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Multi-Value Numerical Modeling for Special Differential Problems

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Introduction

The subject of this thesis is the analysis and development of new numerical methods for Ordinary Differential Equations (ODEs). This studies are motivated by the fundamental role that ODEs play in applied mathematics and applied sciences in general. In particular, as is well known, ODEs are successfully used to describe phenomena evolving in time, but it is often very difficult or even impossible to find a solution in closed form, since a general formula for the exact solution has never been found, apart from special cases. The most important cases in the applications are systems of ODEs, whose exact solution is even harder to find; then the role played by numerical integrators for ODEs is fundamental to many applied scientists. It is probably impossible to count all the scientific papers that made use of numerical integrators during the last century and this is enough to recognize the importance of them in the progress of modern science. Moreover, in modern research, models keep getting more complicated, in order to catch more and more peculiarities of the physical systems they describe, thus it is crucial to keep improving numerical integrator's efficiency and accuracy.

The first, simpler and most famous numerical integrator was introduced by Euler in 1768 and it is nowadays still used very often in many situations, especially in educational settings because of its immediacy, but also in the practical integration of simple and well-behaved systems of ODEs. Since that time, many mathematicians and applied scientists devoted their time to the research of new and more efficient methods (in terms of accuracy and computational cost). The development of numerical integrators followed both the scientific interests and the technological progress of the ages during whom they were developed. In XIX century, when most of the calculations were executed by hand or at most with mechanical calculators, Adams and Bashfort introduced the first linear multistep methods (1855) and the first Runge-Kutta methods appeared (1895-1905) due to the early works of Carl Runge and Martin Kutta. Both multistep and Runge-Kutta methods generated an incredible amount of research and of great results, providing a great understanding of them and making them very reliable in the numerical integration of a large number of practical problems.

It was only with the advent of the first electronic computers that the computational cost started to be a less crucial problem and the research efforts started to move towards the development of problem-oriented methods. It is probably possible to say that the first class of problems that needed an ad-hoc numerical treatment was that of *stiff* problems. These problems require highly stable numerical integrators (see Section 1.7) or, in the worst cases, a reformulation of the problem itself.

Crucial contributions to the theory of numerical integrators for ODEs were given in the XX century by J.C. Butcher, who developed a theory of order for Runge-Kutta

methods based on rooted trees and introduced the family of General Linear Methods together with K. Burrage, that unified all the known families of methods for first order ODEs under a single formulation. General Linear Methods are multistage-multivalued methods that combine the characteristics of Runge-Kutta and Linear Multistep integrators.

In recent times, the researchers started to develop new methods designed for the efficient solution of particular problems, i.e. taking into account the specific expression and properties of the problem itself and paying attention to the preservation of the intrinsic structures of the solutions in the numerical approximation. This is for example the case of exponentially fitted methods, introduced by L. Gr. Ixaru, which are especially designed for oscillatory or periodic problems. Another important example is that of geometric integrators, that are also one of the main topics of the present thesis. The main idea behind such integration techniques is that of preserving the geometric properties of the solution of an ODE system, such as the presence of invariants or the belonging of the solution to a particular surface. This is for example the case of conservative mechanical systems or of systems with space constraints. It is obvious that the numerical solution of such problems must share these properties of the exact one, or its practical usefulness would be poor and even its significance would be lost. We can think for example to the motion of planets of the Solar System, which move on closed planar trajectories (ellipses): we need a numerical integrator to provide closed trajectories, or the approximation of the motion would be completely useless.

The main result achieved in this thesis is the construction of four nearly-conservative methods belonging to the family of General Linear Methods. In particular, two of these methods proved to be very efficient also compared to classical methods both in terms of computational cost and accuracy. We also studied some theoretical aspects of these techniques, highlighting the presence of parasitic components in the numerical approximation and finding a condition for their boundedness. Parasitic components arise in the application of General Linear Methods due to their multivalued nature and they cannot be completely removed, but only controlled, in order to avoid them to destroy the overall accuracy of the numerical scheme. We found an algebraic condition under which the parasitic components give a bounded contribution to the numerical solution and this is small enough to avoid the perturbation of the geometric properties that we aim to preserve. We also addressed the question of which link exists between the accuracy of a numerical scheme and its ability to preserve geometric invariants, providing a Theorem regarding the family of non-parasitic B-series methods.

Another important class of problems that deserves a special treatment is that of the special second order autonomous ODE presented in Section 2.2. For these problems, R. D'Ambrosio, E. Esposito and B. Paternoster introduced a general family of numerical methods extending the ideas of General Linear Methods. This new family is called the General Linear Nyström (GLN) methods family. The original contribution to this theory that is presented in this thesis is the formulation of an algebraic theory of the order based on a particular set of bi-colored rooted trees. Since GLNs are multivalued methods, an initial approximation of the starting values must be provided by the user. This can be avoided by forging our methods around the so-called *Nordsieck vector*, i.e. requiring our method to approximate the solution

and its derivatives, whose initial approximations can be computed exactly from the initial value provided by the problem. We studied in deep this important subclass of numerical integrators, exploiting the expression of the order conditions and proving a theorem where the explicit expression of the local truncation error has been found.

The thesis is organized as follows: the first Chapter is devoted to basic definitions and properties concerning ODEs and numerical methods. In particular, the well-posedness problem is addressed and a few examples from the applications are presented. We also introduce numerical methods and their basic properties, such as order and stability. The methods presented in this Chapter are the classical Linear Multistep and Runge-Kutta families. Chapter 2 is devoted to General Linear Methods, both for first and second order differential problems. In this Chapter we introduce the theory of order for General Linear Nyström methods and the other results discussed above. The discussion on geometric integration is performed in Chapter 3, where we present more in detail the geometric properties of ODE systems and of numerical methods and introduce the concept of G-symplecticity, that is the main conservation property we require General Linear Methods to possess. The final Chapter concerns the topics studied by the author in two academic visits to the Department of Computer Science of the University of Oxford, namely the extraction on cardiac tissue structure information from a particular Magnetic Resonance Imaging technique.

Part I

Chapter 1

Ordinary Differential Equations: Mathematical Background and Introduction to Numerical Integration

In this Chapter, we will give the basic definitions and concepts regarding the theory of Ordinary Differential Equations (ODEs). In particular, we recall the general formulation of a system of ODEs, we give a short classification of various types of ODEs and a list of examples. The question of existence and uniqueness of a solution, that is fundamental in Numerical Analysis, is answered by means of the classical Cauchy's Theorem and some basic stability and geometric properties are listed.

