= \frac{c_i^q}{q!} + \frac{(-1)^q}{q!} - \frac{1}{(q-2)!}\sum_{j=1}^{m} a_{ij}c_j^{q-2}, \quad i = 1, ..., m,\ q = 2, 3, ... \\ \hat{C}_q &= \frac{1}{q!} + \frac{(-1)^q}{q!} - \frac{1}{(q-2)!}\sum_{j=1}^{m} b_j c_j^{q-2},\ q = 2, 3, ... \end{aligned}$$

As a consequence, we can give the following definition.

Definition 3.3.1

The $i-th$ internal stage (3.1.3) of a two-step hybrid method has order p_i if

$$C_{i2} = 0,\ C_{i3} = 0,\ \ldots,\ C_{ip_i+1} = 0, \quad C_{ip_i+2} = 0, \tag{3.3.5}$$

while the external stage (3.1.2) has order p if

$$\hat{C}_2 = 0,\ \hat{C}_3 = 0,\ \ldots,\ \hat{C}_{p+1} = 0, \quad \hat{C}_{p+2} = 0. \tag{3.3.6}$$

We know that necessary condition for a two-step hybrid method (3.1.2), (3.1.3) to have order p is that the external stage must have order p, i.e.

$$b^T c^{q-2} = \frac{1 + (-1)^q}{q(q-1)}, \quad q = 2, 3, ..., p+1, \tag{3.3.7}$$

where the vector power is componentwise. In order to look for conditions that are also sufficient, in line to Albercht's approach, we need to look at the global error. We omit the details achieving order conditions, because they can be found in [30]. The table 3.1 shows the set of order conditions up to 4.

Order	Order conditions
1	$\sum_i b_i = 1$
2	$\sum_i b_i c_i = 0$
3	$\sum_i b_i c_i^2 = \frac{1}{6}$ $\sum_i \sum_j b_i a_{ij} = \frac{1}{12}$
4	$\sum_i b_i c_i^3 = 0$ $\sum_i \sum_j b_i c_i a_{ij} = \frac{1}{12}$ $\sum_i \sum_j b_i a_{ij} c_j = 0$

Table 3.1: Order conditions for two-step hybrid methods (3.1.2), (3.1.3) of order up to 4.

3.3.2 Constructive technique of mixed-trigonometrically fitted two-step hybrid methods

Now we show the construction of some two-step hybrid methods for the numerical solution of second order ODEs, whose solutions depend on one or more frequencies, which at the moment we suppose can be estimated in advance. In particular, we require that both the internal and external stages of the resulting methods exactly integrate linear combinations of the following basis functions:

$$\{1, x, \ldots, x^q, cos(\omega_i x), sin(\omega_i x),\ q, i = 1, 2, \ldots\} \tag{3.3.8}$$

depending on the frequencies ω_i, with i, q such that the dimension of the basis is $m + 2$, so $2i + q = m + 1$.

The case of mixed basis follows the idea of using mixed interpolation of type

$$acos(\omega x) + bsin(\omega x) + \sum_{i=0}^{m-1} c_i x^i, \tag{3.3.9}$$

presented in [42] and used in [31]. In each case the vector $\mathbf{c}$ is considered to be free. Each c_i, $i = 1, 2, ..., m$ can be chosen in order to improve the stability properties of

the methods or, imposing a special set of constraints in the implicit case, in order to achieve superconvergence.

Methods with constant coefficients

In order to derive s-stage methods of type (3.1.2), (3.1.3) with constant coefficients, we annihilate the linear operators (3.3.3)-(3.3.4) on the functional basis

$$\{1, x, x^2, ..., x^q\} \tag{3.3.10}$$

with $q = s + 1$. It trivially happens that

$$\begin{aligned} L_i[1; h] &= \hat{L}[1; h] = 0, \quad i = 1,\ 2, ...,\ m, \\ L_i[x; h] &= \hat{L}[x; h] = 0, \quad i = 1,\ 2, ...,\ m, \end{aligned}$$

while, for $2 \leq k \leq q$, it is

$$\begin{aligned} L_j[x^k; h] &= 0,\ i = 1,\ 2, ...,\ m \quad \Leftrightarrow \quad \frac{c_i^k + (-1)^k c_i}{k(k-1)} = \sum_{j=1}^{m} a_{ij} c_j^{k-2} \\ \hat{L}[x^k; h] &= 0 \quad \Leftrightarrow \quad \frac{1 + (-1)^k}{k(k-1)} = \sum_{i=1}^{m} b_i c_i^{k-2}. \end{aligned}$$

Therefore, we have obtained the set of conditions

$$\begin{cases} \dfrac{c_i^k + (-1)^k c_i}{k(k-1)} = \displaystyle\sum_{j=1}^{m} a_{ij} c_j^{k-2} \\ \dfrac{1 + (-1)^k}{k(k-1)} = \displaystyle\sum_{j=1}^{m} b_j c_j^{k-2}, \end{cases} \tag{3.3.11}$$

for $i = 1,\ 2, ...,\ m$ and $2 \leq k \leq q$, which is a system of $m(m + 1)$ equations in the unknowns a_{ij}, b_i, for $i,\ j = 1,\ 2, ...,\ m$.

Remark 3.3.1

It is easy to verify that the methods obtained by solving the order conditions (3.3.11) are equal to the methods described in the previous section and in [37], which are based on collocation through algebraic polynomials, and have been derived by extending the multistep collocation technique described in [53]. Therefore conditions (3.3.11) are the order conditions for collocation methods within class (3.1.2), (3.1.3).

Methods with parameters depending on one frequency

In order to derive numerical methods for second order ODEs whose solution depends on the frequency ω, a priori known, we consider the function basis $\{1, x, \ldots, x^q, cos(\omega x), sin(\omega x),\ q = 1, 2, \ldots\}$.

In particular, to derive two-stage methods, we consider $\{1, cos(\omega x), sin(\omega x)\}$ as function basis and we impose that the numerical method exactly integrates second order ODEs whose solution is a linear combination of the basis functions. In this way we obtain the class of trigonometrically fitted two-step hybrid methods. As it automatically happens that

$$L_j[1; h] = \hat{L}[1; h] = 0,\ j = 1, 2,$$

we need to impose the following set of conditions

$$L_j[\cos \omega x; h] = 0, \quad j = 1, 2, \qquad \hat{L}[\cos \omega x; h] = 0, \tag{3.3.12}$$

$$L_j[\sin \omega x; h] = 0, \quad j = 1, 2, \qquad \hat{L}[\sin \omega x; h] = 0, \tag{3.3.13}$$

which constitutes a 6×6 linear system in the unknowns $a_{11},\ a_{12},\ a_{21},\ a_{22},\ b_1,\ b_2$.

In order to construct methods with 3 or more stages, we impose that the numerical method exactly integrates second order ODEs whose solution is a linear combination of the basis function

$$\{1, x, x^2, ...x^{m-1}, cos(\omega x), sin(\omega x)\}$$

depending on the frequency ω. In this case we obtain ***mixed-trigonometrically fitted two-step hybrid methods***. As also $L_j[x; h] = \hat{L}[x; h] = 0,\ j = 1, ..., m$, it is sufficient to impose that

$$L_j[x^q; h] = 0, \quad \hat{L}[x^q; h] = 0, \quad j = 1, ..., m,\ q = 2, ..., m-1, \tag{3.3.14}$$

$$L_j[\cos \omega x; h] = 0, \quad \hat{L}[\cos \omega x; h] = 0, \quad j = 1, 2, ..., m, \tag{3.3.15}$$

$$L_j[\sin \omega x; h] = 0, \quad \hat{L}[\sin \omega x; h] = 0, \quad j = 1, 2, ..., m. \tag{3.3.16}$$

It arises a system of $m(m+1)$ conditions in the unknowns a_{ij}, b_i, $i, j = 1, 2, ..., m$. This system is equivalent to the following set of conditions:

$$\begin{aligned}
\sum_{i=1}^{m} b_i c_i^{q-2} &= \frac{1+(-1)^q}{q(q-1)}, \quad q = 2, ...m, \\
\sum_{j=1}^{m} a_{ij} c_j^{q-2} &= c_i^q \frac{1+(-1)^q c_i}{q(q-1)}, \quad i = 1, 2, ..., m, \quad q = 2, ..., m, \\
\sum_{i=1}^{m} b_i \cos(c_i\theta) &= 2\frac{(1-\cos\theta)}{\theta^2}, \\
\sum_{j=1}^{m} a_{ij} \cos(c_j\theta) &= -\frac{\cos(c_i\theta) + 1 + c_i + c_i\cos\theta}{\theta^2} \quad i = 1, 2, ..., m, \\
\sum_{i=1}^{m} b_i \sin(c_i\theta) &= 0, \\
\sum_{j=1}^{m} a_{ij} \sin(c_j\theta) &= \frac{c_i \sin(\theta) - \sin(c_i\theta)}{\theta^2} \quad i = 1, 2, ..., m,
\end{aligned}$$

where $\theta = \omega h$. In both cases, the coefficients of the resulting methods are subjected to heavy numerical cancellation, so it is necessary to represent them through their expansion in power series of θ. Now we list the coefficients of some methods.

1. Two-stage methods

The solution of the system (3.3.12) for $m = 2$ is

$$\begin{aligned}
a_{11} &= -\frac{(\sin((c_1-c_2)\theta) + (1+c_1)\sin(c_2\theta) - c_1\sin((1+c_2)\theta))}{\theta^2\sin((c_1-c_2)\theta)}, \\
a_{12} &= \frac{((1+c_1)\sin(c_1\theta) - c_1\sin((1+c_1)\theta))}{\theta^2\sin((c_1-c_2)\theta)} \\
a_{21} &= \frac{(-((1+c_2)\sin(c_2\theta)) + c_2\sin((1+c_2)\theta))}{\theta^2\sin((c_1-c_2)\theta)} \\
a_{22} &= \frac{((1+c_2)\sin(c_1\theta) - c_2\sin((1+c_1)\theta) - \sin((c_1-c_2)\theta))}{\theta^2\sin((c_1-c_2)\theta)} \\
b_1 &= \frac{2(-1+\cos(\theta))\sin(c_2\theta)}{\theta^2\sin((c_1-c_2)\theta)} \\
b_2 &= \frac{-2(-1+\cos(\theta))\sin(c_1\theta)}{\theta^2\sin((c_1-c_2)\theta)}
\end{aligned}$$

where $\theta = \omega h$. The coefficients expressed in this form are not of practical utility, because they are subject to heavy numerical cancellation: this is the reason why we handle their Taylor series expansion. For brevity, we give only the Taylor series expansion of the coefficients of the two stage method having $c = [3/4, 1]$

$$\begin{aligned}
a_{11} &= \frac{91}{32} - \frac{4375}{6144}\theta^2 + \frac{198451}{2949120}\theta^4 - \frac{263429}{75497472}\theta^6 + \frac{62606173}{543581798400}\theta^8 \\
&- \frac{4225415771}{1607262661509120}\theta^{10} + O(\theta^{12}) \\
a_{12} &= -\frac{35}{16} + \frac{287}{768}\theta^2 - \frac{475}{18432}\theta^4 + \frac{2921}{2949120}\theta^6 - \frac{5149}{212336640}\theta^8 \\
&+ \frac{1606607}{3923981107200}\theta^{10} + O(\theta^{12}) \\
a_{21} &= 4 - \frac{23}{24}\theta^2 + \frac{2071}{23040}\theta^4 - \frac{24019}{5160960}\theta^6 + \frac{4565341}{29727129600}\theta^8 \\
&- \frac{110038253}{31391848857600}\theta^{10} + O(\theta^{12}) \\
a_{22} &= -3 + \frac{1}{2}\theta^2 - \frac{11}{320}\theta^4 + \frac{71}{53760}\theta^6 - \frac{2503}{77414400}\theta^8 \\
&+ \frac{3719}{6812467200}\theta^{10} + O(\theta^{12}) \\
b_1 &= 4 - \frac{23}{24}\theta^2 + \frac{2071}{23040}\theta^4 - \frac{24019}{5160960}\theta^6 + \frac{4565341}{29727129600}\theta^8 \\
&- \frac{110038253}{31391848857600}\theta^{10} + O(\theta^{12}) \\
b_2 &= -3 + \frac{1}{2}\theta^2 - \frac{11}{320}\theta^4 + \frac{71}{53760}\theta^6 - \frac{2503}{77414400}\theta^8 \\
&+ \frac{3719}{6812467200}\theta^{10} + O(\theta^{12}).
\end{aligned}$$

This representation of the coefficients is very expressive, because it allows us to easily consider what follows. First of all we can notice that, for $\theta \to 0$, these coefficients tend to the ones of the corresponding polynomial collocation method. Moreover, we can also easily derive the order of the resulting methods:

$$\begin{aligned}
b_1 + b_2 &= 1 + O(\theta^2) \\
b_1 c_1 + b_2 c_2 &= O(\theta^2) \\
b_1 c_1^2 + b_2 c_2^2 &= -c_1 c_2 + O(\theta^2).
\end{aligned}$$

Therefore, the method has algebraic order 2. The stability region in the (ν, θ)-plane of the methods corresponding to some values of c_1 and c_2 are drawn in fig. 3.1.

2. Three stage mixed trigonometrically fitted methods depending on one frequency.

Solving the system of equations for $m = 3$, we derive the coefficients of three stage methods depending on one frequency. We omit their expression because it is huge and it has no practical utility because of the heavy numerical cancellation it is subject to. In our numerical experiment we have used the Taylor expansion of the coefficients. We consider the method corresponding to $(c_1, c_2, c_3) = (\frac{1}{2}, \frac{3}{4}, 1)$:

$$\begin{aligned}
a_{11} &= \frac{7}{2} - \frac{1081\theta^2}{2560} + \frac{251761\theta^4}{10321920} - \frac{1384021\theta^6}{1651507200} + O(\theta^8) \\
a_{12} &= -\frac{21}{4} + \frac{2293\theta^2}{3840} - \frac{163169\theta^4}{5160960} + \frac{279607\theta^6}{275251200} + O(\theta^8) \\
a_{13} &= \frac{17}{8} - \frac{1343\theta^2}{7680} + \frac{24859\theta^4}{3440640} - \frac{293621\theta^6}{1651507200} + O(\theta^8)
\end{aligned}$$

$$\begin{aligned}
a_{21} &= \frac{693}{128} - \frac{78169\theta^2}{122880} + \frac{431851\theta^4}{11796480} - \frac{3163721\theta^6}{2516582400} + O(\theta^8) \\
a_{22} &= -\frac{511}{64} + \frac{18403\theta^2}{20480} - \frac{279851\theta^4}{5898240} + \frac{5752283\theta^6}{3774873600} + O(\theta^8) \\
a_{23} &= \frac{413}{128} - \frac{32249\theta^2}{122880} + \frac{42617\theta^4}{3932160} - \frac{2013403\theta^6}{7549747200} + O(\theta^8)
\end{aligned}$$

$$\begin{aligned}
a_{31} &= \frac{22}{3} - \frac{17\theta^2}{20} + \frac{2953\theta^4}{60480} - \frac{129767\theta^6}{77414400} + O(\theta^8) \\
a_{32} &= -\frac{32}{3} + \frac{6\theta^2}{5} - \frac{3827\theta^4}{60480} + \frac{78647\theta^6}{38707200} + O(\theta^8) \\
a_{33} &= \frac{13}{3} - \frac{7\theta^2}{20} + \frac{437\theta^4}{30240} - \frac{27527\theta^6}{77414400} + O(\theta^8)
\end{aligned}$$

$$\begin{aligned}
b_1 &= \frac{22}{3} - \frac{17\theta^2}{20} + \frac{2953\theta^4}{60480} - \frac{129767\theta^6}{77414400} + O(\theta^8) \\
b_2 &= -\frac{32}{3} + \frac{6\theta^2}{5} - \frac{3827\theta^4}{60480} + \frac{78647\theta^6}{38707200} + O(\theta^8) \\
b_3 &= \frac{13}{3} - \frac{7\theta^2}{20} + \frac{437\theta^4}{30240} - \frac{27527\theta^6}{77414400} + O(\theta^8)
\end{aligned}$$

We can verify the order of this method, applying the set of order conditions [30]

$$\begin{aligned}
\sum_{i=1}^{3} b_i &= 1 + O(\theta^2) \\
\sum_{i=1}^{3} b_i c_i &= O(\theta^2) \\
\sum_{i=1}^{3} b_i c_i^2 &= \frac{1}{6} + O(\theta^2) \\
\sum_{i=1}^{3}\sum_{j=1}^{3} b_i a_{ij} &= \frac{1}{12} + O(\theta^2) \\
\sum_{i=1}^{3} b_i c_i^3 &= O(\theta^2).
\end{aligned}$$

Therefore, the method has algebraic order 3. The stability region is drawn in fig. 3.2.

Remark 3.3.2

It is possible to prove that, for $\theta \to 0$, the coefficients of the resulting trigonometrically–fitted method tend to the coefficient of the corresponding collocation two–step hybrid methods, derived as shown in section 3.3.2 or in [37]. Therefore the two and three stage methods, above described, are the trigonometric based collocation methods within class (3.1.2), (3.1.3).

Methods with parameters depending on two frequencies

We now deal with the case of second order ODEs whose solution depends on two frequencies ω_1 and ω_2, both estimated in advance. We require that the methods must exactly solve the problem when its solution is linear combination of the basis functions

$$\{1, x, \ldots, x^{s-3}, cos(\omega_1 x), sin(\omega_1 x), cos(\omega_2 x), sin(\omega_2 x)\}, \tag{3.3.17}$$

with $s \geq 4$. In order to derive such methods, we impose the following set of conditions

$$\begin{aligned} L_j[\cos\omega_1 x; h] &= 0, \quad \hat{L}[\cos\omega_1 x; h] = 0, \quad j = 1, \ldots, m \\ L_j[\sin\omega_1 x; h] &= 0, \quad \hat{L}[\sin\omega_1 x; h] = 0, \quad j = 1, \ldots, m \\ L_j[\cos\omega_2 x; h] &= 0, \quad \hat{L}[\cos\omega_2 x; h] = 0, \quad j = 1, \ldots, m \\ L_j[\sin\omega_2 x; h] &= 0, \quad \hat{L}[\sin\omega_2 x; h] = 0, \quad j = 1, \ldots, m. \end{aligned} \tag{3.3.18}$$

Then if we are interested in methods with 4 stages, we only have to solve the system (3.3.18) in the unknowns $a_{ij}, b_i, \quad i, j = 1, ..., 4$. It has now become clear that, if we annihilate also

$$L_j[x^q; h] = 0, \ \hat{L}[x^q; h] = 0, \quad j = 1, 2, ..., m, \ q = 2, 3..., m-3, \tag{3.3.19}$$

more stages are necessary. The methods derived by solving (3.3.18) have parameters depending on $\theta_1 = \omega_1 h$ and $\theta_2 = \omega_2 h$.

3. Four stage methods depending on two frequencies.

We now consider four stage methods of order 4 depending on two frequencies. The following method comes out setting $(c_1, c_2, c_3, c_4) = (0, \frac{1}{3}, \frac{2}{3}, 1)$. We report some terms of the Taylor series expansion of its coefficients.

$$\begin{aligned} a_{11} &= 0 \\ a_{12} &= 0 \\ a_{13} &= 0 \\ a_{14} &= 0 \\ a_{21} &= \frac{13676040 - 658854\theta_2^2}{16533720} - \frac{\theta_1^2(355781160 - 6480270\theta_2^2)}{8928208800} + O(\theta_1^4) + O(\theta_2^4) \\ a_{22} &= -\frac{71}{54} + \frac{833\theta_2^2}{9720} + \frac{\theta_1^2(510095880 - 35167230\theta_2^2)}{5952139200} + O(\theta_1^4) + O(\theta_2^4) \end{aligned}$$

$$
\begin{aligned}
a_{23} &= \frac{26}{27} - \frac{7\theta_2^2}{135} + \theta_1^2 \frac{-(\frac{7}{135}) + (533\theta_2^2)}{367416} + O(\theta_1^4) + O(\theta_2^4) \\
a_{24} &= \frac{-8368920 + 198450\theta_2^2}{33067440} + \frac{\theta_1^2(21432600 - 103626\theta_2^2)}{3571283520} + O(\theta_1^4) + O(\theta_2^4) \\
a_{31} &= \frac{539}{324} - \frac{929\theta_2^2}{11664} + \theta_1^2 \frac{\frac{-929}{11664} + (27443\theta_2^2)}{18895680} + O(\theta_1^4) + O(\theta_2^4) \\
a_{32} &= -\frac{137}{54} + \frac{37\theta_2^2}{216} + \frac{\theta_1^2(203915880 - 14061762\theta_2^2)}{1190427840} + O(\theta_1^4) + O(\theta_2^4) \\
a_{33} &= 42661080 - 2285010\theta_2^2 - \frac{\theta_1^2(246781080 - 6909354\theta_2^2)}{2380855680} + O(\theta_1^4) + O(\theta_2^4) \\
a_{34} &= -8368920 + 198450\theta_2^2 + \frac{\theta_1^2(21432600 - 103626\theta_2^2)}{1785641760} + O(\theta_1^4) + O(\theta_2^4) \\
a_{41} &= \frac{5}{2} - \frac{43\theta_2^2}{360} + \frac{\theta_1^2(-8777160 + 160110\theta_2^2)}{73483200} + O(\theta_1^4) + O(\theta_2^4) \\
a_{42} &= -\frac{15}{4} + \frac{37\theta_2^2}{144} + \frac{\theta_1^2(7552440 - 520722\theta_2^2)}{29393280} + O(\theta_1^4) + O(\theta_2^4) \\
a_{43} &= 3 - \frac{7\theta_2^2}{45} + \frac{\theta_1^2(-5715360 + 160110\theta_2^2)}{36741600} + O(\theta_1^4) + O(\theta_2^4) \\
a_{44} &= -\frac{3}{4} + \frac{13\theta_2^2}{720} + \frac{\theta_1^2(2653560 - 12690\theta_2^2)}{146966400} + O(\theta_1^4) + O(\theta_2^4) \\
b_1 &= \frac{5}{2} - \frac{43\theta_2^2}{360} + \frac{\theta_1^2(-8777160 + 160110\theta_2^2)}{73483200} + O(\theta_1^4) + O(\theta_2^4) \\
b_2 &= -\frac{15}{4} + \frac{37\theta_2^2}{144} + \frac{\theta_1^2(7552440 - 520722\theta_2^2)}{29393280} + O(\theta_1^4) + O(\theta_2^4) \\
b_3 &= \frac{3 - (7\theta_2^2)}{45} + \frac{\theta_1^2(-5715360 + 160110\theta_2^2)}{36741600} + O(\theta_1^4) + O(\theta_2^4) \\
b_4 &= -\frac{3}{4} + \frac{13\theta_2^2}{720} + \frac{\theta_1^2(2653560 - 12690\theta_2^2)}{146966400} + O(\theta_1^4) + O(\theta_2^4)
\end{aligned}
$$

Figures 3.3 and 3.4 show the stability region of this method and other methods, obtained in correspondence of different values of the abscissa.

Remark 3.3.3

Also in this case, for $\theta_1 \to 0$ *and* $\theta_2 \to 0$*, the coefficients of the derived methods tend to the coefficients of the two–step collocation hybrid methods, derived in section 3.3.2 and [37]. Therefore the four stage method derived by (3.3.18) is the two frequencies trigonometric based collocation methods within class (*3.1.2*), (*3.1.3*).*

3.3.3 Linear stability analysis

We handle the linear stability analysis [79], [101], [102] of the obtained methods. We consider the cases of methods with coefficients depending on one or two frequencies.

Methods depending on one frequency

We now analyse the stability properties of mixed trigonometrically fitted methods depending on one frequency. In [32] the authors discussed the modifications introduced in the linear stability analysis, when the parameters depend on one fitted frequency ω. As a consequence of the presence of the fitted frequency ω, the interval of stability now becomes a two-dimensional region for the one parameter family of methods.
In this analysis, we denote the stability matrix as $M(\nu^2, \theta)$ and

$$R(\nu^2, \theta) = \frac{1}{2} trace(M(\nu^2, \theta)),\ P(\nu^2, \theta) = det(M(\nu^2, \theta)), \tag{3.3.20}$$

because it depends not only on $\nu^2 = \lambda^2 h^2$ but also on $\theta = \omega h$.
The eigenvalues of the stability matrix $M(\nu^2, \theta)$ satisfy the following equation

$$\xi^2 - 2R(\nu^2, \theta)\xi + P(\nu^2, \theta) = 0. \tag{3.3.21}$$

It is known in literature (see [31], [32], [63]) that methods such that

$$|P(\nu^2, \theta)| \equiv 1, \tag{3.3.22}$$

i.e. the roots of (3.3.21) lie on the unit circle, are of particular interest. For example, Runge–Kutta Nyström methods based on polynomial approximations with symmetric abscissas c_i in $[0, 1]$, have an interval of periodicity, but they are not P–stable, if collocation based. If (3.3.22) holds, the study of periodicity can be developed just looking at the stability function $R(\nu^2, \theta)$, in agreement with the following definition, [32].

Definition 3.3.2

For a trigonometrically fitted method of the type (3.1.2), (3.1.3) satisfying $|P(\nu^2, \theta)| \equiv 1$, *we define the primary interval of periodicity as the largest interval* $(0, h_0)$ *such that* $|R(\nu^2, \theta)| < 1$, *for all steplengths* $h \in (0, h_0)$. *If, when* h_0 *is finite,* $|R(\nu^2, \theta)| < 1$ *also for* $\gamma < h\delta$, *where* $\gamma > h_0$, *then the interval* (γ, δ) *is a secondary interval of periodicity.*

Exponentially fitted linear multistep methods in [32] verify (3.3.22), but only for few methods in the literature condition (3.3.22) holds. In our analysis, we found that for two-stage methods (3.1.2), (3.1.3) the values of the abscissas such that $|P(\nu^2, \theta)| \equiv 1$ are only $c_1 = 0, c_2 = 1$. We relax the definition 2 of region of stability in [32], in order to consider also methods for which $P(\nu^2, \theta) < 1$, in the following way [45]:

Definition 3.3.3

A region of stability Ω *is a region of the* (ν, θ) *plane, such that* $\forall(\nu^2, \theta) \in \Omega$

$$P(\nu^2, \theta) < 1, \quad |R(\nu^2, \theta)| < \frac{1}{2}(P(\nu^2, \theta) + 1). \tag{3.3.23}$$

Any closed curve defined by $P(\nu^2, \theta) \equiv 1$ *and* $|R(\nu^2, \theta)| = \frac{1}{2}(P(\nu^2, \theta) + 1)$ *is a stability boundary.*

Fig. 3.1 and fig. 3.2 show some examples of stability regions for one–frequency depending methods, in the cases $m = 2$ and $m = 3$.

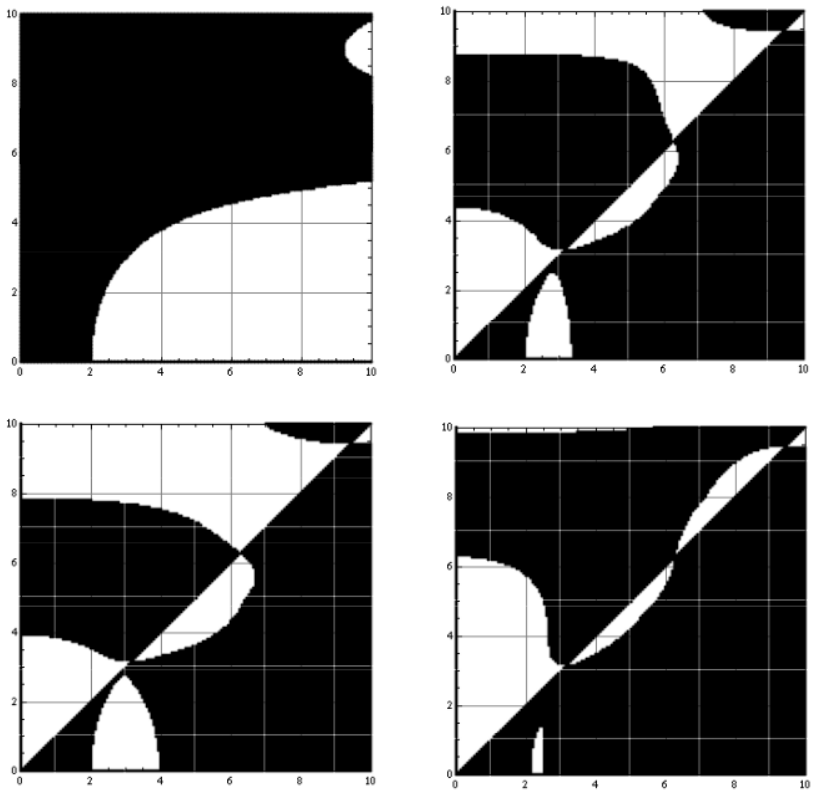

Figure 3.1: Regions of stability in the (ν, θ)–plane for the two-step methods for $m = 2$ with nodes $(0, 1)$, $(\frac{1}{7}, \frac{6}{7})$, $(\frac{1}{10}, \frac{9}{10})$, $(\frac{3}{4}, 1)$ respectively.

Methods depending on two frequencies

We now consider the linear stability analysis of methods depending on two frequencies. As stated before, for methods with constant coefficient, the stability region is an interval on the real axis, while methods depending on one frequency have bidimensional stability region. At the best of our knowledge this is the first time in which the bidimensional stability region are considered.

In the case of methods depending on the values of two frequencies, ω_1, ω_2, op-

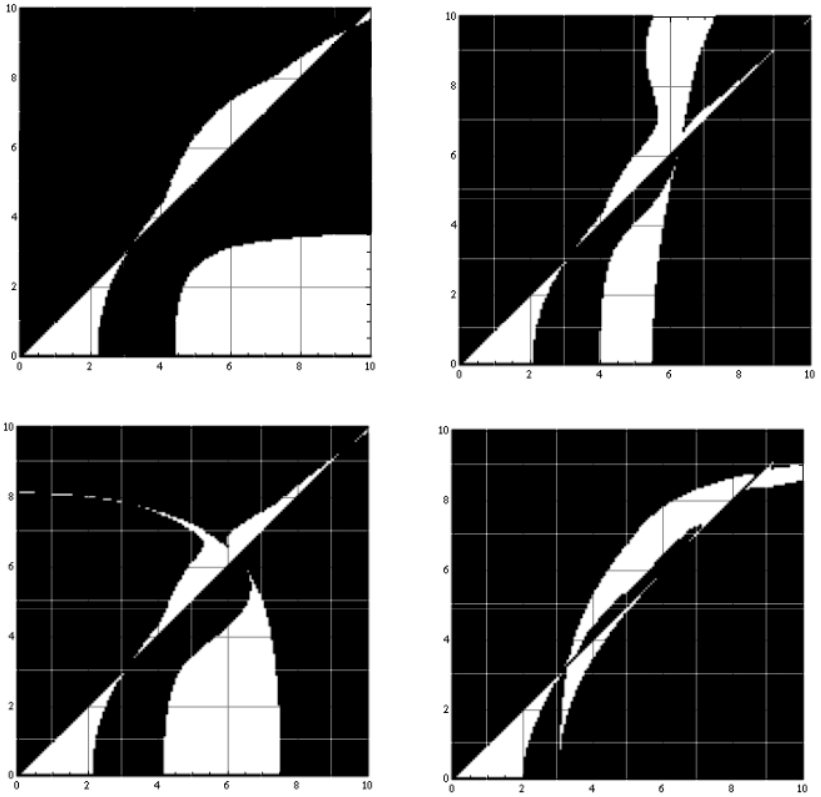

Figure 3.2: Regions of stability in the (ν, θ)–plane for the two-step methods for $m = 3$ with nodes $(0, \frac{1}{2}, 1)$, $(\frac{1}{4}, \frac{1}{2}, \frac{3}{4})$, $(\frac{1}{9}, \frac{1}{2}, \frac{8}{9})$, $(\frac{1}{2}, \frac{3}{4}, 1)$ respectively.

portunely adapting the approach that Coleman and Ixaru in [32] introduced for one frequency depending methods, the stability region becomes tridimensional. We now denote the stability matrix of the methods as $M(\nu^2, \theta_1, \theta_2)$, with $\nu^2 = \lambda^2 h^2, \theta_1 = \omega_1 h, \theta_2 = \omega_2 h$. Its eigenvalues satisfy the following equation

$$\xi^2 - 2R(\nu^2, \theta_1, \theta_2)\xi + P(\nu^2, \theta_1, \theta_2) = 0, \tag{3.3.24}$$

where $R(\nu^2, \theta_1, \theta_2) = \frac{1}{2}\text{trace}(M(\nu^2, \theta_1, \theta_2))$ and $P(\nu^2, \theta_1, \theta_2) = \det(M(\nu^2, \theta_1, \theta_2))$ are rational functions of ν^2. The definition of stability region for two frequencies de-

pending methods can now be adapted as follows, [45]:

Definition 3.3.4

A three dimensional region Ω *of the* $(\nu^2, \theta_1, \theta_2)$ *space is said to be the region of stability of the corresponding two-frequencies depending method if* $\forall(\nu^2, \theta_1, \theta_2) \in \Omega$

$$P(\nu^2, \theta_1, \theta_2) < 1, \quad |R(\nu^2, \theta_1, \theta_2)| < \frac{1}{2}(P(\nu^2, \theta_1, \theta_2) + 1). \tag{3.3.25}$$

Any closed curve defined by

$$P(\nu^2, \theta_1, \theta_2) \equiv 1, \quad |R(\nu^2, \theta_1, \theta_2)| = \frac{1}{2}(P(\nu^2, \theta_1, \theta_2) + 1). \tag{3.3.26}$$

is a stability boundary for the method.

Fig. 3.4 shows an example of three dimensional stability region, while fig. 3.3 shows the projection of three dimensional regions on a particular plane.

3.4 Numerical Results

We now show some numerical results we have obtained applying our families of solvers to some linear and nonlinear problems depending on one or two frequencies, in order to test the accuracy of the derived methods and also to compare them with ones already considered in literature for second order ODEs.