1.1 Introduction

An *Ordinary Differential Equation* (ODE) (compare [1, 2, 26, 77, 109]) of order n is an equation of the form

$$F(y^{(n)}(x), y^{(n-1)}(x), \dots, y'(x), y(x), x) = 0, \quad (1.1)$$

where F is defined in a subset of \mathbb{R}^{n+2} and takes values in \mathbb{R} and the unknown function is $y : \mathbb{R} \rightarrow \mathbb{R}$. An ODE is said to be in *normal form* if in (1.1) it is possible to isolate the maximum order derivative, i.e.

$$y^{(n)}(x) = f(y^{(n-1)}(x), \dots, y'(x), y(x), x), \quad (1.2)$$

with $f : \mathbb{R}^{n+1} \rightarrow \mathbb{R}$. Notation (1.1) can be extended to *systems* of ODEs

$$\begin{cases} F_1(y_1^{(n)}, y_2^{(n)}, \dots, y_d^{(n)}, \dots, y_1', y_2', \dots, y_d', y_1, y_2, \dots, y_d, x) = 0 \\ F_2(y_1^{(n)}, y_2^{(n)}, \dots, y_d^{(n)}, \dots, y_1', y_2', \dots, y_d', y_1, y_2, \dots, y_d, x) = 0 \\ \vdots \\ F_d(y_1^{(n)}, y_2^{(n)}, \dots, y_d^{(n)}, \dots, y_1', y_2', \dots, y_d', y_1, y_2, \dots, y_d, x) = 0, \end{cases}$$

by considering F and the unknown function y taking values in \mathbb{R}^d .

A first result concerning systems of ODEs is that an equation of order n can always be written as a system of n first order equations. In fact, if we consider an order n equation (in normal form, to simplify the notations)

$$y^{(n)}(x) = f(y^{(n-1)}(x), \dots, y'(x), y(x), x),$$

defining

$$\begin{cases} z_1 = y \\ z_2 = y' \\ \vdots \\ z_n = y^{(n-1)}, \end{cases}$$

we obtain the first order system

$$\begin{cases} z'_1 = z_2 \\ z'_2 = z_3 \\ \vdots \\ z'_{n-1} = z_n \\ z'_n = f(z_n, z_{n-1}, \dots, z_1, x). \end{cases}$$

Note that this procedure can be applied recursively to systems of d equations of order n , thus obtaining a system of nd first order equations. It is then convenient and exhaustive to introduce the following vector notation

$$y' = f(x, y) \tag{1.3}$$

with $y : \mathbb{R} \rightarrow \mathbb{R}^d$ and $f : \mathbb{R}^{d+1} \rightarrow \mathbb{R}^d$. A *solution* of (1.3) is a function $\bar{y} : \mathbb{R} \rightarrow \mathbb{R}^d$ such that $\bar{y}' = f(x, \bar{y})$.

Depending on the properties of the function f , equation (1.3) can be further classified, e.g. if f is linear with respect to y , the equation is said to be *linear*, if f do not depend explicitly on x , then the equation is called *autonomous*.

Example 1.1.1. The forced Van Der Pol oscillator [64] describes an electrical or mechanical oscillator with non-linear attenuation

$$\begin{cases} y'_1 = y_2 \\ y'_2 = b(1 - y_1^2)y_2 - \omega^2 y_1 + a \cos(\Omega * x) \end{cases}$$

and is an example of first order system of two equations depending on four parameters a, b, ω, Ω .

We observe that a system (1.3) can always be written in the autonomous form, just rewriting the unknown vector function y as a $d + 1$ -sized vector, being the new component the identity function of x , i.e.

$$\begin{cases} y'_1 = f_1(y_{d+1}, y_1, y_2, \dots, y_d) \\ y'_2 = f_2(y_{d+1}, y_1, y_2, \dots, y_d) \\ \vdots \\ y'_d = f_d(y_{d+1}, y_1, y_2, \dots, y_d) \\ y'_{d+1} = 1. \end{cases}$$

1.1.1 The Initial Value Problem

As observed in the Introduction, ODEs are a fundamental tool to model phenomena evolving in time. In many practical applications, ODEs are given together with an *initial condition*, describing the status of the system at a certain point in time. We define then an *Initial Value Problem* (IVP) as a system of ODEs coupled with an initial condition, i.e.

$$\begin{cases} y' = f(x, y) \\ y(x_0) = y_0. \end{cases} \quad (1.4)$$

A solution of (1.4) is a solution \bar{y} of the ODE such that $\bar{y}(x_0) = y_0$. For the numerical treatment that will follow in next Sections, it is fundamental to understand when an IVP is a Hadamard well-posed problem, i.e. when

- there exist a solution;
- the solution is unique;
- the solution has a continuous dependency on the data.

In order to recall some results concerning well-posedness, we need the definition of Lipschitz-continuous function.

Definition 1.1.1. A function $f : [a, b] \times \mathbb{R}^d \rightarrow \mathbb{R}^d$ is *Lipschitz-continuous* with respect to the second argument if there exist a real number L , called *Lipschitz constant*, such that

$$\|f(x, y_1) - f(x, y_2)\| \leq L\|y_1 - y_2\| \quad (1.5)$$

for each $x \in [a, b]$.

The first two points of well-posedness are answered by the classical [1, 2, 11, 26, 77, 109]

Theorem 1.1.1 (Cauchy's Existence and Uniqueness). Given an IVP

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

if f is continuous in an open neighborhood of the initial condition (x_0, y_0) , uniformly with respect to x and Lipschitz-continuous with respect to y , then there exist an unique solution of the given IVP.

Under the same hypotheses it can be proved that the solution depends continuously on the data, that is the third condition to be satisfied in order to have a well posed problem.

Theorem 1.1.2. Given an IVP

$$\begin{cases} y' = f(x, y) \\ y(x_0) = y_0 \end{cases}, x \in [x_0, X], \quad (1.6)$$

consider the *perturbed* problem

$$\begin{cases} y' = \tilde{f}(x, y) \\ y(x_0) = \tilde{y}_0 \end{cases}, x \in [x_0, X], \quad (1.7)$$

being f, \tilde{f} defined and continuous in $[x_0, X] \times \mathbb{R}^d$.

Let y and \tilde{y} be solutions respectively of (1.6) and of (1.7). If there exists an $\epsilon \in \mathbb{R}$ such that

$$\|f(x, \eta) - \tilde{f}(x, \eta)\| \leq \epsilon$$

for each $x \in [x_0, X]$ and for each $\eta \in \mathbb{R}^d$ and f is Lipschitz-continuous with Lipschitz constant L , then

$$\|y(x) - \tilde{y}(x)\| \leq \|y_0 - \tilde{y}_0\| e^{L(x-x_0)} + \frac{\epsilon}{L} (e^{L(x-x_0)} - 1),$$

thus providing an upper bound for the normed difference between the solutions of the given problems.

1.2 Examples

ODEs arise naturally as models in a large number of applied sciences. In this Section some examples are collected and analysed.

1.2.1 Models from Life Sciences

Example 1.2.1 (Population Growth). Population growth models apply to a number of areas of applied and social sciences, such as Biology, Chemistry, Demography, Economics, Immunology and Physics. Aiming to introduce a basic model, we consider an isolated population, i.e. a population such that the only causes of variation in the number of elements are birth and death. The *Malthusian Model* [41] describing the growth of such a population is the following ODE

$$N'(t) = (\lambda - \mu)N(t) \tag{1.8}$$

where $N(t)$ is the number of elements at time t and λ, μ are respectively the birth and death rates. If we fix an initial condition $N(0) = N_0$, the solution of (1.8) is an exponential

$$N(t) = N_0 \exp \frac{\lambda - \mu}{\mu} t.$$

Malthusian model provides an indefinitely growing solution for the number of individuals in a population, then it is not realistic for long time-spans. An improvement can be introduced using the so called *carrying capacity* parameter K , i.e. a parameter controlling the growth of the solution and related to the environment where the population is set. Such a modification leads to the *logistic model* [41]

$$N'(t) = \frac{\lambda - \mu}{\mu} N(t) \left(1 - \frac{N}{K} \right)$$

whose solution grows up to a certain level of saturation and then remains stable asymptotically. More recent models take into account a larger number of factors and are very specialized for each field of application. One can think for example to a time-varying carrying capacity, to models embedding catastrophes or multiple population, or to stochastic models [41].

Next examples are taken from Immunology[116] [76].

Let v be the number of free viruses infecting a body and let x and y be the number of uninfected and infected cells respectively. Uninfected cells are produced at a rate λ and die at a rate d . Such new born cells are susceptible of infection if they meet a virus and become infected with rate β . Infected cells die at a rate a . The viruses population elements die at a rate u but each infected cell produces a number of new viruses; let k be the rate of birth of the viruses in an infected cell. Combining those information, we get to the following three-populations model [116]

$$\begin{cases} x' = \lambda - dx - \beta xv \\ y' = \beta xv - ay \\ v' = ky - uv. \end{cases}$$

Example 1.2.2. We present a recent model describing an infection of influenza A virus. Its mathematical expression presents an embedding of ODEs and PDEs. We denote respectively with T and I the number of uninfected and infected target cells and with T_a and I_a their apoptotic ¹ counterparts.

$$\begin{cases} \frac{dT}{dt} = \mu T - r^{Inf} T - K_T^{Apo} T, \\ \frac{\partial I}{\partial t} + \frac{\partial I}{\partial \tau} = - \left(k_T^{Apo} + k_t^{Apo}(\tau) \right) I(t, \tau), \\ \frac{dT_a}{dt} = h_T^{Apo} T - r^{inf} T_a - k^{Lys} T_a, \\ \frac{dI_a}{dI} = \int_0^\infty \left(k_T^{Apo} - k_I^{Apo}(\tau) \right) I(t, \tau) d\tau + r^{Inf} T_a - k^{Lys} I_a, \end{cases}$$

where

$$\mu = \left[\frac{\mu_{max}}{T_{max}} \left(T_{max} - T - \int_0^\infty I(t, \tau) d\tau \right) \right]_+.$$

Here μ is the specific growth rate of uninfected cells and k_T^{Apo} their apoptosys rate (analogous notation is used for infected cells). The parameters r^{Inf} , T_{max} and μ_{max} are respectively the infection rate, the maximum concentration of cells and the maximum specific rate.

We observe that this model follows two time scales, the absolute time t and the cells age τ .

Example 1.2.3. The FitzHugh-Nagumo model [112, 61]

$$\begin{cases} \frac{dv}{dt} = c_1 v(v - a)(1 - v) - c_2 w + i_{app} \\ \frac{dw}{dt} = b(v - c_3 w) \end{cases} \quad (1.9)$$

contains an example of cubic equation. The variable v describes the transmembrane potential in a living cell, while w is called *recovery variable* and was introduced to improve the original model. The parameters a, b, c_1, c_2, c_3 can be adjusted to simulate different types of cell.

1.2.2 Models from Physics

Newton's second law, connecting the force applied on a material point of mass m with the acceleration it receives in an inertial system [70, 75], is a second order ODE

$$\mathbf{F} = m\mathbf{a}. \quad (1.10)$$

¹Apoptosys is the process which naturally leads living cells to die.

Example 1.2.4. In a more rigorous fashion, let $y(t)$ be the position of the material point at time t in \mathbb{R}^3 , equation (1.10) takes the form

$$y''(t) = F(t, y, y').$$

Some particular classical examples are the harmonic oscillator

$$y'' = -\omega^2 y,$$

and the motion of a body under the gravity force into the void

$$y'' = -\mathbf{g}.$$

Example 1.2.5. Another example of a second order ODE in Physics, in particular in the field of electromagnetism [75], is

$$LI'' + RI' + C^{-1}I = f(t)$$

describing the current $I(t)$ in an *LRC* circuit with applied power $f(t)$.

Example 1.2.6. The radial Schrödinger equation

$$y'' + (E - V(x))y = 0 \tag{1.11}$$

is a fundamental equation of quantum physics describing the behaviour of a particle in a spherically symmetric potential $V(x)$. E is the energy associated to the system and the interest in this equation is generally twofold

- in its IVP formulation, it provides the trajectory followed by the particle;
- in its formulation as a boundary value problem it provides the admissible values of the energy E , that are the eigenvalues.

1.2.3 Other Problems

Ill-Posed Problems

In Numerical Analysis, a problem is said to be *ill-posed* if it is not well-posed, i.e. if one or more of the conditions of well-posedness are not satisfied (see Section 1.1.1). In this Section, we will see an example of problem where the f function in (1.3) is not continuous[55], failing to satisfy the hypotheses of Theorem 1.1.1.

Example 1.2.7. We consider the problem of modeling the flow of water through a porous media in a realistic environment [55, 60], so that the flow of water is controlled by atmospheric events and is then discontinuous. We consider a slab of soil and let $\theta(t) \in [0, 1[$ be the volumetric moisture content and L the thickness of the slab. Then θ satisfies the following ODE

$$L \frac{d\theta}{dt} = I(t) - D(t)$$

being $D(t)$ the rate of drainage below the slab and $I(t)$ the rate of infiltration, respectively given by

$$D(t) = \frac{1}{B} \left(\Psi(t) + \frac{L}{2} \right) \quad I(t) = \min \left\{ Q(t), \frac{-Psi(t)}{A} \right\}.$$

being Ψ the soil matric potential ², A and B some characteristic times and $Q(t)$ the discontinuous volumetric rainfall rate. For such a problem, neither Cauchy's Theorem and Theorem 1.1.2 hold, thus we can't even tell if a solution exists. Numerical integration is still possible for some discontinuous problems, see for example [55].