Test 1. We consider the following test equation

$$\begin{cases} y''(x) = -25y(x), \quad x \in [0, 2\pi], \\ y'(0) = y'_0, \\ y(0) = 1 \end{cases} \tag{3.4.1}$$

whose exact solution is $y(x) = \cos(5x)$, so it depends on the frequency $\omega = 5$. We solve this problem using the following solvers:

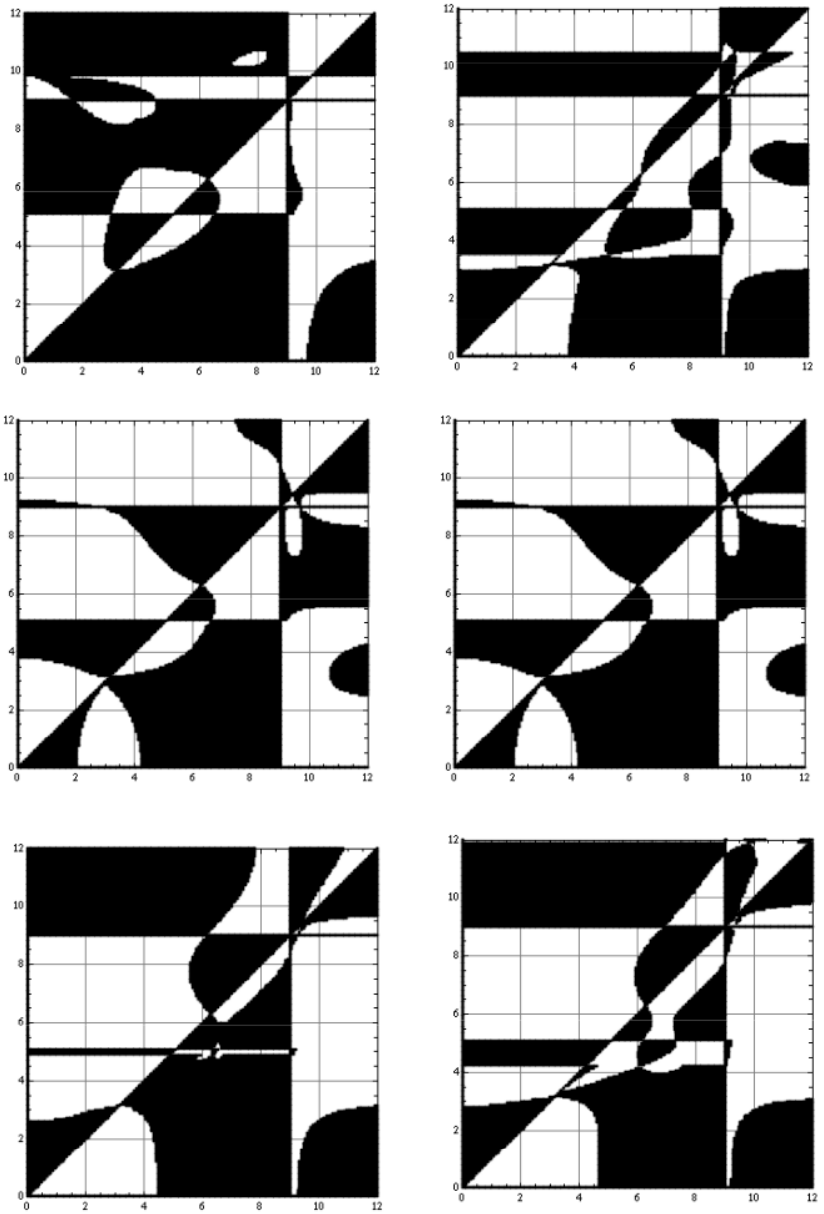

Figure 3.3: Regions of stability in the (ν, θ_1)–plane for the two-step methods for $m = 4$ with nodes $(0, \frac{1}{3}, \frac{2}{3}, 1)$, $(0, \frac{1}{10}, \frac{9}{10}, 1)$, $(0, \frac{2}{5}, \frac{3}{5}, 1)$, $(0, \frac{9}{20}, \frac{11}{20}, 1)$, $(\frac{1}{4}, \frac{3}{4})$, $(\frac{1}{5}, \frac{4}{5})$ respectively.

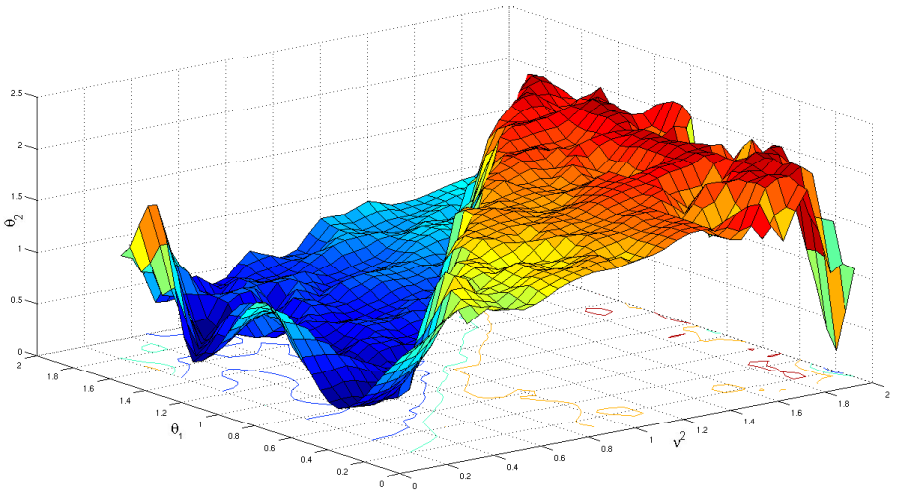

Figure 3.4: Region of stability in the $(\nu^2, \theta_1, \theta_2)$–plane for the two-step methods for $m = 4$ with nodes $(0, \frac{1}{3}, \frac{2}{3}, 1)$.

- COLEM: two–step hybrid method, [30],

$$\begin{array}{c|cc} \frac{1}{\sqrt{6}} & \frac{1+\sqrt{6}}{12} & 0 \\ -\frac{1}{\sqrt{6}} & -\frac{\sqrt{6}}{12} & \frac{1}{12} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \tag{3.4.2}$$

- TRIGFIT1: trigonometrically fitted two–step hybrid method, with 2 stages and order 2, $c = [0, 1]$, derived in 3.3.2,

- TRIGFIT2: trigonometrically fitted two–step hybrid method, with 2 stages and order 2, $c = [0, 3/4]$, derived in 3.3.2,

- TRIGFIT3: trigonometrically fitted two–step hybrid method, with 2 stages and order 2, $c = [3/4, 1]$, derived in 3.3.2,

- POL: two–step hybrid method derived in 3.3.2, with 2 stages and order 2;

- MTRIGFIT: mixed–trigonometrically fitted two–step hybrid method, with 3 stages and order 3,$c = [1/3, 1/2, 1]$, derived in 3.3.2,

- TRIGFIT4S: trigonometrically fitted two–step hybrid method, with 4 stages and order 4, $c = [0, 1/3, 2/3, 1]$, derived in 3.3.2,

The tables shows the global error in the final point of the integration interval, while *cd* is the number of the correct digits. Table 2 compares the new methods

Method	$h = \pi/64$	cd	$h = \pi/128$	cd
COLEM	0.07313	1.1358	0.0042	2.3698
TRIGFIT1	4.21885e-15	14.3748	4.44089e-16	15.3525
TRIGFIT2	4.44089e-15	14.3525	4.44090e-16	15.3530
TRIGFIT3	2.88658e-15	14.539	8.88178e-16	15.0515
POL	0.00286835	2.54236	0.0006948	3.158135
MTRIGFIT	2.22045e-15	14.6536	1.11466e-13	13.9529

Table 3.2: Numerical results for the problem (3.4.1).

with classical ones, having constant coefficients. Trigonometrically fitted methods would solve this kind of problem exactly, of course, in exact arithmetic. The errors are the effect of the accumulation of round off errors in finite precision calculation.

Test 2. The Prothero-Robinson problem

$$y'' + v^2[y - \cos(10x)]^3 = -100y, \quad x \in [0, 20\pi], \tag{3.4.3}$$

with $v >> 0$, $y(0) = 1$, $y'(0) = 0$, whose exact solution is $y(x) = \cos(10x)$, is an example of nonlinear equation, depending on the frequency $\omega = 10$.

Numerical results show that trigonometrically fitted methods and mixed-trigonometrically fitted ones are both *exact* also for this nonlinear problem. Small differences in nu-

Method	$h = \pi/8$	cd	$h = \pi/16$	cd	$h = \pi/32$	cd
TRIGFIT1	4.4409e-16	15.35	8.8818e-15	14.05	6.2172e-15	14.21
TRIGFIT2	1.7745e-15	14.75	4.2188e-15	14.37	6.8834e-15	14.16
TRIGFIT3	1.9984e-15	14.6993	4.21885e-15	14.3748	6.88338e-15	14.1622
MTRIGFIT	9.4058e-13	12.066	1.48992e-13	12.8268	2.18714e-14	13.6601

Table 3.3: Numerical results for the problem (3.4.3).

merical errors are due to the round-off errors.

Test 3. We test our methods also on a well known example of stiff system, from [63, 79]

$$y''(t) = \begin{pmatrix} \mu - 2 & 2\mu - 2 \\ 1 - \mu & 1 - 2\mu \end{pmatrix} y(t), \quad y(0) = \begin{pmatrix} 2 \\ -1 \end{pmatrix}, \; y'(0) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad t \in [0, 20\pi], \tag{3.4.4}$$

where μ is an arbitrary parameter. The exact solution is $y_1(t) = 2\cos t,\ y_2(t) = -\cos t$, i.e. it is independent on μ. When $\mu = 2500$, then (3.4.4) is Kramarz's system [63], which is often used in numerical experiments on stiffness in second order ODEs.

The eigenvalues of the coefficient matrix of the system (3.4.4) are -1 and $-\mu$, so that the analytical solution of the system exhibits the two frequencies 1 and $\sqrt{\mu}$, but the initial conditions eliminate the high frequency component, which corresponds to $\sqrt{\mu}$ when $\mu >> 1$. Notwithstanding this, its presence in the general solution of the system dictates strong restrictions on the choice of the stepsize, so that the system exhibits the phenomenon of *periodic stiffness* [82].

The behaviour of our class of solvers is still similar to the one shown in the previous cases. The choice of the stepsize is such that the methods result stable, and it is possible to integrate this problem with a large stepsize. On the contrary,

Method	$h = \pi/2$	cd	$h = \pi/4$	cd
TRIGFIT3	2.33916e-10	9.63094	1.95534e-9	8.70878
MTRIGFIT	1.44983e-8	7.83868	5.01173e-8	7.30001
TRIGFIT4S	3.80591e-10	9.41954	9.65342e-8	7.01532

Table 3.4: Numerical results for the problem 3.4.4.

methods with constant coefficients are stable only for small values of the stepsize. Anyway Table 4 shows that here we are in the presence of an unstability effect. A natural conclusion is that the advantage of using versions based on trigonometrically fitted coefficients is that they allow obtaining highly accurate results at values of the stepsize which are still big, well before that the unstability effect becomes severe.

STOCHASTIC DIFFERENTIAL EQUATIONS

Chapter 4

Preliminary notions for Stochastic Differential Equations

This chapter provides a short introduction to the numerical treatment of Stochastic Ordinary Differential Equations (SDEs). First we supply some basic notions of probability theory and stochastic calculus, then we give an overview on numerical treatment of stochastic differential equations.

4.1 Introduction

The general form of a stochastic ordinary differential equation (SDE) that will be considered in this thesis is

$$dX(t) = f(t, X(t))dt + G(t, X(t))dW(t) \tag{4.1.1}$$

where W denotes an s-dimensional Wiener process given on the probability space $(\Omega, \mathcal{F}, P)$ with a filtration $(\mathcal{F}_t)_{t\geq 0}$. The drift and diffusion functions are given as $f : [0, T] \times \mathbb{R}^d \to \mathbb{R}^d$ and $G = (g_1, \ldots, g_s) : [0, T] \times \mathbb{R}^d \to \mathbb{R}^{d\times s}$, respectively.
The SDE (4.1.1) is an abbreviation of the stochastic integral equation

$$\begin{aligned} X(\tau)|_0^t &= \int_0^t f(\tau, X(\tau))d\tau + \int_0^t G(\tau, X(\tau))dW(\tau), \\ X(0) &= X_0, \quad t \in [0, T], \end{aligned} \tag{4.1.2}$$

where the first integral is a regular Riemann or Lebesgue integral and the second one is a stochastic integral, which can be interpreted in many ways. In this thesis we work with Itô stochastic differential equations.

It is because analytical solutions are rare for differential equations systems that numerical approximations, equipped with an error estimation, have been developed.

To make this thesis 'self-contained' we recall the basic notions of probability theory and stochastic processes, then we proceed to define the stochastic integral with respect to a Wiener process and to give the Itô formula. Finally we give a brief overview on numerical approximation of the solution of SDEs.

4.2 A general model of two interacting populations

A stochastic differential equation is an important model in science and engineering when noise affects behavior. In this section we will briefly introduce a model of two interacting populations, for more details see [4]. We will follow this procedure:

- a discrete stochastic model for the process is developed by listing the possible changes along with the corresponding probabilities for a short time step Δt,
- the expected change and covariance matrix of the change is calculated for the discrete stochastic process,
- the stochastic differential equation system is obtained by letting the expected change divided by Δt be the drift coefficient and the square root of the covariance matrix divided by Δt be the diffusion coefficient.

This procedure provides in a natural manner an Itô stochastic differential equation model, rather than a Stratonovich stochastic differential equation model.

The approach is applicable to populations of the same species or different species. Let the sizes of the two populations at time t denoted by $x_1(t)$ and $x_2(t)$. Important parameters of the populations are denoted by $b_1,\ d_1,\ b_2,\ d_2,\ m_{12},\ m_{21}$. The parameters b_i and d_i are per capita birth and death rates, respectively, for population i and m_{ij} is the rate of population i which is transformed to population j. For geographically isolated populations, m_{ij} may represent the migration rate of population i to j. For a population undergoing an epidemic, m_{12} may represent the rate a susceptible becomes infected and m_{21} may represent the rate an infected recovers. Each parameter may depend on population sizes x_1 and x_2 and time t, i.e. $b_i = b_i(x_1, x_2, t),\ \ d_i = d_i(x_1, x_2, t)$ and $m_{ij} = m_{ij}(x_1, x_2, t)$, where it is assumed that each parameter is a smooth function of $x_1,\ x_2$, and t. For notational simplicity, the dependence of the parameters on $x_1,\ x_2$ and t is often not explicitly written.
In a small time interval Δt, there are seven possibilities for a population change Δx neglecting multiple births, deaths or transformations in time Δt which have probabilities of order $(\Delta t)^2$. For example $\Delta x_4 = [0, 1]^T$ represents a birth in population x_2 with probability $p_4 = b_2 x_2 \Delta t$. Notice that $\sum_{i}^{7} p_i = 1$. In the following table we show the possible changes in the population system, with the corresponding probabilities.

Change	*Probability*
$\Delta x_1 = [-1, 0]^T$	$p_1 = d_1 x_1 \Delta t$
$\Delta x_2 = [-1, 1]^T$	$p_2 = m_{12} x_1 \Delta t$
$\Delta x_3 = [0, -1]^T$	$p_3 = d_2 x_2 \Delta t$
$\Delta x_4 = [0, 1]^T$	$p_4 = b_3 x_2 \Delta t$
$\Delta x_5 = [1, -1]^T$	$p_5 = m_{21} x_2 \Delta t$
$\Delta x_6 = [1, 0]^T$	$p_6 = b_1 x_1 \Delta t$
$\Delta x_7 = [0, 0]^T$	$p_7 = 1 - \sum_{i=1}^{6} p_i$

It is now of interest to find the mean change $\mathbb{E}[\Delta x]$ and the covariance matrix $\mathbb{E}[\Delta x(\Delta x)^T]$ for the time interval Δt. Neglecting terms of $(\Delta t)^2$,

$$\mathbb{E}[\Delta x] = \sum_{j=1}^{7} p_j \Delta x_j = \begin{pmatrix} b_1 x_1 - d_1 x_1 - m_{12} x_1 + m_{21} x_2 \\ b_2 x_2 - d_2 x_2 - m_{21} x_2 + m_{12} x_1 \end{pmatrix} \Delta t \tag{4.2.1}$$

and

$$\begin{aligned} \mathbb{E}[\Delta x(\Delta x)^T] &= \sum_{j=1}^{7} p_j \Delta x_j (\Delta x_j)^T \\ &= \begin{pmatrix} b_1 x_1 + d_1 x_1 + m_{12} x_1 + m_{21} x_2 & -m_{12} x_1 - m_{21} x_2 \\ -m_{12} x_1 - m_{21} x_2 & b_2 x_2 + d_2 x_2 + m_{21} x_2 + m_{12} x_1 \end{pmatrix} \Delta t. \end{aligned} \tag{4.2.2}$$

As the product $\mathbb{E}[\Delta x](\mathbb{E}[\Delta x])^T$ is of order $(\Delta t)^2$, the covariance matrix V is set equal to $\mathbb{E}[\Delta x(\Delta x)^T]/\Delta t$. It is simple to show that V is positive definite and hence has a positive definite square root B. The vector μ and the matrix V are defined as

$$\mu = \mathbb{E}[\Delta x]/\Delta t = \sum_{j=1}^{7} p_j \Delta x_j = \begin{pmatrix} b_1 x_1 - d_1 x_1 - m_{12} x_1 + m_{21} x_2 \\ b_2 x_2 - d_2 x_2 - m_{21} x_2 + m_{12} x_1 \end{pmatrix} \tag{4.2.3}$$

$$V = \begin{pmatrix} b_1 x_1 + d_1 x_1 + m_{12} x_1 + m_{21} x_2 & -m_{12} x_1 - m_{21} x_2 \\ -m_{12} x_1 - m_{21} x_2 & b_2 x_2 + d_2 x_2 + m_{21} x_2 + m_{12} x_1 \end{pmatrix}. \tag{4.2.4}$$

Following the discussion in [4], the stochastic differential equation model for the dynamics of two interacting populations has the form

$$dx = \mu(t, x_1, x_2)dt + B(t, x_1, x_2)dW(t), \tag{4.2.5}$$

with $x(0) = x_0$ and where $W(t)$ is the two-dimensional Wiener process. The equation (4.2.5) is a stochastic differential equation system that describes the population dynamics; notice that if the matrix B is set equal to zero, then (4.2.5) reduces to a standard deterministic model for population dynamics.