Large systems of ODEs

Large systems of ODEs may arise naturally for example in the analysis of circuits, but here we introduce them as a discretization of a Partial Differential Equation with the method of lines.

Example 1.2.8. Consider the linear advection equation

$$u_t + vu_x = 0$$

and discretize the spatial derivative with a finite difference

$$u_x \approx \frac{u_i - u_{i-1}}{h}$$

being h the discretization step. The method of lines provides then the following approximation

$$\frac{du}{dt} = -v \frac{u_i - u_{i-1}}{h}, \quad i = 1, \dots, N$$

which is a system of N ODEs.

1.3 Hamiltonian Systems

Hamiltonian systems are a class of ODEs mainly used in modeling mechanical systems. This Section is devoted to the description of the basic properties of such systems. Some examples are shown.

1.3.1 History and Motivations

Mechanics is the branch of Physics studying the motion of bodies by means of Differential Equations. The first equations of mechanics appeared in Galilei's and Newton's works, in particular the former introduced the celebrated equation (1.10). In 1788, Lagrange introduced his *Analytical Mechanics*, making the analysis of mechanical systems easier also in complex cases. The main simplification introduced by Lagrange was the adoption of *generalized coordinates* (q_1, q_2, \dots, q_d) to describe the state of a system with d degrees of freedom. For example, a material point that is bonded to move on a surface will have two degrees of freedom, so its motion can be described using only two variables instead of the three required in Newtonian Mechanics. Let $T = T(q, \dot{q})$ be the kinetic energy of a system with d degrees of freedom and $U = U(q)$ its potential energy, we define the **Lagrangian function** of the system as the difference

$$\mathcal{L} = \mathcal{T} - \mathcal{U}.$$

²i.e. the energy per unit volume of water required to transfer an infinitesimal quantity of water from a reference pool to the reference air pressure and temperature point.

At each time point, the generalized coordinates of the system satisfy the so-called *Lagrange's equations of motion*

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{q}} \right) = \frac{\partial \mathcal{L}}{\partial q}$$

providing a system of d second order ODEs. W.R. Hamilton introduced a further simplification adopting the so-called *conjugate momenta*

$$p_k = \frac{\partial \mathcal{L}}{\partial \dot{q}}(q, \dot{q}) \quad k = 1, \dots, d \quad (1.12)$$

in place of the generalized velocities \dot{q} . The Lagrangian function can be rewritten as the so-called *Hamiltonian function*

$$\mathcal{H}(p, q) := p^T \dot{q} - \mathcal{L}(q, \dot{q}),$$

where \dot{q} can be expressed in terms of p and q by means of equation(1.12). *Hamilton's equations of motion* [34, 57, 59, 63, 66, 97] are given by

$$\begin{cases} \dot{p}_k = -\frac{\partial \mathcal{H}}{\partial q_k} \\ \dot{q}_k = \frac{\partial \mathcal{H}}{\partial p_k} \end{cases} \quad k = 1, \dots, d \quad (1.13)$$

providing a system of $2d$ first order ODEs .

1.3.2 Examples

We provide a few examples of Hamiltonian systems. Other and more complex examples are given in Section 3.1

Example 1.3.1 (Harmonic Oscillator). A simple harmonic oscillator is a system made by a material point (we assume here of unitary mass) linked to a spring. The equations of motion are

$$\begin{cases} p' = -q \\ q' = p \end{cases}$$

with the Hamiltonian

$$\mathcal{H} = \frac{p^2}{2} + \frac{q^2}{2}.$$

Example 1.3.2 (Simple Pendulum). A simple pendulum is a mechanical system made by an unitary mass connected to an inextensible rope of negligible mass. If we assume the gravity force to be unitary, the equations of motion are

$$\begin{cases} p' = -\sin q \\ q' = p \end{cases}$$

and the Hamiltonian function is

$$\mathcal{H} = \frac{p^2}{2} - \cos q.$$

Example 1.3.3 (Kepler's Problem). The following Hamiltonian system describes the motion of a planet around the origin, where a fixed sun is supposed to lie

$$\begin{cases} q_1' = p_1 \\ q_2' = p_2 \\ p_1' = \frac{-q_1}{(q_1^2 + q_2^2)^{\frac{3}{2}}} \\ p_2' = \frac{-q_2}{(q_1^2 + q_2^2)^{\frac{3}{2}}}. \end{cases}$$

The Hamiltonian function has the form

$$\mathcal{H} = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}}.$$

1.3.3 Geometric properties of Hamiltonian systems

Hamiltonian systems are widely studied in the field of geometric numerical integration, since they own two important conservation properties: energy conservation and the symplecticity of the flow [59, 70]. Concerning the preservation of the total energy, we observe that the Hamiltonian function of each Hamiltonian system is a first integral of the system itself. This can be verified immediately just deriving \mathcal{H} with respect to the time variable

$$\frac{d\mathcal{H}}{dt} = \sum_i \frac{\partial \mathcal{H}}{\partial p_i} \frac{dp_i}{dt} + \frac{\partial \mathcal{H}}{\partial q_i} \frac{dq_i}{dt} \quad (1.14)$$

evaluating (1.14) in a solution of the system we obtain

$$\frac{d\mathcal{H}}{dt} = \sum_i \frac{dq_i}{dt} \frac{dp_i}{dt} - \frac{dp_i}{dt} \frac{dq_i}{dt} = 0.$$

We are not going into the mathematical details of symplecticity of the flow, since such a treatment would require advanced mathematical tools that are beyond the purposes of this work (for more details, see [70]).

We will give here a geometric idea of what symplecticity of the flow of an Hamiltonian system means. We first recall the definition of *flow* of a dynamical system as the operator

$$\Psi(p(0), q(0)) \mapsto (p(t), q(t)).$$

Such an operator is said to be symplectic if it preserves volumes. In particular, in the case of a system with one degree of freedom, that will provide a two dimensional domain for Ψ , the flow is symplectic if it preserves oriented areas.

1.3.4 Quadratic Invariants

Consider an homogeneous ODE

$$y' = f(y). \quad (1.15)$$

A quadratic function

$$I(y) = y^T Q y \quad (1.16)$$

where Q is a symmetric matrix is an invariant for (1.15) if, and only if

$$y^T Q f(y) = 0.$$

Example 1.3.4 (Inertial motion of a rigid body). Euler's equations for the inertial motion of a rigid body are

$$\begin{cases} \dot{\omega}_x = \left(\frac{I_{yy}-I_{zz}}{I_{xx}}\right)\omega_y\omega_z \\ \dot{\omega}_y = \left(\frac{I_{zz}-I_{xx}}{I_{yy}}\right)\omega_z\omega_x \\ \dot{\omega}_z = \left(\frac{I_{xx}-I_{yy}}{I_{zz}}\right)\omega_x\omega_y \end{cases}$$

where $\omega_x, \omega_y, \omega_z$ are the components of the angular speed along the principal axes of inertia and I_{xx}, I_{yy}, I_{zz} are the principal inertia momenta. This system possesses two quadratic invariants, namely the kinetic energy K and the square norm of the angular momentum A , i.e.

$$K = \frac{1}{2} \begin{bmatrix} \omega_x & \omega_y & \omega_z \end{bmatrix} \begin{bmatrix} I_{xx} & 0 & 0 \\ 0 & I_{yy} & 0 \\ 0 & 0 & I_{zz} \end{bmatrix} \begin{bmatrix} \omega_x \\ \omega_y \\ \omega_z \end{bmatrix},$$

$$A = \begin{bmatrix} \omega_x & \omega_y & \omega_z \end{bmatrix} \begin{bmatrix} I_{xx}^2 & 0 & 0 \\ 0 & I_{yy}^2 & 0 \\ 0 & 0 & I_{zz}^2 \end{bmatrix} \begin{bmatrix} \omega_x \\ \omega_y \\ \omega_z \end{bmatrix}.$$

1.4 Introduction to Numerical Integration

The numerical integration of an IVP by means of classical integrators usually involves working on a *discretized* version of the IVP itself, thus introducing an intrinsic error, that is called *Local Truncation Error (LTE)*. A numerical method is said to be *consistent* if LTE tends to zero with the integration step going to zero.

1.4.1 Finite Differences

Before going into the details of numerical integrators, it is appropriate to recall a classical method for the approximation of derivatives: finite differences.

By definition, the first derivative of a function f in a point x is given by the limit

$$f'(x) = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}$$

if it exists. Neglecting the limit operator and taking a fixed value for h we obtain an approximation of $f'(x)$

$$f'(x) = \frac{f(x+h) - f(x)}{h} + O(h)$$

involving the so-called *first order forward difference* [4, 106, 108]

$$\Delta_h[f](x) = \frac{f(x+h) - f(x)}{h}. \tag{1.17}$$

Another first order approximation of $f'(x)$ can be obtained using the *first order backward difference*

$$\nabla_h[f](x) = \frac{f(x) - f(x-h)}{h},$$

while the *central difference*

$$\delta_h[f](x) = \frac{f(x + \frac{1}{2}h) - f(x - \frac{1}{2}h)}{h}$$

provides a second order approximation.

Higher order finite differences, useful to approximate higher order derivatives, can be obtained by means of recursive application of the first order ones. An example that is widely used is the *second order central difference*

$$\delta_h^2[f](x) = \frac{f(x + h) - 2f(x) + f(x - h)}{h^2}$$

providing an approximation of $f''(x)$.

1.4.2 The Euler's method

We consider an IVP

$$\begin{cases} y' = f(x, y) \\ y(x_0) = y_0 \end{cases}, x \in [x_0, X] \quad (1.18)$$

and approximate the first derivative just with a first order difference (1.17). The differential equation in (1.18) becomes

$$y(x_0 + h) - y(x_0) = hf(x_0, y(x_0)) + O(h).$$

Neglecting the $O(h)$ term, we get one step of the Euler's method.

$$y(x_0 + h) \approx y(x_0) + hf(x_0, y(x_0)) \quad (1.19)$$

and iterating on a fixed stepsize discretization of $[x_0, X]$:

$$\Delta = \{x_0 + nh, n = 0, 1, \dots, N\},$$

we obtain the following approximation of the solution

$$y_{n+1} = y_n + hf(x_n, y_n), \quad n = 0, 1, \dots, N - 1. \quad (1.20)$$

The numerical approximation of (1.18) is no more a differential equation, but a *discretized* version of it. Classical numerical integrators do not deal with the continuous problem, but with a discretization of it, usually by means of a difference equation. New problems then arise at this step: is the discretized problem well-posed? Is it a good approximation to the original problem?

1.4.3 Difference Equations

A *difference equation* [56] is a recurrence relation, i.e. a relation involving the values of a function in a discrete number of points, formally

$$F(y_n, y_{n+1}, \dots, y_{n+k}) = 0, \quad (1.21)$$

where k is the **order** of the equation. We are interested in finding a *solution* of (1.21), that is a sequence of values that makes (1.21) an identity. Definitions of

linearity, homogeneity and expression in normal form can be given and are analogous to those given for ODEs.

Many numerical methods produce linear difference equation with constant coefficients, namely of the form

$$\alpha_k y_{n+k} + \alpha_{k-1} y_{n+k-1} + \cdots + \alpha_0 y_n = g_n, \quad (1.22)$$

being g_n the *forcing term*.

Example 1.4.1. The equation

$$y_{n+1} - y_n = n - 2$$

is first-order, linear and constant coefficients with forcing term $g_n = n - 2$. Given the initial value of the solution, we can obtain the whole sequence just applying recursively the equation. Another example is the Euler's method formula (1.20).

Well-posedness of difference equations is crucial in the analysis of numerical integrators. The following theorem is the analogous of Theorem 1.1.1 for equations like (1.22)

Theorem 1.4.1. The linear difference equation of order k with constant coefficients

$$\alpha_k y_{n+k} + \alpha_{k-1} y_{n+k-1} + \cdots + \alpha_0 y_n = g_n$$

has a unique solution for each k -uple of initial values.

The following result gives much insight in what can happen to the solutions of (1.22)

Theorem 1.4.2. Consider the equation (1.22),

1. if $g_n = 0$ and $y_0 = y_1 = \cdots = y_{k-1} = 0$, then the only solution is a sequence of zeros;
2. if $\{y_n\}$ and $\{z_n\}$ are solutions, then $\{Ay_n + Bz_n\}$ is a solution for each $A, B \in \mathbb{R}$;

A system of k linearly independent solutions³ of (1.22) is said **fundamental system** of solutions. We now consider the homogeneous equation

$$\alpha_k y_{n+k} + \alpha_{k-1} y_{n+k-1} + \cdots + \alpha_0 y_n = 0 \quad (1.23)$$

and search for its solutions of the form $\{y_n\} = \{z^n\}$, $z \neq 0$. Substituting in (1.23), we obtain

$$\alpha_k z^{n+k} + \alpha_{k-1} z^{n+k-1} + \cdots + \alpha_0 z^n = 0$$

that is equivalent to

$$\alpha_k z^k + \alpha_{k-1} z^{k-1} + \cdots + \alpha_0 = 0. \quad (1.24)$$

The polynomial at first member in (1.24) is called *characteristic polynomial* of eqreflinom and $\{z^n\}$ is a solution of (1.23) if and only if z is a root of the characteristic polynomial, moreover, the following result holds

³The sequences $\{y_n\}$ and $\{z_n\}$ are said to be **linearly independent** in $n = n_0$ if and only if the only combination $\{Ay_n + Bz_n\} = 0$ is the one with $A = 0, B = 0$ for each $n - n_0 = 0, 1, \dots, k - 1$.