4.3 Some basic notions of probability theory

Now we state only those definitions which are of direct relevance to this thesis, for further details see for example [61], [62], [68].

Definition 4.3.1

A probability space $(\Omega, \mathcal{F}, P)$ consist of the sample space Ω, which is the set of all possible outcomes, a σ-algebra $\mathcal{F}$ of subset of Ω, called events, and a probability measure P on $\mathcal{F}$.

Definition 4.3.2

A σ-algebra $\mathcal{F}$ of subsets of Ω satisfies the following properties:

1. $\Omega \in \mathcal{F}$,
2. $A \in \mathcal{F} \Rightarrow A^c = \{\omega \in \Omega \ \ s.t. \ \ \omega \notin A\} \in \mathcal{F}$,
3. $\{A_n\}_{n\geq 1}, \ A_n \in \mathcal{F}, \ n \geq 1 \Rightarrow \bigcup_{n=1}^{\infty} A_n \in F$.

Definition 4.3.3

A probability measure P on $\mathcal{F}$ must satisfy

1. $P(\Omega) = 1$,
2. $A \in \mathcal{F} \Rightarrow P(A) \geq 0$,
3. $P(A^c) = 1 - P(A)$,
4. $A_i \cap A_j = \emptyset \ for \ i = j \Rightarrow P(\bigcup_{n=1}^{\infty} A_n) = \sum_{n=1}^{\infty} P(A_n)$.

Definition 4.3.4

A filtration $\{\mathcal{F}_t\}_{t\geq 0}$ *is a family of sub* σ*-algebras of* $\mathcal{F}$ *with* $\mathcal{F}_s \subset \mathcal{F}_t$ *for* $0 \leq s \leq t < \infty$.

Definition 4.3.5

A random variable $X(\omega),\ \omega \in \Omega$ *is a Gaussian random variable if it has the Gaussian (or Normal) density function*

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp \frac{-(x-\mu)^2}{2\sigma^2}, \tag{4.3.1}$$

where μ *is the mean and* σ^2 *the variance of the Normal Distribution* $\mathcal{N}(\mu, \sigma^2)$*. If* $\mu = 0,\ \sigma = 1$*, the distribution is called standard Normal distribution.*

Let X and $X_k,\ k \geq 1$, be random variables. The following four convergence modes are very important:

- *Almost Sure Convergence* ($X_k \xrightarrow{a.s.} X$): the sequence $\{X_k\}$ converges almost surely (a.s.) or with probability 1 to X if

$$P(\{\omega \in \Omega : lim_{k\to\infty} X_k(\omega) = X(\omega)\}) = 1;$$

- *Convergence in Probability* ($X_k \xrightarrow{P} X$): the sequence $\{X_k\}$ converges in probability to the random variable X if for all positive ϵ the relation

$$P(|X_k - X| > \epsilon) \to 0, k \to \infty \quad \text{holds;}$$

- L^p*-Convergence* ($X_k \xrightarrow{L^p} X$): let $p > 0$, the sequence $\{X_k\}$ converges in L^p or in p-th mean to X if $\mathbb{E}[|X_k|^p + |X|^p] < \infty$ for all k and $\mathbb{E}|X_k - X|^p \to 0,\ k \to \infty$;

- *Convergence in Distribution* ($X_k \xrightarrow{d} X$): the sequence $\{X_k\}$ converges in distribution, or converges weakly to the random variable X if for all bounded, continuous functions f, $\mathbb{E}[f(X_k)] \to \mathbb{E}[f(X)],\ k \to \infty$.

Observe that $(X_k \xrightarrow{a.s.} X) \Rightarrow (X_k \xrightarrow{P} X) \Rightarrow (X_k \xrightarrow{d} X)$.
$(X_k \xrightarrow{d} X) \Rightarrow (X_k \xrightarrow{P} X)$ if and only if X is constant.
$(X_k \xrightarrow{P} X) \not\Rightarrow (X_k \xrightarrow{a.s.} X)$ but there always exists a subsequence k_l such that $(X_k \xrightarrow{P} X) \Rightarrow (X_{k_l} \xrightarrow{a.s.} X)$.

4.4 The theory of stochastic differential equations

4.4.1 Stochastic processes

Definition 4.4.1

Let be in the probability space $(\Omega, \mathcal{F}, P)$, and let consider an arbitrary set I. A family $\{X(t)\}_{t\in I}$ of $\mathbb{R}^d$-valued random variables is called a stochastic processes with parameter set I and state space $\mathbb{R}^d$.

Observe that for each fixed $t \in I$ we have a random variable $\omega \in \Omega \to X(t,\omega) \in \mathbb{R}^d$. In the other hand, for each fixed $\omega \in \Omega$ we have a function $t \in I \to X(t,\omega) \in \mathbb{R}^d$, which is called a sample path (or trajectory) of the process.

Definition 4.4.2

A stochastic process $X(t)$ is adapted to a filtration $\{\mathcal{F}_t\}_{t\geq 0}$ if, for every $t \geq 0$, $X(t)$ is $\mathcal{F}_t$-measurable.

Brownian motion is the name given to the irregular movement of particles, suspended in a fluid, observed by the Scottish botanist Robert Brown in 1828. Louis Bachelier (1900), Albert Einstein (1905) and Nobert Wiener (1923) began developing the mathematical theory of Brownian motion, but Wiener was the first to put Brownian motion on a firm mathematical basis.

Definition 4.4.3

Let $(\Omega, \mathcal{F}, P)$ be a probability space with a filtration $\{\mathcal{F}_t\}_{t\geq 0}$. A standard one-dimensional Wiener process is a real-valued $\{\mathcal{F}_t\}$-adapted process $W(t)_{t\geq 0}$ with the following properties:

1. $W(0) = 0$ *almost surely;*

2. *for* $0 \leq s < t < \infty$, *the increment* $W(t) - W(s)$ *is normally distributed with mean zero and variance* $t - s$ $((W(t) - W(s)) \equiv \mathcal{N}(0, t - s))$;

3. *for* $0 \leq s < t < \infty$, *the increment* $W(t) - W(s)$ *is independent of* $\mathcal{F}_s$.

If $W(t)$ is a Wiener process and $0 \leq t_0 < t_1 < \cdots < t_k < \infty$, then the increments $W(t_i) - W(t_{i-1}),\ 1 \leq i \leq k$ are independent and we say that it has independent increments. Moreover, the distribution of $W(t_i) - W(t_{i-1})$ depends only on the difference $t_i - t_{i-1}$ and we say that the Wiener process has stationary increments.

Definition 4.4.4

An s-dimensional Wiener process $W(t)$ *is a vector* $(W_1(t), W_2(t), \ldots, W_s(t))$ *of* s *independent one dimensional Wiener process.*

4.4.2 Stochastic Integrals

Now we shall introduce the stochastic integral

$$\int_0^t G(\tau, X(\tau))dW(\tau) \tag{4.4.1}$$

with respect to an s-dimensional Wiener process $W(t)$ for a class of $d \times s$ matrix valued stochastic processes $\{G(\tau, X(\tau))\}$. For almost all $\omega \in \Omega$, the Wiener trajectory is nowhere differentiable. The variance of the Wiener process satisfies $Var(W(t)) = t$, so this increases as time increases even though the mean stays at 0. Because of this, typical sample paths of a Wiener process attain larger values in magnitude as time progresses, and consequently the sample paths of the Wiener process are not of bounded variation; hence the integral can not be defined as a Riemann-Stieltjes integral in the classical calculus way.

An approximation of the stochastic integral by the sums

$$\sum_{i=1}^{N} G(\tau_i, X(\tau_i))[W(t_i) - W(t_{i-1})] \tag{4.4.2}$$

converges in the mean square sense to different values of this integral, for various $\tau_i \in [t_{i-1}, t_i]$.

In particular for $\tau_i = t_{i-1}$ the integral is known as the *Itô integral* and this leads to a calculus based on Itô chain rule.

If $\tau_i = \frac{t_i + t_{i-1}}{2}$ then the resulting integral is the *Stratonovich integral*.

In order that the Itô stochastic integral $\int_0^t X(t)dW(t)$ be defined, for $X(t)$ a real-valued stochastic process with respect to the Wiener process $W(t)$, it is necessary that $X(t)$ and $W(t)$ are both defined on the same probability space $(\Omega, \mathcal{F}, P)$. It is also necessary that $X(t)$ be non-anticipating, by which it is meant that information about $X(t)$ does not depend on event occurring after time t. The stochastic Itô integral has some nice properties.

Theorem 4.4.1

Let $f, g \in \mathcal{M}^2([a,b];\mathbb{R})$, where $\mathcal{M}^2([a,b];\mathbb{R})$ is the space of all real-valued measurable $\{\mathcal{F}_t\}$-adapted stochastic processes $f \in L^2([a,b],\mathbb{R})$ such that $E(\int_a^b |f|^2 ds) < \infty$ almost surely; and let α, β be two real numbers. Then

1. $\int_a^b f(t)dW(t)$ *is $\mathcal{F}_b$-measurable,*
2. $E\int_a^b f(t)dW(t) = 0$,
3. $E|\int_a^b f(t)dW(t)|^2 = E\int_a^b |f(t)|^2 dt$,
4. $\int_a^b [\alpha f(t) + \beta g(t)]dW(t) = \alpha \int_a^b f(t)dW(t) + \beta \int_a^b g(t)dW(t)$.

In this thesis we will deal with SDEs in Itô form, for this reason we will introduce only the Itô calculus; for more details on Itô and Stratonovich calculus see [47], [68].

4.4.3 Itô's formula

We have introduced the Itô stochastic integrals, however as for classical Lebesgue integrals, the basic definition of the integrals is not very convenient in evaluating a given integral. We shall now establish the stochastic version of the chain rule for Itô

integrals, the Itô formula, that plays a key role in stochastic analysis.
Consider the stochastic differential equation (4.1.2), then, for a given function F and with certain smoothness, measurability and boundedness properties on F, f and g in (4.1.2) to guarantee the existence, pathwise uniqueness and bounded second moments, the multi-dimensional stochastic chain rule gives

$$dF(t,X) = \Big(\frac{\partial F}{\partial t} + \frac{\partial F}{\partial X}f + \frac{1}{2}trace\Big(GG^T\frac{\partial^2 F}{\partial X^2}\Big)\Big)dt + \frac{\partial F}{\partial X}GdW. \tag{4.4.3}$$

In the scalar case we have

$$dF(t,X) = \Big(\frac{\partial F}{\partial t} + \frac{\partial F}{\partial X}f + \frac{1}{2}\Big(\frac{\partial^2 F}{\partial X^2}g^2\Big)\Big)dt + \frac{\partial F}{\partial X}gdW. \tag{4.4.4}$$

4.4.4 Itô or Stratonovich?

There is much discussion in the literature about when to use the Itô instead of the Stratonovich interpretation of the integral, [22], [62], and while both approaches are appropriate, the choice depends on the modeling process that leads to the SDE formulation. As stated before in this thesis we are interested in Itô SDEs, to distinguish the Stratonovich form of the SDEs, we use the symbol $\circ$. Indeed, it is possible to convert from one interpretation to the other in order to take advantage of the particular features of one of the approaches as appropriate.

Theorem 4.4.2

If $X(t)$ satisfies the Itô SDE

$$dX(t) = f(t,X(t)dt + G(t,X(t))dW(t), \tag{4.4.5}$$

then it is also a solution of the Stratonovich SDE

$$dX(t) = \Big(f(t,X(t)) - \frac{1}{2}\frac{\partial G}{\partial X}(t,X(t))G(t,X(t))\Big)dt + G(t,X(t)) \circ dW(t). \tag{4.4.6}$$

4.4.5 Stochastic Differential Equations

Definition 4.4.5

A process $X = \{X(t)\}_{t\in[0,T]}$, on $(\Omega, \mathcal{F}, \{\mathcal{F}_t\}, P)$, with values in $\mathbb{R}^d$, is called a strong solution of the stochastic differential equation (4.1.2), with respect to the fixed Wiener process W and the initial condition X_0, if the following properties hold:

1. *X is adapted to the filtration $\{\mathcal{F}_t\}_{t\in[0,T]}$;*

2. *X has continuous sample paths;*

3. *the integrals in (4.1.2) exist, X_0 is $\mathcal{F}_t$-measurable and independent of W;*

4. *for all $t \in [0, T]$*

$$X(t) = X_0 + \int_0^t f(s, X(s))ds + \int_0^t G(s, X(s))dW(s), \tag{4.4.7}$$

holds almost surely.

Let the initial condition and the Wiener process be given. Then the solution $X(t)$ of the SDE should be determined in a non-ambiguous way.

Theorem 4.4.3

Suppose that the drift coefficient f, and the diffusion one G, satisfy the global Lipschitz and linear growth conditions:

$$||f(t,x) - f(t,y)|| + ||G(t,x) - G(t,y)|| \leq k||x - y||, \tag{4.4.8}$$

$$||f(t,x)||^2 + ||G(t,x)||^2 \leq k^2(1 + ||x||^2), \tag{4.4.9}$$

for every $t \in [0, T]$, $x, y \in \mathbb{R}^d$, where k is a positive constant. Let X_0 be a $\mathbb{R}^d$-valued random vector, independent of the Wiener process W and with $\mathbb{E}(||X_0||^2)^{2l} < \infty$, for some $l \in \mathbb{N}$. Then there exists a continuous, adapted process $X = X(\cdot)$ which is a unique strong solution of SDE relative to W, with initial condition X_0.

4.5 Stochastic Multiple Integrals

Now we shall introduce some notations in order to allow us to formulate Itô Taylor (and analogously Stratonovich-Taylor) expansions in a way that will simplify the presentation. A multiple Itô integral is defined as

$$I_{j_1,j_2,\ldots,j_l}^{t_1,t_2}(f) := \int_{t_1}^{t_2} \int_{t_1}^{s_1} \ldots \int_{t_1}^{s_{l-1}} f(s_l, X(s_l)) dW_{j_1}(s_1) \ldots dW_{j_l}(s_l) \tag{4.5.1}$$

where $dW_0(s) = ds$. If $f \equiv 1$ then we write $I_{j_1,j_2,\ldots,j_l}^{t_1,t_2}$.
Similarly we can define a multiple Stratonovich integral as

$$J_{j_1,j_2,\ldots,j_l}^{t_1,t_2}(f) := \int_{t_1}^{t_2} \int_{t_1}^{s_1} \ldots \int_{t_1}^{s_{l-1}} f(s_l, X(s_l)) \circ dW_{j_1}(s_1) \cdots \circ dW_{j_l}(s_l). \tag{4.5.2}$$

Example:

$$I_0^{t_1,t_2} = \int_{t_1}^{t_2} dW_0(s) = t_2 - t_1; \tag{4.5.3}$$

$$I_r^{t_1,t_2} = \int_{t_1}^{t_2} dW_r(s) = W_r(t_2) - W_r(t_1) \simeq \sqrt{t_2 - t_1}\mathcal{N}(0,1). \tag{4.5.4}$$

Some multiple stochastic integrals can be expressed in terms of lower multiple integrals, while other must be approximated.
There are also some relationships between stochastic integrals; for example

$$I_0 I_r = I_{0r} + I_{r0} \tag{4.5.5}$$

$$I_{rr} = \frac{I_r^2 - I_0}{2} \tag{4.5.6}$$

$$I_r = J_r \tag{4.5.7}$$

$$J_0 J_r = J_{0r} + J_{r0} \tag{4.5.8}$$

$$J_{rr} = \frac{J_r^2}{2} \tag{4.5.9}$$

$$I_{rr} = J_{rr} - \frac{I_0}{2}. \tag{4.5.10}$$

It is also necessary, when studying the order of convergence of numerical methods, to be able to determine the expected value of multiple stochastic integrals. The

following lemma, see [70] and [71], provides a means of calculating these expected values.

Lemma 4.5.1

For every function $f \in [0,T] \times \mathbb{R}^d \Rightarrow \mathbb{R}^d$ such that $|f(t,x)| \leq k(1+|x|^2)^{\frac{1}{2}}$, it holds for all $t, t+h \in [0,T]$ that:

$$\begin{aligned} \mathbb{E}(I^{t,t+h}_{(j_1,j_2,\ldots,j_l)}(f)) &= 0, \text{ if } j_k = 0 \text{ for at least one } \ k = 1,\ldots,l, \quad (4.5.11) \\ |I^{t,t+h}_{(j_1,j_2,\ldots,j_l)}(f)| &= O(h^{l_1+\frac{l_2}{2}}), \end{aligned}$$

where l_1 is the number of null indices while l_2 is the number of non zero indices.

In the implementation of the numerical method, these integrals have to be simulated together with the Wiener increments, this can be done following [49], [62], [70], [71].

4.6 Itô Taylor Expansions

In order to derive the expansions, the Itô formula is applied successively to the SDE (4.1.2).