Theorem 1.4.3. Let z_1, z_2, \dots, z_k be the roots of the characteristic polynomial of equation (1.23), then

- if $z_i \neq z_j$ for each $i \neq j$, then $\{\{z_1^n\}, \{z_2^n\}, \dots, \{z_k^n\}\}$ is a fundamental system of solutions for (1.23);
- if z_i is a multiple root of order $l > 1$, then $\{z_i^n\}, \{nz_i^n\}, \dots, \{n^{l-1}z_i^n\}$ are solutions and a fundamental system of solutions can be obtained just joining this set of solutions with those related to the other roots.

In view of some observations concerning stability, it is important to analyze the behavior of the solutions of a difference equation, in particular we distinguish three cases

1. z is a simple real root, then $\{z^n\}$ is a solution of (1.23) it diverges if $|z| > 1$, while it goes to zero if $|z| < 1$ and is bounded if $|z| = 1$;
2. z is a complex root, then its conjugate \bar{z} is a root. If $z = \alpha + i\beta$, the corresponding solutions are $\{z^n\} = \{(\alpha + i\beta)^n\}$ and $\{\bar{z}^n\} = \{(\alpha - i\beta)^n\}$, corresponding, if $z = \rho(\cos \theta + i \sin \theta)$, to the trigonometric form

$$\{\rho^n \sin n\theta\} \quad , \quad \{\rho^n \cos n\theta\},$$

thus oscillating in $[-\rho, \rho]$;

3. z is a multiple root of order l : we obtain l solutions $\{z^n\}, \{nz^n\}, \dots, \{n^{l-1}z^n\}$, diverging if $|z| \geq 1$ and going to zero if $|z| < 1$.

In numerical integration we obviously want our approximation to be bounded, so we only consider as good those methods whose associated difference equation has a characteristic polynomial with roots of modulus less or equal than one but being the roots of modulus one simple. This is a first “raw“ definition of stability. Method (1.20) is a linear first-order difference equation, whose characteristic polynomial is $z - 1$.

1.5 Linear Multistep Methods

Consider an IVP

$$\begin{cases} y' = f(x, y) \\ y(x_0) = y_0. \end{cases}, \quad x \in [x_0, X] \quad (1.25)$$

and a discretization $\{x_i\}$ of the interval $[x_0, X]$. The general expression of a k -step Linear Multistep Method (LMM) [11, 71, 86] is

$$\sum_{j=0}^k \alpha_j y_{n+j} = h \sum_{j=0}^k \beta_j f(t_{n+j}, y_{n+j}). \quad (1.26)$$

Example 1.5.1. Integrating the ODE in (1.25) in a subinterval of the discretization $[x_i, x_{i+1}]$ we obtain

$$y(x_{i+1}) - y(x_i) = \int_{x_i}^{x_{i+1}} f(\tau, y) d\tau. \quad (1.27)$$

Approximating the integral in (1.27) with different quadrature formulas gives rise to different LMM, e.g.

- using a trapezoidal formula and neglecting the associated error we obtain

$$y_{i+1} - y_i = \frac{h}{2} (f(x_{i+1}, y_{i+1}) + f(x_i, y_i)),$$

called again *trapezoidal rule*;

- using as approximation the surface of a rectangle based in x_i, x_{i+2} and of height $f(x_{i+1})$ we obtain the *mid-point rule*

$$y_{i+2} - y_i = 2hf(x_{i+1}, y_{i+1}).$$

These two examples are useful to the purpose of introducing the issues that are generally related to the application of LMM, in fact the mid-point rule is a two step method, needing a starting value that is generally not provided by the problem. Such a starting value is often obtained applying a one step method or using other strategies. In trapezoidal rule the unknown value y_{i+1} appears as a variable of the function f , giving rise to a generally non linear equation.

Definition 1.5.1. A LMM (1.26) is called *explicit* if $\alpha_k = 0$, otherwise it is called *implicit*.

Remark 1.5.1. Implicit methods involve the solution of a non linear equation or system of equations, that is generally effectively solved using fixed-point iterations. In equation (1.26) it is possible to rescale the coefficients in such a way that $\alpha_k = 1$. If we assume the method to be implicit, we can write

$$y_{n+k} = - \sum_{j=0}^{k-1} \alpha_j y_{n+j} + h \sum_{j=0}^k \beta_j f(x_{n+j}, y_{n+j}). \quad (1.28)$$

This can be viewed as a fixed point iteration $x = g(x)$ and it can be numerically solved by means of an iterative procedure

$$x^{(k+1)} = g(x^{(k)})$$

which is convergent e.g. if g is a contraction⁴. In equation (1.28), if we collect in A the terms independent from y_{n+k} we have the following expression for g

$$g(y) = A + h\beta_k f(x_{n+k}, y).$$

We want this function to be a contraction

$$|g(y_1) - g(y_2)| = |h\beta_k (f(x_{n+k}, y_1) - f(x_{n+k}, y_2))| \leq |h\beta_k L| |y_1 - y_2|$$

where L is the Lipschitz constant of the function f .

The fixed point iteration is then convergent if $h < \frac{1}{|\beta_k|L}$.

⁴A function $g : \mathbb{R} \rightarrow \mathbb{R}$ is a contraction if and only if $|g(x) - g(y)| \leq L|x - y|$, with $L < 1$.

1.5.1 Consistency and Order Conditions of LMM

Associated to a LMM

$$\sum_{j=0}^k \alpha_j y_{n+j} = h \sum_{j=0}^k \beta_j f(x_{n+j}, y_{n+j}),$$

is a difference operator [86]

$$L[y(x); h] = \sum_{j=0}^k \alpha_j y(x + jh) - h \beta y'(x + jh). \quad (1.29)$$

The operator L , if evaluated in the solution y of an IVP, returns the residual of the solution itself in the method, i.e. the LTE. We are interested in finding conditions on the coefficients of the method for LTE being of a certain order. To do that, we write the Taylor's expansion of L in a neighborhood of x

$$\begin{aligned} L[y(x); h] &= \sum_{j=0}^k \alpha_j \left[y(x) + jhy'(x) + \frac{j^2 h^2}{2} y''(x) + \dots + \frac{j^q h^q}{q!} y^{(q)}(x) + \dots \right] - \\ &\quad - h \sum_{j=0}^k \beta_j \left[y'(x) + jhy''(x) + \frac{j^2 h^2}{2} y'''(x) + \dots + \frac{j^q h^q}{q!} y^{(q+1)}(x) + \dots \right] \end{aligned}$$

and collect the coefficients of the derivatives of y

$$\begin{aligned} c_0 &= \sum_{j=0}^k (\alpha_j) \\ c_1 &= \sum_{j=0}^k (j\alpha_j - \beta_j) \\ c_2 &= \sum_{j=0}^k \left(\frac{j^2 \alpha_j}{2} - j\beta_j \right) \\ &\vdots \\ c_q &= \sum_{j=0}^k \left(\frac{j^q \alpha_j}{q!} - \frac{j^{q-1} \beta_j}{(q-1)!} \right) \end{aligned} \quad (1.30)$$

Definition 1.5.2. A LMM has *order* p if its coefficients c_i defined in (1.30), are zero for each i less than or equal to p and c_{p+1} is not zero. c_{p+1} is called *main term of LTE*.

Definition 1.5.3. A LMM is *consistent* if its order is at least one.

1.5.2 Zero-stability and Convergence

Zero-stability of a LMM is related to the stability of the underlying difference operator [11, 86].

Definition 1.5.4. We consider a LMM (1.26). The polynomials

$$\rho(z) = \sum_{j=0}^k \alpha_j z^j$$

and

$$\sigma(z) = \sum_{j=0}^k \beta_j z^j$$

are respectively called *first and second characteristic polynomial* of the method.

Applying the results shown in Section (1.4.3) we can give the following

Definition 1.5.5. A LMM is *zero-stable* if the roots of its first characteristic polynomial are all less or equal to one in modulus and those whose modulus is equal to one are simple.

Convergence, as we will see more in detail in next sections, is the property of a method ensuring the numerical approximation to tend to the exact solution as the stepsize goes to zero. In order to give a suitable definition of convergence for LMM, we need to take into account the necessity of starting values that may affect the overall integration process. Following [86], we define convergence of LMM as follows

Definition 1.5.6. Consider an IVP and let y be its solution and $y_n(h)$ the numerical approximation provided by a k -step LMM method (1.26) with stepsize h . The LMM is *convergent* if

$$\lim_{\substack{h \rightarrow 0, n \rightarrow +\infty \\ nh = x - x_0}} y_n(h) = y(x)$$

for each k -uple of starting values

$$y_\mu = \eta_\mu(h), \quad \mu = 0, \dots, k-1$$

such that

$$\lim_{h \rightarrow 0} \eta_\mu(h) = y_0. \tag{1.31}$$

Condition (1.31) ensures that the starting values are close enough to the only exact value of the solution that is given us, i.e. the initial value.

Definition 1.5.6 can be hard to verify. In practical construction processes, the following equivalence is very useful.

Theorem 1.5.1. A Linear Multistep Method is convergent if and only if it is zero-stable and consistent.

1.6 Runge-Kutta Methods

Runge-Kutta methods (RK) [11, 71, 86] are single-step multi-stage methods. Their complexity relies on a higher number of function evaluation per step, making the

maximum profit out of the given initial value. A Runge-Kutta method is defined by the following procedure

$$\begin{cases} K_i = f(t_n + c_i h, y_n + h \sum_{j=1}^s a_{ij} K_j), & i = 1, \dots, s \\ y_{n+1} = y_n + h \sum_{i=1}^s b_i K_i, \end{cases} \quad (1.32)$$

or, equivalently

$$\begin{cases} Y_i = y_n + h \sum_{j=1}^s a_{ij} f(t_n + c_j h, Y_j), & i = 1, \dots, s \\ y_{n+1} = y_n + h \sum_{i=1}^s b_i f(t_n + c_i h, Y_i). \end{cases}$$

Each step of the computation is further divided into two phases

1. solving the nonlinear system in the first equation of (1.32) in order to compute the values K_i , called *inner stages* of the method;
2. computing the approximation y_{n+1} using the second equation in (1.32).

Remark 1.6.1. The computation of the stages is the most computationally expensive task of each step, requiring the numerical solution of a nonlinear system. The dimension of this system, usually denoted with s is the number of stages of the method. A fixed point iteration procedure can be used in order to solve the system, being it in a fixed point form already. In some cases, however, fixed point iterations do not converge and Newton's method can be used effectively.

RK methods are usually denoted with a tableaux

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \dots & a_{1s} \\ c_2 & a_{21} & a_{22} & \dots & a_{2s} \\ \vdots & \vdots & \ddots & & \vdots \\ c_s & a_{s1} & a_{s2} & \dots & a_{ss} \\ \hline & b_1 & b_2 & \dots & b_s, \end{array}$$

called *Butcher's tableaux* or *Butcher's array* [11, 71, 86]; using a matrix notation $A = (a_{ij})$, $c = (c_1, \dots, c_s)$, $b = (b_1, \dots, b_s)$, it becomes

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

Coefficients b_i are called *weights* of the method and c_i are called *abscissae* or *nodes*.

A Runge-Kutta method is said *explicit* if its coefficient matrix A is strictly lower triangular, otherwise we say that the method is *implicit*. Explicit methods require a lower computational effort in the computation of the stages, since one can solve the non-linear equations in (1.32) sequentially.

Example 1.6.1. We can write the Euler's method and the mid-point rule as RK methods respectively as

$$\begin{array}{c|c} 0 & \\ \hline & 1 \end{array}, \quad \begin{array}{c|cc} 0 & & \\ & 1 & 1 \\ \hline & & \frac{1}{2} \quad \frac{1}{2} \end{array}.$$

The following methods have order 3 and 4 respectively [11]

$$\begin{array}{c|cc} 0 & & \\ \frac{1}{2} & \frac{1}{2} & \\ 1 & -1 & 2 \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}, \quad \begin{array}{c|ccc} 0 & & & \\ \frac{1}{2} & \frac{1}{2} & & \\ \frac{1}{2} & 0 & \frac{1}{2} & \\ 1 & 0 & 0 & 1 \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array}.$$

Radau II method (order 3, 2 stages) has the tableaux [11]

$$\begin{array}{c|cc} \frac{1}{3} & \frac{1}{3} & 0 \\ & 1 & 1 & 0 \\ \hline & \frac{3}{4} & \frac{1}{4} \end{array}.$$

The following methods are based on Gaussian nodes and have respectively order 4 and 6. Gauss methods achieve the maximal order with a fixed number of stages, i.e. $2s$ if s is the number of stages[11, 71, 70].

$$\begin{array}{c|cc} \frac{3-\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\ \frac{3+\sqrt{3}}{6} & \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \tag{1.33}$$

$$\begin{array}{c|ccc} \frac{1}{2} - \frac{\sqrt{15}}{10} & \frac{5}{36} & \frac{2}{9} - \frac{\sqrt{15}}{15} & \frac{5}{36} - \frac{\sqrt{15}}{30} \\ \frac{1}{2} & \frac{5}{36} + \frac{\sqrt{15}}{24} & \frac{2}{9} & \frac{5}{36} - \frac{\sqrt{15}}{24} \\ \frac{1}{2} + \frac{\sqrt{15}}{10} & \frac{5}{36} + \frac{\sqrt{15}}{30} & \frac{2}{9} + \frac{\sqrt{15}}{15} & \frac{5}{36} \\ \hline & \frac{5}{18} & \frac{4}{9} & \frac{5}{18} \end{array}$$

1.6.1 Order Conditions

The theory we present in this Section was developed by Butcher, who found a link between the order of a RK method and the elements of the set of rooted trees (see [11]). This theory simplified a lot the study and construction of RK methods and nowadays it is still actual and still many papers and new theories are based on it. Starting from the ideas of this theory we developed an algebraic theory of order for General Linear Nyström methods for second order ODEs in Section 2.2.1. Many relevant and fundamental contributions have also been given by Hairer and his co-authors (see for example [71, 70]) and by Chartier, Faou and Murua [23].