Let $C^{k-1,k}$ denote the class of all functions, F from $[0,T] \times \mathbb{R}^d$ to $\mathbb{R}^d$ having continuous partial derivatives up to order $k-1$ with respect to the first variable and, in addition, continuous partial derivatives of order k with respect to the second variable. We introduce operators Λ_0 and Λ_r, $r = 1,\ldots,s$, defined on $C^{1,2}$ and $C^{0,1}$, respectively, by

$$\Lambda_0 F = F'_t + F'_x[f] + \frac{1}{2}\sum_{r=1}^{s} F''_{xx}[g_r, g_r]\,, \quad \Lambda_r F = F'_x[g_r]\,, \quad r = 1,\ldots,s. \qquad (4.6.1)$$

Here and subsequently the square brackets are used to denote elementary differentials, see, e.g., [27]. Using the operators (4.6.1) and the notation for multiple stochastic integrals (4.5), the Itô formula for a function F in $C^{1,2}$ and the solution X of (4.1.2) reads

$$F(t,X(t)) = F(u,X(u)) + I_0^{u,t}(\Lambda_0 F) + \sum_{r=1}^{m} I_r^{u,t}(\Lambda_r F), \quad 0 \leq u < t \leq T. \qquad (4.6.2)$$

Applying the Itô formula to the drift and diffusion coefficients f, g_r, which are assumed to be in $C^{1,2}$, and inserting the results into the SDEs (4.1.2) leads to the first terms of the Itô-Taylor (or Wagner-Platen) expansion of the solution $X(t)$ for $0 \leq u < t \leq T$:

$$\begin{aligned} X(t) &= X(u) + I_0^{u,t}(f) + \sum_{r=1}^{s} I_r^{u,t}(g_r) \qquad (4.6.3) \\ &= X(u) + f(u, X(u)) I_0^{u,t} + \sum_{r=1}^{s} g_r(u, X(u)) I_r^{u,t} \\ &\quad + I_{00}^{u,t}(\Lambda_0 f) + \sum_{r=1}^{s} \left(I_{r0}^{u,t}(\Lambda_r f) + I_{0r}^{u,t}(\Lambda_0 g_r) \right) + \sum_{r,q=1}^{s} I_{qr}^{u,t}(\Lambda_q g_r) \,. \end{aligned}$$

4.7 An Overview on Numerical Methods for Stochastic Differential Equations

Unfortunately explicitly solvable SDEs are rare in practical applications. Over last decades an increasing number of numerical methods for the approximation of the solution of a stochastic differential equation have been developed. Obviously such methods should be implementable on digital computers. They often involve the simulation of a large number of different sample paths in order to estimate various statistical features of the solution.

The most efficient and widely applicable approach to solving SDEs seems to be the simulation of sample paths of time discrete approximations on digital computers. This is based on a finite discretization of the sample paths step by step at the discretization times. The simulated sample paths can then be analysed by usual statistical methods to determine how good the approximation is and in what sense it is close to the exact solution. An advantage of considerable practical importance of this approach is that the computational costs such as time and memory required increase only polynomially with the dimension of the problem.

Simulation studies and theoretical investigations showed that not all heuristic time

discrete approximations of a SDE converge in a usual sense to the solution process as the maximum step size tends to zero. In particular, it was found that one cannot simply use a deterministic numerical methods for ordinary differential equations. So a careful and systematic investigation of different methods is needed in order to select a sufficiently efficient method for the task at hand.

Now we introduce the Euler-Maruyama scheme and we give the definitions of strong and weak approximations.

Let us consider a SDE (4.1.1) and a discretisation $0 < t_1 < \cdots < t_n = T$ of the time interval $[0, T]$. The Euler-Maruyama scheme is defined by

$$\begin{aligned} y_0 &= X_0 \\ y_{n+1} &= y_n + h_n f(t_n, y_n) + G(t_n, y_n) I_r^{t_n, t_n+h_n}, \end{aligned} \tag{4.7.1}$$

with $h_n = t_{n+1} - t_n$, $I_r^{t_n,t_n+h_n} = W(t_{n+1}) - W(t_n)$, $n = 0, 1, ..., N-1$. In order to determine the order of accuracy of a discrete time approximation we need a criterion. We can distinguish between situations where a good pathwise approximation is required and situations we are interested in approximating expectations of functionals of the Itô process. If we are interested in pathwise approximations required in direct simulations, we follow the concept of strong convergence.

Definition 4.7.1

We say that a discrete time approximation Y converges strongly with order p at time T if there exists a positive constant C, which does not depend on the maximum stepsize $\mathbf{h}$, and a h_0 such that

$$\mathbb{E}[||X(t) - Y(t)||] \leq C\mathbf{h}^p \tag{4.7.2}$$

holds for each $\mathbf{h} \in]0, h_0[$.

In contrast to deterministic schemes we have to point out that the strong order of convergence needs not to be integer valued in the stochastic setting.

On the other hand, if we are interested in the approximation of some higher moment

or of the expectation of some functional $f : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$ of the solution, we need to consider the rate of weak convergence. Let $C_P^d(\mathbb{R}, \mathbb{R}^n)$ denote the space of d times continuously differentiable functions $f \in C^d(\mathbb{R}, \mathbb{R}^n)$ for which all the partial derivatives up to order d have polynomial growth.

Definition 4.7.2

We say that a discrete time approximation Y with maximum stepsize $\mathbf{h}$ converges weakly with order p to X at time T, as $\mathbf{h}$ goes to 0, if for each $f \in C_P^{2(p+1)}(\mathbb{R}, \mathbb{R}^d)$ there exist positive constant C, which does not depend on $\mathbf{h}$, and h_0 such that

$$|\mathbb{E}[f(X_T)] - \mathbb{E}[f(Y_T)]| \leq C\mathbf{h}^p \tag{4.7.3}$$

holds for each $\mathbf{h} \in]0, h_0[$.

It is possible to prove that the Euler-Maruyama method converges with weak order $p = 1$ in contrast to the strong order 0.5.

It is easy to construct schemes of higher order of convergence than this scheme. It is possible to calculate strong and weak schemes of arbitrarily high order of convergence using stochastic Taylor expansions. However these methods are not very handsome for high orders p. We have to calculate the partial derivatives appearing in the expansion and we have to simulate the multiple stochastic integrals.

As a result of this, the development of efficient numerical methods focuses on schemes where we are able to approximate multiple stochastic integrals by random variables in a simple way and we are interested in derivatives free schemes.

Chapter 5

Analysis of SRK methods using Albrecht's approach

We consider stochastic methods of Runge-Kutta type (SRK) for Itô stochastic ordinary differential equations (SDEs) and introduce Albrecht's approach for their analysis. We show its advantages in the convergence analysis and in the derivation of order conditions for the method as well as for the internal stages.

5.1 Introduction

There is a rich literature on stochastic Runge-Kutta schemes. In one of the first papers on this topic, Rümelin [91] considered the mean-square convergence of explicit Runge-Kutta schemes, where only increments of the Wiener process were used for the approximation of the diffusion term. He proved that the stochastic improved Euler (or Heun) scheme converges in the mean-square sense to the solution of the Stratonovich version of the SDEs (4.1.2). For SDEs with a scalar Wiener process or with commutative noise the order of mean-square convergence of this scheme is 1. He also treated scalar SDEs as well as systems of equations driven by a multi-dimensional Wiener process. In the papers [17, 18, 19, 21, 22] the authors also have studied classes of stochastic Runge-Kutta methods for Stratonovich SDEs and have developed schemes up to order 1.5 in the mean-square sense. To obtain appropriate order conditions in a systematic way they have generalised the theory of Butcher trees to the stochastic setting.

An approach to approximate Itô and Stratonovich SDEs with a scalar Wiener process with convergence of order 1 is presented in [72]. For the Itô case this goal is achieved by including terms into the schemes that involve the square root of the step-size. Additionally using terms that involve mixed classical stochastic integrals, schemes with order 1.5 are developed in [86] for Itô SDEs with scalar noise. Further, strong convergence of stochastic Runge-Kutta methods and Runge-Kutta-type methods have been discussed in [15, 62, 71]. In the context of weak approximations of SDEs stochastic Runge-Kutta methods have been studied, e.g., in [85, 87, 88, 89, 90].

5.2 The methods and Albrecht's idea, stochastic version.

Let us consider a deterministic grid $t_0 < t_1 < \ldots < t_N = T$ with stepsizes

$h_n := t_{n+1} - t_n$, we denote by Y_n the numerical approximation of the exact solution value $X(t_n)$ at the time-point t_n generated by a numerical scheme of the form

$$\begin{aligned} y_0 &= X_0, \\ y_{n+1} &= y_n + h_n \sum_{i=1}^{m} \beta_i f(t_n + c_i h_n, Y_i^{[n]}) + \sum_{i=1}^{m} \Upsilon_i(t_n + \hat{c}_i h_n, \hat{Y}_i^{[n]}) I^{t_n, t_n+h_n} \\ Y_i^{[n]} &= y_n + h_n \sum_{j=1}^{m} a_{ij} f(t_n + c_j h_n, Y_j^{[n]}) + \sum_{j=1}^{m} \Psi_j(t_n + \hat{c}_j h_n, \hat{Y}_j^{[n]}) I^{t_n, t_n+c_j h_n}, \\ \hat{Y}_i^{[n]} &= y_n + h_n \sum_{j=1}^{m} \hat{a}_{ij} f(t_n + c_j h_n, Y_j^{[n]}), \quad i = 1, ..., m. \end{aligned} \tag{5.2.1}$$

The weights $c_i, \hat{c}_i$ are chosen as $c = Ae,\ \hat{c} = \hat{A}e$, with $e = (1, \cdots, 1)^T$. The functions Υ and Ψ are finite sums of appropriate terms

$$\begin{aligned} \Upsilon_j(t,x) I^{t_n, t_n+h_n} &= \sum_{r=1}^{s} \gamma_j g_r(t,x) I_r^{t_n, t_n+h_n} + \sum_{r=1}^{s} \eta_j g_r(t,x) \frac{I_{r0}^{t_n, t_n+h_n}}{h_n} + \cdots \\ \Psi_j(t,x) I^{t_n, t_n+c_i h_n} &= \sum_{r=1}^{s} b_{ij} g_r(t,x) I_r^{t_n, t_n+c_i h_n} + \sum_{r=1}^{s} d_{ij} g_r(t,x) \frac{I_{r0}^{t_n, t_n+c_i h_n}}{h_n} + \cdots \end{aligned} \tag{5.2.2}$$

I^{t_n, t_n+h_n} denotes a collection of multiple stochastic integrals $I_{r_1, r_2, ..., r_j}^{t_n, t_n+h_n}$ over the subinterval $[t_n, t_n + h_n] \subseteq [0, T]$, or also terms involving combinations of stochastic integrals. Further, we denote by $|\cdot|$ the Euclidean norm in $\mathbb{R}^d$, by $\|\cdot\|$ the corresponding induced matrix norm and by $\|Z\|_{L_2} := (\mathbb{E}|Z|^2)^{1/2}$ the norm of a vector-valued square-integrable random variable $Z \in L_2(\Omega, \mathbb{R}^d)$.

We use this generic notation in order to cover all Runge-Kutta methods considered in this thesis. The methods that we analyse could be also drift-implicit. In that case one has to consider the solvability of the implicit equation to arrive at a method that can be described by (5.2.1). The required techniques are analogous to those in the deterministic setting as described, e.g., in [52, Thm. II.7.2].

The starting point in the construction of new methods is the derivation of order conditions. In this context there are mainly two way to do this:

- Taylor expansions, widely introduced and used by Kloeden [62].

- Butcher trees, extended in the stochastic framework by Burrage and Burrage [22]. They expanded the rooted trees theory, well known in the deterministic context, [25], by the use of bi-coloured nodes for the stochastic setting.

We have extended the classical approach introduced by Albrecht in 1987, [2], in the deterministic context. Applying Albrecht's approach to a Stochastic Runge–Kutta method we are able to linearise it and so we can carry out our analysis as done in the context of multistep linear methods, [13], [14]. Moreover we are also able to provide stage order conditions, up to now never considered.
Remember that we denote by $X(t)$, the value of the exact solution of the SDEs (4.1.2) at time t that satisfies the initial condition $X(0) = X_0$. We define

$$\begin{aligned}
\mathcal{Z}_{n+1} &:= [Y_1^{[n]}, \dots, Y_m^{[n]}, \hat{Y}_1^{[n]}, \dots, \hat{Y}_m^{[n]}, y_{n+1}]^T \qquad (5.2.3)\\
F(t_n, \mathcal{Z}_{n+1}; h_n) &:= [f(t_n + c_1 h_n, Y_1^{[n]}), \dots, f(t_n + c_m h_n, Y_m^{[n]}),\\
&\quad f(t_n + \hat{c}_1 h_n, \hat{Y}_1^{[n]}), \dots, f(t_n + \hat{c}_m h_n, \hat{Y}_m^{[n]}), f(t_{n+1}, y_{n+1})]^T\\
\mathcal{G}(t_n, \mathcal{Z}_{n+1}; h_n) &:= [G(t_n + c_1 h_n, Y_1^{[n]}), \dots, G(t_n + c_m h_n, Y_m^{[n]}),\\
&\quad G(t_n + \hat{c}_1 h_n, \hat{Y}_1^{[n]}), \dots, G(t_n + \hat{c}_m h_n, \hat{Y}_m^{[n]}), G(t_{n+1}, y_{n+1})]^T
\end{aligned}$$

We can rewrite the Runge-Kutta method as a linear multistep method

$$\begin{aligned}
\mathcal{Z}_0 &= X_0,\\
\mathcal{Z}_{n+1} &= \mathcal{A}\mathcal{Z}_n + h_n \mathcal{B} F(t_n, \mathcal{Z}_{n+1}; h_n) + \Gamma(t_n, \mathcal{Z}_{n+1}; h_n) I^{t_n, t_n + h_n}\\
&\quad + \Xi(t_n, \mathcal{Z}_{n+1}; h_n) I^{t_n, t_n + c h_n}, \qquad (5.2.4)
\end{aligned}$$

where Γ and Ξ are the tensorial version of Υ and Ψ

$$\begin{aligned}
\Gamma(t_n, \mathcal{Z}_{n+1}; h_n) I^{t_n, t_n + h_n} &= \mathcal{C}_1 \mathcal{G}(t_n, \mathcal{Z}_{n+1}; h_n) I_r^{t_n, t_n + h_n}\\
&+ \mathcal{C}_2 \mathcal{G}(t_n, \mathcal{Z}_{n+1}; h_n) \frac{I_{r0}^{t_n, t_n + h_n}}{h_n} + \cdots \qquad (5.2.5)\\
\Xi(t_n, \mathcal{Z}_{n+1}; h_n) I^{t_n, t_n + c h_n} &= \mathcal{D}_1 \mathcal{G}(t_n, \mathcal{Z}_{n+1}; h_n) I_r^{t_n, t_n + c h_n}\\
&+ \mathcal{D}_2 \mathcal{G}(t_n, \mathcal{Z}_{n+1}; h_n) \frac{I_{r0}^{t_n, t_n + c h_n}}{h_n} + \cdots
\end{aligned}$$

and $\mathcal{A}$, $\mathcal{B}$, $\mathcal{C}_k$, $\mathcal{D}_k$ are block matrices of dimension $(2m+1)\times(2m+1)$. For example

$$\mathcal{A}=\begin{pmatrix} 0_{mm} & 0_{mm} & e \\ 0_{mm} & 0_{mm} & e \\ 0_m & 0_m & 1 \end{pmatrix},\ \mathcal{B}=\begin{pmatrix} A & 0_{mm} & 0_m \\ \hat{A} & 0_{mm} & 0_m \\ \beta^T & 0_m & 0 \end{pmatrix} \tag{5.2.6}$$

with $A=(a_{ij})_{i,j=1}^m$, $\hat{A}=(\hat{a}_{ij})_{i,j=1}^m$, $\beta=[\beta_1,\ldots,\beta_m]$, 0_{mm} is the $m\times m$ null matrix and 0_m is the m null vector. The matrices $\mathcal{C}_k,\ \mathcal{D}_k,\ k=1,2,\ldots,$ depend on the particular method, in the sense that they depend on how many and which multiple integrals we use. As Albrecht did for deterministic ODEs, we can associate with the method (5.2.4) some linear differential operators. We define

$$\begin{aligned}
\mathcal{L}[X(t_n);h_n] &:= X(t_n+h_n)-X(t_n)-h_n\sum_{i=1}^m \beta_i f(t_n+c_ih_n,X(t_n+c_ih_n)) \\
&- \sum_{i=1}^m \Upsilon(t_n+\hat{c}_ih_n,X(t_n+\hat{c}_ih_n))I^{t_n,t_n+h_n}, \qquad (5.2.7)\\
\mathcal{L}_i[X(t_n);h_n] &:= X(t_n+c_ih_n)-X(t_n)-h_n\sum_{j=1}^m a_{ij} f(t_n+c_jh_n,X(t_n+c_jh_n)) \\
&- \sum_{j=1}^m \Psi_j(t_n+\hat{c}_jh_n,X(t_n+\hat{c}_jh_n))I^{t_n,t_n+c_ih_n}, \qquad (5.2.8)\\
\hat{\mathcal{L}}_i[X(t_n);h_n] &:= X(t_n+\hat{c}_ih_n)-X(t_n)-h_n\sum_{j=1}^m \hat{a}_{ij} f(t_n+c_jh_n,X(t_n+c_jh_n)). \\
& \qquad (5.2.9)
\end{aligned}$$

5.3 Convergence framework

We list now some definitions we use in the following section.

Definition 5.3.1

We call the stochastic Runge-Kutta method (5.2.1) *for the approximation of the solution of the SDEs* (4.1.2) *mean-square convergent if the global error* $X(t_n)-X_n$ *satisfies*

$$\max_{n=1,\ldots,N}\|X(t_n)-X_\ell\|_{L_2}\to 0 \text{ as } h\to 0, \tag{5.3.1}$$

we say it is mean-square convergent with order γ ($\gamma > 0$) *if the global error satisfies*

$$\max_{\ell=1,\dots,N} \|X(t_\ell) - X_\ell\|_{L_2} \leq C \cdot h^\gamma, \tag{5.3.2}$$

with a grid-independent constant $C > 0$.

We aim to conclude mean square convergence from local properties of the method by means of numerical stability in the mean-square sense. Numerical stability concerns the influence of perturbations of the right-hand side of the discrete scheme on the global solution of that discrete scheme. Sources of perturbations may be the local error, round-off errors or defects in the approximate solution of implicit schemes. The mean-square stability estimate of the global error is based on the mean square norm and on the conditional mean of the perturbations. Thus we consider the following discrete system, the perturbed form of (5.2.4),

$$\begin{aligned} \mathcal{Z}_0 &= X_0 + \delta_0 \\ \mathcal{Z}_{n+1} &= \mathcal{A}\mathcal{Z}_n + h_n \mathcal{B} F(t_n, \mathcal{Z}_{n+1}; h_n) + \Gamma(t_n, \mathcal{Z}_{n+1}; h_n) I^{t_n, t_n+h_n} \\ &+ \Xi(t_n, \mathcal{Z}_{n+1}; h_n) I^{t_n, t_n+ch_n} + \delta_n, \end{aligned} \tag{5.3.3}$$

we suppose that the perturbations δ_n, $n = 0, \cdots, N-1$ are $\mathcal{F}_{t_n}$-measurable and that $\delta_n \in L_2(\Omega, \mathbb{R}^n)$.

Remark 5.3.1

Sometimes it is useful to represent the perturbations in the form $\delta_n = R_n + S_n$, *where* S_n *is* $\mathcal{F}_{t_n}$*-measurable with* $\mathbb{E}(S_n|\mathcal{F}_{t_{n-1}}) = 0$.

We state the following definitions.

Definition 5.3.2

A function $F : [0,T] \times \mathbb{R}^n \to \mathbb{R}^n$ *satisfies a uniform Lipschitz condition with respect to its second variable if there exists a positive constant* L_F *such that*

$$|F(t,x) - F(t,y)| \leq L_F |x - y| \quad \forall\ x, y \in \mathbb{R}^n,\ t \in [0,T]. \tag{5.3.4}$$

A function $\Gamma : [0,T]\times\mathbb{R}^n \to \mathbb{R}^{n\times s}$ *satisfies a uniform Lipschitz condition with respect to its second variable if there exists a positive constant* L_Γ *such that*

$$|F(t,x) - F(t,y)| \le L_\Gamma |x-y| \quad \forall\ x,y \in \mathbb{R}^n,\ t \in [0,T]. \tag{5.3.5}$$

Let $C^{l,l-1}$ *denote the class of all functions from* $[0,T]\times\mathbb{R}^n$ *to* $\mathbb{R}^n$ *having continuous partial derivatives up to order* $l-1$ *and, in addition, continuous partial derivatives of order* l *with respect to the first variable.*
Let C^K *denote the class of function* $z : [0,T]\times\mathbb{R}^n \to \mathbb{R}^n$ *that satisfy a linear growth condition in the form*

$$|z(t,x)| \le K(1+|x|^2)^{\frac{1}{2}},\ \forall x \in \mathbb{R}^n, t \in [0,T]. \tag{5.3.6}$$

Now we give the formal definition of mean square stability and consistency.

Definition 5.3.3

We call the stochastic Runge-Kutta method (5.2.1) numerically stable in the mean-square sense if there exist constants $h_0 > 0$ *and* $S > 0$ *such that for all stepsizes* $h < h_0$ *and for all* $\mathcal{F}_{t_n}$*-measurable perturbations* $\delta_n \in L_2(\Omega,\mathbb{R}^n)$ $(n = 0,\dots,N)$ *and all their representations, the following inequality holds*

$$\max_{n=0,\dots,N} \|X_n - \tilde{X}_n\|_{L_2} \le S\Big\{ \max_{n=0,\dots,k-1} \|\delta_n\|_{L_2} + \max_{n=k,\dots,N} \big(\frac{\|R_n\|_{L_2}}{h} + \frac{\|S_n\|_{L_2}}{h^{1/2}}\big)\Big\}, \tag{5.3.7}$$

where $(X_n)_{n=1}^N$ *and* $(\tilde{X}_n)_{n=1}^N$ *are the solutions of the (5.2.4) and the perturbed discrete system (5.3.3), respectively.*

We refer to S as the stability constant and to (5.3.7) as the stability inequality.

Definition 5.3.4

We call the stochastic Runge-Kutta method (5.2.1) for the approximation of the solution of the SDEs (4.1.2) mean-square consistent if the local error $\mathcal{L}[X(t_n);h_n]$ *satisfies*

$$h^{-1}\ \|\mathbb{E}(\mathcal{L}[X(t_n);h_n]|\mathcal{F}_{t_n})\|_{L_2} \to 0 \text{ for } h \to 0, \quad \text{and}$$

$$h^{-1/2}\ \|\mathcal{L}[X(t_n);h_n]\|_{L_2} \to 0 \text{ for } h \to 0. \tag{5.3.8}$$

We call the Runge-Kutta method (5.2.1) for the approximation of the solution of the SDEs (4.1.2) mean-square consistent of order γ ($\gamma > 0$), *if the local error* $\mathcal{L}[X(t_n);h_n]$ *satisfies*

$$\begin{aligned} &\|\mathbb{E}(\mathcal{L}[X(t_n);h_n]|\mathcal{F}_{t_n})\|_{L_2} \le \overline{c}\cdot h^{\gamma+1}\ ,\ \text{and} \\ &\|\mathcal{L}[X(t_n);h_n]\|_{L_2} \le c\cdot h^{\gamma+\frac{1}{2}}\ ,\quad n=1,\dots,N\ , \end{aligned} \tag{5.3.9}$$

with constants $c\,,\ \overline{c}>0$ *only depending on the SDEs and its solution.*

We remind the reader that consistency is only concerned with the local error. In the case that we disregard other sources of errors in (5.3.3) we only have to deal with perturbations $\delta_n = \mathcal{L}[X(t_n);h_n]$. Following [65], we can consider the general class of multistep methods

$$\sum_{j=1}^{k}\alpha_j y_{n+j} = h\Phi_f(t_n,y_n,y_{n+1},\dots,y_{n+k};h_n) + \Phi_\Upsilon(t_n,y_n,y_{n+1},\dots,y_{n+k};h_n)I^{t_n,t_n+h_n}.$$

Let us notice that our stochastic Runge–Kutta method (5.2.1) falls in the previous class for $k=1,\ \alpha_0=-1,\ \alpha_1=1$ and

$$\Phi_f(t_n,y_n,y_{n+1},\dots,y_{n+k};h_n) \;=\; \sum_{i=1}^{m}\beta_i f(t_n+c_ih_n,Y_i^{[n]}) \tag{5.3.10}$$

$$\Phi_\Upsilon(t_n,y_n,y_{n+1},\dots,y_{n+k};h_n) \;=\; \sum_{i=1}^{m}\Upsilon_i(t_n+\hat{c}_ih_n,\hat{Y}_i^{[n]}). \tag{5.3.11}$$

Now we can state the following definition, [13].

Definition 5.3.5

The characteristic polynomial of (5.2.1) is given by

$$\rho(\zeta) = \alpha_1\zeta^m + \alpha_2\zeta^{m-1} + \cdots + \alpha_m. \tag{5.3.12}$$

The stochastic Runge–Kutta method (5.2.1) is said to fulfill Dahlquist's root conditions if

1. *the roots of $\rho(\zeta)$ lie on or within the unit circle,*

2. *the roots on the unit circle are simple.*

Lemma 5.3.1 (A discrete version of Gronwall's lemma)
Let a_ℓ, $\ell = 1, \ldots, N$, and C_1, C_2 be non-negative real numbers and assume that the inequalities

$$a_\ell \leq C_1 + C_2 \frac{1}{N} \sum_{i=1}^{\ell-1} a_i, \quad \ell = 1, \ldots, N, \tag{5.3.13}$$

are valid. Then we have

$$\max_{\ell=1,\ldots,N} a_\ell \leq C_1 \exp(C_2). \tag{5.3.14}$$

5.3.1 Results

A this point we will prove the main results about consistency and convergence.

Theorem 5.3.2
The stochastic Runge–Kutta method is mean-square consistent of order γ if

$$\|R_n\|_{L_2} \leq c_1 \cdot h_n^{\gamma+1}, \text{ and } \|S_n\|_{L_2} \leq c \cdot h_n^{\gamma+\frac{1}{2}}, \quad n = 1, \ldots, N \tag{5.3.15}$$

for any representation of the local error $\mathcal{L}[X(t_n); h_n]$.

Proof:
To prove the first part, we consider, as we say in Remark 5.3.1, the following representation of the local error $\mathcal{L}[X(t_n); h_n] = R_n + S_n$, with $\mathbb{E}(S_n|\mathcal{F}_{t_{n-1}}) = 0$, such that

$$\|R_n\|_{L_2} \leq c_1 \cdot h_n^{\gamma+1}, \text{ and } \|S_n\|_{L_2} \leq c \cdot h_n^{\gamma+\frac{1}{2}}, \quad n = 1, \ldots, N. \tag{5.3.16}$$

With these hypotheses we have

$$\left\|\mathbb{E}(\mathcal{L}[X(t_n); h_n]|\mathcal{F}_{t_{n-1}})\right\|_{L_2} = \left\|\mathbb{E}(R_n|\mathcal{F}_{t_{n-1}})\right\|_{L_2} \leq \|R_n\|_{L_2} \leq c_1 \cdot h_n^{\gamma+1}. \tag{5.3.17}$$

Now let us consider the Euclidian norm of the local error, where, for $h \leq 1$,

$$\begin{aligned} \|\mathcal{L}[X(t_n); h_n]\|_{L_2} &= \|R_n + S_n\|_{L_2} \leq \|R_n\|_{L_2} + \|S_n\|_{L_2} \\ &\leq c_1 h^{\gamma+1} + c h^{\gamma+\frac{1}{2}} \leq (c_1 + c) h^{\gamma+\frac{1}{2}} = \bar{c} \cdot h_n^{\gamma+\frac{1}{2}}. \quad (5.3.18) \end{aligned}$$

♢

Theorem 5.3.3

The stochastic $\mathcal{A}$-method (5.2.4) is numerically stable in the mean-square sense for every continuous f, Γ_j and Ξ_j satisfying the uniform Lipschitz condition (5.3.2) *if and only if its characteristic polynomial $\rho(\zeta)$ satisfies Dahlquist's root condition given in Definition 5.3.5.*

Proof:

Necessity: This part can be proved as in the deterministic case, i.e., we take the equation $X'(t) = 0$, then the functions f, Γ_j and Ξ_j satisfy obviously the uniform Lipschitz condition. Then we follow the proof of Thm 6.3.3 in [48].

Sufficiency: Let us define $e_{n+1} = \mathcal{Z}_{n+1} - \tilde{\mathcal{Z}}_{n+1}$, where $\mathcal{Z}_{n+1},\ \tilde{\mathcal{Z}}_{n+1}$ are the solutions of (5.2.4) and (5.3.3), respectively. Then

$$\begin{aligned} e_{n+1} &= \mathcal{Z}_{n+1} - \tilde{\mathcal{Z}}_{n+1} \\ &= \mathcal{A}(\mathcal{Z}_n - \tilde{\mathcal{Z}}_n) + \\ &+ h_n \mathcal{B}[F(t_n, \mathcal{Z}_{n+1}; h_n) - F(t_n, \tilde{\mathcal{Z}}_{n+1}; h_n)] + \\ &+ \mathcal{C}_1[\Gamma(t_n, \mathcal{Z}_{n+1}; h_n) - \Gamma(t_n, \tilde{\mathcal{Z}}_{n+1}; h_n)] I^{t_n, t_n+h_n} + \\ &+ \mathcal{C}_2[\Xi(t_n, \mathcal{Z}_{n+1}; h_n) - \Xi(t_n, \tilde{\mathcal{Z}}_{n+1}; h_n)] I^{t_n, t_n+ch_n} - \delta_n. \end{aligned}$$

For simplicity of notation, we set

$$\begin{aligned} \Delta F_n &= [F(t_n, \mathcal{Z}_{n+1}; h_n) - F(t_n, \tilde{\mathcal{Z}}_{n+1}; h_n)], \\ \Delta \Gamma_n &= [\Gamma(t_n, \mathcal{Z}_{n+1}; h_n) - \Gamma(t_n, \tilde{\mathcal{Z}}_{n+1}; h_n)], \\ \Delta \Xi_n &= [\Xi(t_n, \mathcal{Z}_{n+1}; h_n) - \Xi(t_n, \tilde{\mathcal{Z}}_{n+1}; h_n)], \end{aligned}$$

and obtain, after iterating once the above equation for e_{n+1},

$$\begin{aligned} e_{n+1} &= \mathcal{A}\{\mathcal{A}[\mathcal{Z}_{n-1} - \tilde{\mathcal{Z}}_{n-1}] + h_{n-1}\mathcal{B}\Delta F_{n-1} + \mathcal{C}_1\Delta\Gamma_{n-1}I^{t_{n-1},t_{n-1}+h_{n-1}} \\ &+ \mathcal{C}_2\Delta\Xi_{n-1}I^{t_{n-1},t_{n-1}+ch_{n-1}} - \delta_{n-1}\} \\ &+ h_n\mathcal{B}\Delta F_n + \mathcal{C}_1\Delta\Gamma_n I^{t_n,t_n+h_n} + \mathcal{C}_2\Delta\Xi_n I^{t_n,t_n+ch_n} - \delta_n. \end{aligned}$$

After n iteration steps, e_{n+1} takes the form

$$\begin{aligned} e_{n+1} &= \mathcal{A}^n e_0 + \sum_{j=0}^{n} h_j\mathcal{A}^{n-j}\mathcal{B}\Delta F_j + \sum_{j=0}^{n}\mathcal{A}^{n-j}\mathcal{C}_1\Delta\Gamma_j I^{t_j,t_j+h_j} \\ &+ \sum_{j=0}^{n}\mathcal{A}^{n-j}\mathcal{C}_2\Delta\Xi_j I^{t_j,t_j+ch_j} - \sum_{j=0}^{n}\mathcal{A}^{n-j}\delta_j. \end{aligned}$$

Let us consider now a norm $||\cdot||_*$, such that $||\mathcal{A}^n||_*^2 \leq 1$ (see [52]). This is possible if the eigenvalues of the Frobenius matrix $\mathcal{A}$ lie inside the unit circle of the complex plane and they are simple if their modulus is equal to 1. The eigenvalues of $\mathcal{A}$ are the roots of the characteristic polynomial ρ and due to the assumption that Dahlquist's root conditions holds they have the required property.
We now apply $||\cdot||_*^2$ to estimate $||e_{n+1}||_*^2$ and then $E(||e_{n+1}||_*^2)$.

$$\begin{aligned} ||e_{n+1}||_*^2 &\leq 5\{\underbrace{||\mathcal{A}^n e_0||_*^2}_{term\ \ 1} + \underbrace{||\sum_{j=0}^{n} h_j\mathcal{A}^{n-j}\mathcal{B}\Delta F_j||_*^2}_{term\ \ 2} + \underbrace{||\sum_{j=0}^{n}\mathcal{A}^{n-j}\mathcal{C}_1\Delta\Gamma_j I^{t_j,t_j+h_j}||_*^2}_{term\ \ 3} \\ &+ \underbrace{||\sum_{j=0}^{n}\mathcal{A}^{n-j}\mathcal{C}_2\Delta\Xi_j I^{t_j,t_j+ch_j}||_*^2}_{term\ \ 4} - \underbrace{||\sum_{j=0}^{n}\mathcal{A}^{n-j}\delta_j||_*^2}_{term\ \ 5}\}. \end{aligned}$$

Term 1: As we assume that Dahlquist's root condition is satisfied, we immediately get

$$||\mathcal{A}^n e_0||_*^2 = ||\mathcal{A}^n||_*^2||e_0||_*^2 \leq ||e_0||_*^2.$$

Term 2: From the Lipschitz condition (5.3.2) on the function f, we can easily get the uniform Lipschitz condition on F and the following inequalities

$$\begin{aligned} ||\sum_{j=0}^{n} h_j \mathcal{A}^{n-j}\mathcal{B}\Delta F_j||_*^2 &\leq (n+1)\sum_{j=0}^{n}||h_j\mathcal{A}^{n-j}\mathcal{B}\Delta F_j||_*^2 \leq S_2\sum_{j=0}^{n}||h_j\Delta F_j||_*^2 \\ &\leq S_2\mathbf{h}^2L_F^2\sum_{j=0}^{n}||e_j||_*^2 \leq S_2\mathbf{h}^2\sum_{j=0}^{n}||e_j||_*^2, \end{aligned}$$

where S_2 is a constant involving all the constants and $\mathbf{h}$ is the maximum stepsize.

Term 3: As before, from the hypotheses on Γ_j, we have

$$\begin{aligned} ||\sum_{j=0}^{n} \mathcal{A}^{n-j}\mathcal{C}_1\Delta\Gamma_j I^{t_j,t_j+h_j}||_*^2 &\leq (n+1)\sum_{j=0}^{n}||\mathcal{A}^{n-j}\mathcal{C}_1\Delta\Gamma_j I^{t_j,t_j+h_j}||_*^2 \\ &\leq S_3\sum_{j=0}^{n}||\Delta\Gamma_j I^{t_j,t_j+h_j}||_*^2, \end{aligned}$$

where S_3 is a constant. *Term 4:* Using the (5.3.2) hypothesis on Ξ, we obtain

$$\begin{aligned} ||\sum_{j=0}^{n} \mathcal{A}^{n-j}\mathcal{C}_2\Delta\Xi_j I^{t_j,t_j+ch_j}||_*^2 &\leq (n+1)\sum_{j=0}^{n}||\mathcal{A}^{n-j}\mathcal{C}_2\Delta\Xi_j I^{t_j,t_j+ch_j}||_*^2 \\ &\leq S_4\sum_{j=0}^{n}||\Delta\Xi_j I^{t_j,t_j+ch_j}||_*^2. \end{aligned}$$

Term 5:

$$||\sum_{j=0}^{n} \mathcal{A}^{n-j}\delta_j||_*^2 \leq (n+1)\sum_{j=0}^{n}||\mathcal{A}^{n-j}\delta_j||_*^2 \leq S_5\sum_{j=0}^{n}||\delta_j||_*^2.$$

So we have

$$\begin{aligned} ||e_{n+1}||_*^2 &\leq 5\big\{||e_0||_*^2 + S_2\mathbf{h}^2\sum_{j=0}^{n}||e_j||_*^2 + S_3\sum_{j=0}^{n}||\Delta\Gamma_j I^{t_j,t_j+h_j}||_*^2 \\ &+ S_4\sum_{j=0}^{n}||\Delta\Xi_j I^{t_j,t_j+ch_j}||_*^2 + S_5\sum_{j=0}^{n}||\delta_j||_*^2\big\}. \end{aligned}$$

Let consider now $\mathbb{E}[\cdot]$:

$$\mathbb{E}[||e_{n+1}||_*^2] \leq 5\big\{\mathbb{E}[||e_0||_*^2] + S_2\mathbf{h}^2\sum_{j=0}^{n}\mathbb{E}[||e_j||_*^2] + \underbrace{S_3\sum_{j=0}^{n}\mathbb{E}[||\Delta\Gamma_j I^{t_j,t_j+h_j}||_*^2]}_{Term\ \star}$$

$$+ \underbrace{S_4 \sum_{j=0}^{n} \mathbb{E}[||\Delta\Xi_j I^{t_j,t_j+ch_j}||_*^2]}_{Term\ \star\star} + S_5 \sum_{j=0}^{n} \mathbb{E}[||\delta_j||_*^2]\Big\} \tag{5.3.19}$$

Term $\star$: As $\Delta\Gamma_j$ is $\mathcal{F}_{t_j}$-measurable and $\mathbb{E}[\Delta\Gamma_j|\mathcal{F}_{t_{j-1}}] = 0$, we have

$$S_3 \sum_{j=0}^{n} \mathbb{E}[||\Delta\Gamma_j I^{t_j,t_j+h_j}||_*^2] \le S_3 \sum_{j=0}^{n} \mathbb{E}[||\Delta\Gamma_j||_*^2 |I^{t_j,t_j+h_j}|^2] \le S_3\mathbf{h} \sum_{j=0}^{n} \mathbb{E}[||e_j||_*^2 \tag{5.3.20}$$

Term $\star\star$: We proceed as for the term $\star$

$$S_4 \sum_{j=0}^{n} \mathbb{E}[||\Delta\Xi_j I^{t_j,t_j+h_j}||_*^2] \le S_4 \sum_{j=0}^{n} \mathbb{E}[||\Delta\Xi_j||_*^2 |I^{t_j,t_j+ch_j}|^2] \le S_4\mathbf{h} \sum_{j=0}^{n} \mathbb{E}[||e_j||_*^2.$$

Inserting these into the intermediate result (5.3.19), we get

$$\mathbb{E}[||e_{n+1}||_*^2] \;=\; 5\Big\{\mathbb{E}[||e_0||_*^2 + [S_2\mathbf{h}^2 + (S_3+S_4)\mathbf{h}] \sum_{j=0}^{n} \mathbb{E}[||e_j||_*^2 + S_5 \sum_{j=0}^{n} \mathbb{E}[||\delta_j||_*^2\Big\}.$$

We set $[S_2\mathbf{h}^2 + (S_3+S_4)\mathbf{h}] = \frac{S}{N}$, so the previous inequality become

$$\mathbb{E}[||e_{n+1}||_*^2] \;\le\; 5\mathbb{E}[||e_0||_*^2] + 5\frac{S}{N} \sum_{j=0}^{n} \mathbb{E}[||e_j||_*^2] + 5S_5 \sum_{j=0}^{n} \mathbb{E}[||\delta_j||_*^2].$$

We apply now the discrete Gronwall Lemma (5.3.1) and we obtain the intermediate result

$$\max_{1\le n\le N} \mathbb{E}[||e_{n+1}||_*^2] \le \hat{S}\Big\{\mathbb{E}[||e_0||_*^2] + S_5 \sum_{j=0}^{n} \mathbb{E}[||\delta_j||_*^2]\Big\},$$

where $\hat{S} = 5\exp(5S)$. We decompose the perturbations δ_j in $\delta_j = R_j + S_j$, where S_j is $\mathcal{F}_{t_j}$-measurable with $\mathbb{E}[S_j|\mathcal{F}_{t_j}] = 0,\ j = 0, ..., N$. So

$$\sum_{j=0}^{n} \mathbb{E}[||\delta_j||_*^2] = \sum_{j=0}^{n} \mathbb{E}[||R_j + S_j||_*^2] \le \sum_{j=0}^{n} \{\mathbb{E}[||R_j||_*^2] + \mathbb{E}[||S_j||_*^2]\},$$

and

$$\begin{aligned}
\max_{1\le n\le N} \mathbb{E}[||e_{n+1}||_*^2] \;&\le\; \hat{S}\Big\{\mathbb{E}[||e_0||_*^2] + C\sum_{j=0}^{n}\Big[\frac{\mathbb{E}[||R_j||_*^2]}{\mathbf{h}} + \frac{\mathbb{E}[||S_j||_*^2]}{\sqrt{\mathbf{h}}}\Big]\Big\} \\
&\le\; \hat{S}\Big\{\mathbb{E}[||e_0||_*^2] + \max_{1\le n\le N}\Big[\frac{||R_j||_*^2}{\mathbf{h}} + \frac{||S_j||_*^2}{\sqrt{\mathbf{h}}}\Big]\Big\}.
\end{aligned}$$

♢

With the powerful notion of numerical stability in the mean-square sense, together with mean-square consistency the mean-square convergence follows almost immediately.

Theorem 5.3.4

A mean-square consistent stochastic Runge-Kutta method (5.2.1) for the approximation of the solution of SDEs (4.1.2) is mean-square convergent for all continuous f, Γ_j *and* Ξ_j *satisfying a uniform Lipschitz condition* (5.3.2), *if and only if it is numerically stable in the mean-square sense. If, in addition, it is mean-square consistent with order* $\gamma > 0$, *then the method is mean-square convergent with order* γ.

5.4 Order Conditions

To estimate the multiple integrals (4.5.1) we will use Lemma 4.5.11 To analyse the local error of Runge-Kutta schemes we shall use the notation

$$e = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} \in \mathbb{R}^m, \qquad \begin{pmatrix} a_1 \\ \vdots \\ a_m \end{pmatrix} * \begin{pmatrix} b_1 \\ \vdots \\ b_m \end{pmatrix} = \begin{pmatrix} a_1 b_1 \\ \vdots \\ a_m b_m \end{pmatrix}.$$

We will calculate the deterministic multivariate Taylor expansion of the stochastic Runge-Kutta approximation (5.2.1) and we consider the Itô-Taylor expansion of the solution process $X(t)$ of (4.1.2). Then we insert the two expansions into the expression of the local error (5.2.7), and we obtain the conditions which annihilate the corresponding terms. Now we will apply this approach to some particular methods.

5.4.1 Stochastic Runge-Kutta methods with mixed stochastic integrals

Let us consider the class of stochastic Runge-Kutta methods with mixed stochastic integrals introduced in [15],

$$\begin{aligned}
y_0 &= X_0 \qquad (5.4.1)\\
y_{n+1} &= y_n + \sum_{i=1}^{m} \beta_i f(t_n + c_i h_n, Y_i^{[n]}) h_n + \sum_{i=1}^{m}\sum_{r=1}^{s} \gamma_i g_r(t_n + \hat{c}_i h_n, \hat{Y}_i^{[n]})) I_r^{t_n, t_n+h_n} \\
&\quad + \sum_{i=1}^{m}\sum_{r=1}^{s} \eta_i g_r(t_n + \hat{c}_i h, \hat{Y}_i^{[n]})) \frac{I_{r0}^{t_n, t_n+h_n}}{h_n}, \\
Y_i^{[n]} &= y_n + \sum_{j=1}^{m} a_{ij} f(t_n + c_j h_n, Y_j^{[n]}) h_n + \sum_{j=1}^{m}\sum_{r=1}^{s} b_{ij} g_r(t_n \hat{c}_j h_n, \hat{Y}_j^{[n]})) \frac{I_{r0}^{t_n, t_n+h_n}}{h_n}, \\
\hat{Y}_i^{[n]} &= y_n + \sum_{j=1}^{m} \hat{a}_{ij} f(t_n + c_j h_n, Y_j^{[n]}) h_n,
\end{aligned}$$

for $n = 1, \cdots, N-1$ and $i = 1, \cdots, m$. The linear operators associated with the method (5.4.1) are

$$\begin{aligned}
\mathcal{L}[X(t_n); h_n] &:= X(t_n + h_n) - X(t_n) - h_n \sum_{j=1}^{m} \beta_j f(t_n + c_j h_n, X(t_n + c_j h_n)) \\
&- \sum_{j=1}^{m}\sum_{r=1}^{s} \gamma_j g_r(t_n + \hat{c}_j h_n, \hat{X}(t_n + \hat{c}_j h_n)) I_r^{t_n, t_n+h_n} \\
&- \sum_{j=1}^{m}\sum_{r=1}^{s} \eta_j g_r(t_n + \hat{c}_j h_n, X(t_n + \hat{c}_j h_n)) \frac{I_{r0}^{t_n, t_n+h_n}}{h_n}, \qquad (5.4.2)
\end{aligned}$$

$$\begin{aligned}
\mathcal{L}_i[X(t_n); h_n] &:= X(t_n + c_i h_n) - X(t_n) - h_n \sum_{j=1}^{m} a_{ij} f(t_n + c_j h_n, X(t_n + c_j h_n)) \\
&- \sum_{j=1}^{m}\sum_{r=1}^{s} b_{ij} g_r(t_n + \hat{c}_j h_n, X(t_n + \hat{c}_j h_n)) \frac{I_{r0}^{t_n, t_n+h_n}}{h_n}, \qquad (5.4.3)
\end{aligned}$$

$$\hat{\mathcal{L}}_i[X(t_n); h_n] := X(t_n + \hat{c}_i h_n) - X(t_n) - h_n \sum_{j=1}^{m} \hat{a}_{ij} f(t_n + c_j h_n, X(t_n + c_j h_n)). \qquad (5.4.4)$$

In the following calculations all the functions and their derivatives are evaluated at the point $(t_n, X(t_n))$, this argument is usually omitted for simplicity of notation. We consider the Itô-Taylor expansion of the solution process of the given SDE

$$\begin{aligned} X(t_n+h_n)-X(t_n) &= f I_0^{t_n,t_n+h_n} + f'_x[f] I_{00}^{t_n,t_n+h_n} + \sum_{r=1}^{s} g_r I_r^{t_n,t_n+h_n} \\ &+ \sum_{r=1}^{s} g'_{r_x}[f] I_{0r}^{t_n,t_n+h_n} + \sum_{r=1}^{s} f'_x[g_r] I_{r0}^{t_n,t_n+h_n} \\ &+ \rho, \end{aligned} \tag{5.4.5}$$

where

$$\begin{aligned} \rho &= f'_t I_{00}^{t_n,t_n+h_n} + \sum_{r=1}^{s} g'_{r_t} I_{0r}^{t_n,t_n+h_n} + \frac{1}{2}\sum_{r=1}^{s} f''_{xx}[g_r,g_r] I_{00}^{t_n,t_n+h_n} \\ &+ \frac{1}{2}\sum_{r,q=1}^{s} g''_{r_{xx}}[g_q,g_q] I_{0r}^{t_n,t_n+h_n} + \sum_{r,q=1}^{s} I_{rq}^{t_n,t_n+h_n}(\Lambda_r g_q) + I_{000}^{t_n,t_n+h_n}(\Lambda_0\Lambda_0 f) \\ &+ \sum_{r=1}^{s} I_{r00}^{t_n,t_n+h_n}(\Lambda_r\Lambda_0 f) + \sum_{r=1}^{s} I_{00r}^{t_n,t_n+h_n}(\Lambda_0\Lambda_0 g_r) \\ &+ \sum_{r=1}^{s} I_{0r0}^{t_n,t_n+h_n}(\Lambda_0\Lambda_r f) + \sum_{r,q=1}^{s} I_{r0q} I^{t_n,t_n+h_n}(\Lambda_r\Lambda_0 g_q) \\ &+ \sum_{r,q=1}^{s} I_{rq0}^{t_n,t_n+h_n}(\Lambda_r\Lambda_q f). \end{aligned} \tag{5.4.6}$$

Let us calculate now the expansion of the numerical approximation at time $t_n + h_n$

$$\begin{aligned} Y(t_n+h_n) &= h_n\beta^T e f + h_n^2\beta^T A e f'_x[f] + \sum_{r=1}^{s}\beta^T B e f'_x[g_r] h_n \frac{I_{r0}^{t,t+h_n}}{h_n} \\ &+ \sum_{r=1}^{s}\gamma^T e g_r I_r^{t,t+h_n} + \sum_{r=1}^{s}\gamma^T \hat{A} e g'_{r_x}[f] h_n I_r^{t,t+h_n} \\ &+ \sum_{r=1}^{s}\eta^T e g_r \frac{I_{r0}^{t,t+h_n}}{h_n} + \sum_{r=1}^{s}\eta^T \hat{A} e g'_{r_x}[f] h_n \frac{I_{r0}^{t,t+h_n}}{h_n} \\ &+ \mu, \end{aligned} \tag{5.4.7}$$

where

$$\mu = h_n^2\beta^T c f'_t + \sum_{r=1}^{s}\gamma^T \hat{c} g'_{r_t} h_n I_r^{t,t+h_n} + \sum_{r=1}^{s}\eta^T \hat{c} g'_{r_t} h_n \frac{I_{r0}^{t,t+h_n}}{h_n}$$

$$
\begin{aligned}
&+ \quad \frac{1}{2}h_n^3\beta^T Aef''_x[f,f] + h_n^3\beta^T AAef'_x[f'_x[f]] \\
&+ \quad h_n^2\sum_{r=1}^{s}\beta^T[(Be)*(Ae)]f''_{xx}[g_r,f]\frac{I_{r0}^{t,t+h_n}}{h_n} \\
&+ \quad h_n^2\sum_{r=1}^{s}\beta^T ABef'_x[f'_x[g_r]]\frac{I_{r0}^{t,t+h_n}}{h_n} \\
&+ \quad h_n^2\sum_{r=1}^{s}\beta^T B\hat{A}ef'_x[g'_{r_x}[f]]\frac{I_{r0}^{t,t+h_n}}{h_n} \\
&+ \quad \frac{1}{2}h_n\sum_{r,q=1}^{s}\beta^T[Be)*((Be))]f''_{xx}[g_r,g_q]\frac{I_{r0}^{t,t+h_n}}{h_n}\frac{I_{q0}^{t,t+h_n}}{h_n} \\
&+ \quad \frac{1}{2}h_n^2\sum_{r=1}^{s}\gamma^T((\hat{A}e)*(\hat{A}e))g''_{r_{xx}}[f,f]I_r^{t,t+h_n} \\
&+ \quad h_n^2\sum_{r=1}^{s}\gamma^T\hat{A}Aeg'_{r_x}[f'_x[f]]I_r^{t,t+h_n} \\
&+ \quad h_n^2\sum_{r,q=1}^{s}\gamma^T\hat{A}Beg'_{r_x}[f'_x[g_q]]I_r^{t,t+h_n}\frac{I_{q0}^{t,t+h_n}}{h_n} \qquad (5.4.8) \\
&+ \quad \frac{1}{2}h_n^2\sum_{r=1}^{s}\eta^T((\hat{A}e)*(\hat{A}e))g''_{r_{xx}}[f,f]\frac{I_{r0}^{t,t+h_n}}{h_n} \\
&+ \quad h_n^2\sum_{r=1}^{s}\eta^T\hat{A}Aeg'_{r_x}[f'_x[f]]\frac{I_{r0}^{t,t+h_n}}{h_n} \\
&+ \quad h_n^2\sum_{r,q=1}^{s}\eta^T\hat{A}Beg'_{r_x}[f'_x[g_q]]\frac{I_{r0}^{t,t+h_n}}{h_n}\frac{I_{q0}^{t,t+h_n}}{h_n}. \qquad (5.4.9)
\end{aligned}
$$

Finally we insert both our expansions into the expression of the local error

$$
\begin{aligned}
\mathcal{L}[X(t);h_n] \quad &= \quad fI_0^{t_n,t_n+h_n} + f'_x[f]I_{00}^{t_n,t_n+h_n} \\
&+ \quad \sum_{r=1}^{s}g_rI_r^{t_n,t_n+h_n} + \sum_{r=1}^{s}g'_{r_x}[f]I_{0r}^{t_n,t_n+h_n} \\
&+ \quad \sum_{r=1}^{s}f'_x[g_r]I_{r0}^{t_n,t_n+h_n} - h_n\beta^T ef - h_n^2\beta^T Aef'_x[f] \\
&- \quad \sum_{r=1}^{s}\beta^T Bef'_x[g_r]h_n\frac{I_{r0}^{t,t+h_n}}{h_n} - \sum_{r=1}^{s}\gamma^T eg_rI_r^{t,t+h_n} \\
&- \quad \sum_{r=1}^{s}\gamma^T\hat{A}eg'_{r_x}[f]h_nI_r^{t,t+h_n} - \sum_{r=1}^{s}\eta^T eg_r\frac{I_{r0}^{t,t+h_n}}{h_n}
\end{aligned}
$$

$$- \quad \sum_{r=1}^{s} \eta^T \hat{A} e g'_{r_x}[f] h_n \frac{I_{r0}^{t,t+h_n}}{h_n}. \tag{5.4.10}$$

The corresponding terms vanish if the following equations are satisfied

$$\begin{aligned}
h_n \beta^T e f &= f I_0^{t_n,t_n+h_n} \\
h_n^2 \beta^T A e f'_x[f] &= f'_x[f] I_{00}^{t_n,t_n+h_n} \\
\sum_{r=1}^{m} \beta^T B e f'_x[g_r] h_n \frac{I_{r0}^{t,t+h_n}}{h_n} &= \sum_{r=1}^{m} f'_x[g_r] I_{r0}^{t_n,t_n+h_n} \\
\sum_{r=1}^{m} \gamma^T e g_r I_r^{t,t+h_n} &= \sum_{r=1}^{m} g_r I_r^{t_n,t_n+h_n} \\
\sum_{r=1}^{m} \eta^T e g_r \frac{I_{r0}^{t,t+h_n}}{h_n} &= 0 \qquad (5.4.11) \\
\sum_{r=1}^{m} \gamma^T \hat{A} e g'_{r_x}[f] h_n I_r^{t,t+h_n} + \sum_{r=1}^{m} \eta^T \hat{A} e g'_{r_x}[f] h_n \frac{I_{r0}^{t,t+h_n}}{h_n} &= \sum_{r=1}^{m} g'_{r_x}[f] I_{0r}^{t_n,t_n+h_n}.
\end{aligned}$$

So we obtain the order conditions for the coefficient of the stochastic Runge-Kutta method (5.4.1)

$$\beta^T e = 1, \qquad \gamma^T e = 1, \qquad \eta^T e = 0, \tag{5.4.12}$$

$$\beta^T A e = \frac{1}{2}, \qquad \beta^T B e = 1, \tag{5.4.13}$$

$$\gamma^T \hat{A} = 1, \qquad \eta^T \hat{A} e = -1. \tag{5.4.14}$$

Now we consider the expansions in $t_n + c_i h_n$ to derive stage order conditions for $Y_i^{[n]}$, and in $t_n + \hat{c}_i h_n$ to have order conditions for $\hat{Y}_i^{[n]}$. We have for the exact solution

$$X(t_n + c_i h_n) - X(t_n) \quad = \quad f I_0^{t_n,t_n+c_i h_n} + \rho_1, \tag{5.4.15}$$

where

$$\begin{aligned}
\rho_1 &= f'_t I_{00}^{t_n,t_n+c_i h_n} + f'_x[f] I_{00}^{t_n,t_n+c_i h_n} \\
&+ \sum_{r=1}^{m} g_r I_r^{t_n,t_n+c_i h_n} + \sum_{r=1}^{m} g'_{r_t}[f] I_{0r}^{t_n,t_n+c_i h_n} \\
&+ \sum_{r=1}^{m} g'_{r_x}[f] I_{0r}^{t_n,t_n+c_i h_n} + \sum_{r=1}^{m} f'_x[g_r] I_{r0}^{t_n,t_n+c_i h_n}
\end{aligned}$$

$$
\begin{aligned}
&+ \quad \frac{1}{2}\sum_{r=1}^{m} f''_{xx}[g_r,g_r]I_{00}^{t_n,t_n+c_ih_n} + \frac{1}{2}\sum_{r,q=1}^{m} g''_{r_{xx}}[g_q,g_q]I_{0r}^{t_n,t_n+c_ih_n} \\
&+ \quad \sum_{r,q=1}^{m} I_{rq}^{t_n,t_n+c_ih_n}(\Lambda_r g_q) + I_{000}^{t_n,t_n+c_ih_n}(\Lambda_0\Lambda_0 f) \\
&+ \quad \sum_{r=1}^{m} I_{r00}^{t_n,t_n+c_ih_n}(\Lambda_r\Lambda_0 f) + \sum_{r=1}^{m} I_{00r}^{t_n,t_n+c_ih_n}(\Lambda_0\Lambda_0 g_r) \\
&+ \quad \sum_{r=1}^{m} I_{0r0}^{t_n,t_n+c_ih_n}(\Lambda_0\Lambda_r f) + \sum_{r,q=1}^{m} I_{r0q}I^{t_n,t_n+c_ih_n}(\Lambda_r\Lambda_0 g_q) \\
&+ \quad \sum_{r,q=1}^{m} I_{rq0}^{t_n,t_n+c_ih_n}(\Lambda_r\Lambda_q f). \qquad (5.4.16)
\end{aligned}
$$

Then, for the numerical approximation, we have

$$
Y(x_n + c_ih_n) \quad = \quad h_nAef + \mu_1, \qquad (5.4.17)
$$

with

$$
\begin{aligned}
\mu_1 \quad = \quad & h_n^2Acf'_t + h_n^2AAef'_x[f] + \sum_{r=1}^{m} ABef'_x[g_r]h_n\frac{I_{r0}^{t_n,t_n+h_n}}{h_n} \\
&+ \quad \sum_{r=1}^{m} Bg_r\frac{I_{r0}^{t_n,t_n+h_n}}{h_n} + \sum_{r=1}^{m} B\hat{c}g'_{r_t}\frac{I_{r0}^{t_n,t_n+h_n}}{h_n}h_n \\
&+ \quad \sum_{r=1}^{m} B\hat{A}eg'_{r_x}[f]\frac{I_{r0}^{t_n,t_n+h_n}}{h_n}h_n \\
&+ \quad \frac{1}{2}h_n^3AAef''_x[f,f] + h_n^3AAAef'_x[f'_x[f]] \\
&+ \quad h_n^2\sum_{r=1}^{m} A[(Be)*(Ae)]f''_{xx}[g_r,f]\frac{I_{r0}^{t,t+h_n}}{h_n} \\
&+ \quad h_n^2\sum_{r=1}^{m} AABef'_x[f'_x[g_r]]\frac{I_{r0}^{t,t+h_n}}{h_n} \\
&+ \quad h_n^2\sum_{r=1}^{m} AB\hat{A}ef'_x[g'_{r_x}[f]]\frac{I_{r0}^{t,t+h_n}}{h_n} \\
&+ \quad \frac{1}{2}h_n\sum_{r,q=1}^{m} A[Be)*((Be))]f''_{xx}[g_r,g_q]\frac{I_{r0}^{t,t+h_n}}{h_n}\frac{I_{q0}^{t,t+h_n}}{h_n} \\
&+ \quad \frac{1}{2}h_n^2\sum_{r=1}^{m} A((\hat{A}e)*(\hat{A}e))g''_{r_{xx}}[f,f]\frac{I_{r0}^{t,t+h_n}}{h_n} \\
&+ \quad h_n^2\sum_{r=1}^{m} A\hat{A}Aeg'_{r_x}[f'_x[f]]\frac{I_{r0}^{t,t+h_n}}{h_n}
\end{aligned}
$$

$$+ \quad h_n^2 \sum_{r,q=1}^{m} A\hat{A}Beg'_{r_x}[f'_x[g_q]] \frac{I_{r0}^{t,t+h_n}}{h_n} \frac{I_{q0}^{t,t+h_n}}{h_n}. \tag{5.4.18}$$

Finally

$$\mathcal{L}_i[X(t); h_n] \quad = \quad f I_0^{t_n, t_n + c_i h_n} - h_n Aef. \tag{5.4.19}$$

So, from the annihilation of $\mathcal{L}_i[X(t); h_n]$, we obtain the following stage order condition

$$Ae \quad = \quad c. \tag{5.4.20}$$

Analogously when we annihilate $\hat{\mathcal{L}}_i[X(t); h_n]$ we have $\hat{A}e = \hat{c}$.

5.4.2 First-order Runge-Kutta method involving the Itô coefficient ("FRKI" method)

In order to derive in a systematic way order and stage order conditions, we reformulate the First-order Runge–Kutta method, introduced by Nigel Newton in [72], using our notation. Newton showed that this kind of method is asymptotically efficient in the sense that it minimises the leading coefficient in the expansion of the mean-square errors as power series in the sample step size. Observe that Newton considers only SDEs with a scalar Wiener process. The method, in our formulation, is

$$\begin{aligned}
y_0 &= X_0 \\
y_{n+1} &= y_n + hf(t_n + ch, Y^{[n]}) - g_1(t_n + ch, Y^{[n]})\sqrt{h} \\
&+ g_1(t_n + \hat{c}h, \hat{Y}^{[n]})\big[I_1^{t_n, t_n+h} + \sqrt{h}\big], \\
Y^{[n]} &= y_n \\
\hat{Y}^{[n]} &= y_n + \frac{1}{2} g_1(t_n + ch, Y^{[n]})\big[I_1^{t_n, t_n+h} - \sqrt{h}\big],
\end{aligned} \tag{5.4.21}$$

for $n = 1, \cdots, N-1$, only for a scalar Wiener process.

Remark 5.4.1

We consider a more general class which contains the FRKI method:

$$\begin{aligned}
y_0 &= X_0 \qquad (5.4.22)\\
y_{n+1} &= y_n + h_n \sum_{j=1}^{m} \alpha_j f(t_n + c_j h_n, Y_j^{[n]}) \\
&+ \sum_{j=1}^{m} \beta_j g_1(t_n + c_j h_n, Y_j^{[n]}) \sqrt{h_n} \\
&+ \sum_{j=1}^{m} \gamma_j g_1(t_n + \hat{c}_j h_n, +\hat{Y}_j^{[n]}) I_1^{t_n, t_n+h_n} \\
&+ \sum_{j=1}^{m} \delta_j g_1(t_n + \hat{c}_j h_n, \hat{Y}_j^{[n]}) \sqrt{h_n}, \\
Y_i^{[n]} &= y_n \\
\hat{Y}_i^{[n]} &= y_n + \sum_{j=1}^{m} \hat{a}_{ij} g(t_n + c_j h_n, Y_i^{[n]}) I_1^{t_n, t_n+h_n} \\
&+ \sum_{j=1}^{m} \hat{b}_{ij} g(t_n + c_j h_n, Y_i^{[n]}) \sqrt{h_n}.
\end{aligned}$$

The FRKI method has $m = 1$, $\alpha = 1$ $\beta = -1$, $\gamma = 1$, $\delta = 1$, $\hat{a} = \frac{1}{2}$, $\hat{b} = -\frac{1}{2}$.

As usual we define the following operators, where X(t) is the solution of our SDE,

$$\begin{aligned}
\mathcal{L}[X(t_n); h_n] &= X(t_n + h_n) - X(t_n) \\
&- h_n \sum_{j=1}^{s} \alpha_j f(t_n + c_j h_n, X(t_n + c_j h_n)) \\
&- \sum_{j=1}^{s} \beta_j g(t_n + c_j h_n, X(t_n + c_j h_n)) \sqrt{h_n} \\
&- \sum_{j=1}^{s} \gamma_j g(t_n + \hat{c}_j h_n, X(t_n + \hat{c}_j h_n)) I_1^{t_n, t_n+h_n} \\
&- \sum_{j=1}^{s} \delta_j g(t_n + \hat{c}_j h_n, X(t_n + \hat{c}_j h_n)) \sqrt{h_n}, \qquad (5.4.23)
\end{aligned}$$

$$\mathcal{L}_i[X(t_n); h_n] = X(t_n + c_i h_n) - X(t_n), \qquad (5.4.24)$$

$$\hat{\mathcal{L}}_i[X(t_n); h_n] = X(t_n + \hat{c}_i h_n) - X(t_n)$$

$$
\begin{aligned}
&- \sum_{j=1}^{s} \hat{a}_{ij} g(t_n + c_j h_n, X(t_n + c_j h_n)) I_1^{t_n, t_n+h_n} \\
&- \sum_{j=1}^{s} \hat{b}_{ij} g(t_n + c_j h_n, X(t_n + c_j h_n)) \sqrt{h_n}. \qquad (5.4.25)
\end{aligned}
$$

Let us consider now the Itô-Taylor expansion of the exact solution

$$
X(t_n + h) - X(t_n) = f I_0^{t_n, t_n+h_n} + g I_1^{t_n, t_n+h} + g'_x[g] I_{11}^{t_n, t_n+h} + \rho_2. \qquad (5.4.26)
$$

where ρ_2 is the truncation term. For the numerical approximation we have

$$
\begin{aligned}
Y(t_n + h_n) &= h_n \alpha^T e f + \beta^T e g \sqrt{h_n} + \gamma^T e g I_1^{t_n, t_n+h_n} \\
&+ \gamma^T \hat{A} e g'_x[g] (I_1^{t_n, t_n+h_n})^2 + \gamma^T \hat{B} e g'_x[g] I_1^{t_n, t_n+h_n} \sqrt{h_n} \\
&+ \delta^T e g \sqrt{h_n} + \delta^T \hat{A} e g'_x[g] \sqrt{h_n} I_1^{t_n, t_n+h_n} + \delta^T \hat{B} e g'_x[g] h_n + \mu_2, \qquad (5.4.27)
\end{aligned}
$$

again μ_2 is the truncation term. By inserting both expansions in $\mathcal{L}[X(t_n); h_n]$, we obtain

$$
\begin{aligned}
\mathcal{L}[X(t_n); h_n] &= f I_0^{t_n, t_n+h_n} + g I_1^{t_n, t_n+h} + g'_x I_{11}^{t_n, t_n+h} \\
&- h_n \alpha^T e f - \beta^T e g \sqrt{h_n} - \gamma^T e g I_1^{t_n, t_n+h_n} \\
&- \gamma^T \hat{A} e g'_x[g] (I_1^{t_n, t_n+h_n})^2 - \gamma^T \hat{B} e g'_x[g] I_1^{t_n, t_n+h_n} \sqrt{h_n} \\
&- \delta^T e g \sqrt{h_n} - \delta^T \hat{A} e g'_x[g] \sqrt{h_n} I_1^{t_n, t_n+h_n} - \delta^T \hat{B} e g'_x[g] h_n \qquad (5.4.28)
\end{aligned}
$$

The corresponding terms vanish if the following equations are satisfied

$$
\begin{gathered}
h_n \alpha^T e f = f I_0 \\
\beta^T e g \sqrt{h_n} + \gamma^T e g I_1^{t_n, t_n+h_n} + \delta^T e g \sqrt{h_n} = g I_1^{t_n, t_n+h} \\
\gamma^T \hat{A} e g'_x[g] (I_1^{t_n, t_n+h_n})^2 + \gamma^T \hat{B} e g'_x[g] I_1^{t_n, t_n+h_n} \sqrt{h_n} \\
\delta^T \hat{A} e g'_x[g] \sqrt{h_n} I_1^{t_n, t_n+h_n} + \delta^T \hat{B} e g'_x[g] h_n = g'_x I_{11}^{t_n, t_n+h}. \\
(5.4.29)
\end{gathered}
$$

So we get the order conditions for the coefficient of the stochastic Runge–Kutta method (5.4.22)

$$
\alpha^T e = 1
$$

$$\gamma^T e = 1,\ \beta^T e + \delta^T e = 0$$
$$\gamma^T \hat{B} e + \gamma^T \hat{A} e = 0,\ \gamma^T \hat{A} e = \tfrac{1}{2},\ \gamma^T \hat{B} e = -\tfrac{1}{2}. \tag{5.4.30}$$

We can easily notice that the coefficients of the FRKI method (5.4.21), introduced by Newton verify the above order conditions.

Conclusions

We devoted this thesis to the numerical treatment of Ordinary Differential Equations and Stochastic Differential Equations. The problem of the numerical approximation of ODEs could be considered quite old and well known: indeed a rich literature exists. On the other hand the necessity of efficient methods and fast implementations of them, for high dimensional stiff problem make this topic still an open research area, especially the field of multistep Runge–Kutta and General Linear Methods, in order to design efficient and robust mathematical software, with reliable error estimate and variable stepsize implementation.

In this thesis we proposed a new class of continuous two-step m-stage methods for the numerical solution of ordinary differential equations. These methods have uniform order in any point of the integration interval, and stage order equal to the step point order. As a result, they do not suffer from order reduction phenomenon persistent with methods of low stage order. They are constructed using the collocation approach but by relaxing some of the collocation conditions to obtain methods with desirable stability properties. The construction of high order methods which are A-stable and L-stable is a highly nontrivial task. We hope these methods will constitute building blocks of modern software for stiff differential systems.

As concerning the numerical approximation of second order initial value problems, we present new trigonometrically fitted hybrid methods with parameters depending on one and two frequencies and analyse the linear stability properties. We

think that the used technique can be extended to adapt the coefficients of general linear methods to an oscillatory behavior, especially in the context of collocation methods, by modifying the choice of the collocation functions, as done in the context of exponential-fitting. In this context, the parameters of the methods depend of an estimate of the frequencies appearing in the solution. In our approach, at the moment we have considered that a good estimate of the frequencies is a priori known with enough accuracy. An open problem still remains, concerning the choice of the parameters in the basis of functions, that is a good predictions of the frequencies, when they are not known from the knowledge on the problem.

In the second part we have considered numerical methods for Stochastic Differential Equations. This is quite a new topic, in the sense that there exist some numerical methods in general of low order. Only for particular classes of SDEs there are quite efficient methods. Our aim is to derive in a systematic way numerical methods for general s-dimensional SDEs in Itô form. The first step has been to derive order conditions, extending the classical Albrecht approach, already used in the deterministic case. In this way we carry out our analysis as done in the context of multistep linear methods. Moreover we are also able to provide stage order conditions, up to now never considered. This approach seems to us very promising for the analysis and derivation of new numerical methods for SDEs.

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