For the remainder of this Section, in order to simplify the notations, it will be convenient to consider only autonomous initial value problems

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

Butcher's order theory is based on the observation that a biunivocal correspondence can be found between the derivatives of such problem and the elements of the set of rooted trees we will introduce later in this Section. In practice, the order conditions will be found by comparison between the Taylor expansions of the exact solution and the numerical one. In order to exploit this properties, we write the derivatives of y up to order 3

$$y'(x) = f(y(x)) \tag{1.34}$$

$$y''(x) = f'(y(x))y'(x) \tag{1.35}$$

$$= f'(y(x))f(y(x)) \tag{1.36}$$

$$y'''(x) = f''(y(x))(f(y(x)), y'(x)) + f'(y(x))f'(y(x))y'(x) \tag{1.37}$$

$$= f''(y(x))(f(y(x)), f(y(x))) + f'(y(x))f'(y(x))f(y(x)). \tag{1.38}$$

Note that we used the fact that y is a solution of the differential problem, thus $y' = f(y)$ and we need to compute those derivatives essentially by means of Leibnitz's rule. Following Butcher (see [11]), we simplify the notations writing $\mathbf{f} = f(y(x))$, $\mathbf{f}' = f'(y(x))$, $\mathbf{f}'' = f''(y(x))$, \dots , then we observe that these derivatives can be put in correspondence with rooted trees following a simple set of rules

1. a derivative of order n corresponds to a tree with n nodes;
2. each occurrence of f becomes a vertex;
3. a first derivative f' becomes a vertex with one branch;
4. a k -th derivative $f^{(k)}$ becomes a vertex with k branches pointing upwards.

We then obtain Table 1.1 It is now time to introduce a few operators on the set of rooted trees

$$T = \{\bullet, \mathbf{!}, \mathbf{V}, \mathbf{!}, \dots\},$$

namely, for a generic tree $t \in T$,

- $r(t)$ is the order of t , i.e. the number of vertices
- $\sigma(t)$ is the symmetry of t , i.e. the order of the automorphism group of the set of vertices of t

$$\begin{array}{l|l}
y'(x) & = \mathbf{f} \qquad \bullet \mathbf{f} \\
y''(x) & = \mathbf{f}'\mathbf{f} \qquad \begin{array}{c} \bullet \mathbf{f} \\ | \\ \bullet \mathbf{f}' \end{array} \\
y'''(x) & = \mathbf{f}''(\mathbf{f}, \mathbf{f}) \qquad \begin{array}{c} \mathbf{f} \bullet \qquad \bullet \mathbf{f} \\ \diagdown \quad \diagup \\ \bullet \mathbf{f}'' \end{array} \\
& + \mathbf{f}'\mathbf{f}'\mathbf{f} \qquad \begin{array}{c} \bullet \mathbf{f} \\ | \\ \bullet \mathbf{f}' \\ | \\ \bullet \mathbf{f}' \end{array}
\end{array}$$

Table 1.1: Correspondence between derivatives and trees.

t								
$r(t)$	1	2	3	3	4	4	4	4
$\sigma(t)$	1	1	2	1	6	1	2	1
$\gamma(t)$	1	2	3	6	4	8	12	24
$\alpha(t)$	1	1	1	1	1	3	1	1
$\beta(t)$	1	2	3	6	4	24	12	24
$F(t)$	\mathbf{f}	$\mathbf{f}'\mathbf{f}$	$\mathbf{f}''(\mathbf{f},\mathbf{f})$	$\mathbf{f}'\mathbf{f}'\mathbf{f}$	$\mathbf{f}^{(3)}(\mathbf{f},\mathbf{f},\mathbf{f})$	$\mathbf{f}'(\mathbf{f},\mathbf{f}'\mathbf{f})$	$\mathbf{f}'\mathbf{f}''(\mathbf{f},\mathbf{f})$	$\mathbf{f}'\mathbf{f}'\mathbf{f}'\mathbf{f}$

Table 1.2: Operators on trees up to order 4.

- $\gamma(t)$ is the density of t
- $\alpha(t)$ is the number of ways of labelling with an ordered set
- $\beta(t)$ is the number of ways of labelling with an unordered set
- $F(t)(y_0)$ are the elementary differentials.

Elementary differentials are in practice the various differential terms which combination give the derivatives of y (for more rigorous definitions, see [11, 71]). It is now easy to verify that the exact solution of the given problem y can be expanded in Taylor series around x_0 as follows

$$y(x_0 + h) = y_0 + \sum_{t \in T} \frac{\alpha(t) h^{r(t)}}{r(t)!} F(t)(y_0) \quad (1.39)$$

or, equivalently

$$y(x_0 + h) = y_0 + \sum_{t \in T} \frac{h^{r(t)}}{\sigma(t) \gamma(t)} F(t)(y_0)$$

Next step is to write the numerical approximation provided by a RK method as a series of the form (1.39) and compare the corresponding terms between those two series. We consider expression (1.32) of a Runge-Kutta method and, following [70], we put $g_i = hk_i$ and write

$$g_i = hf(u_i), \quad u_i = y_n + \sum_j a_{ij} g_j, \quad y_{n+1} = y_n + \sum_i b_i g_i. \quad (1.40)$$

Now we need to derive these expressions as functions of the stepsize h and evaluate the derivatives in $h = 0$, since we are interested in the value in y_n . Applying Leibnitz's rule, we obtain

$$g_i^{(q)} = h(f^{(q)}(u_i)) + q(f^{(q-1)}(u_i))$$

then, in $h = 0$,

$$g_i^{(q)} = q(f^{(q-1)}(u_i)).$$

In practice we have the same expression of the derivative of the exact solution multiplied by a term q . This allows us to compute the g_i 's derivatives using (1.34), but we find them to depend on the derivative of the u_i terms. These terms are easily computed by linearity, due to the definition of u_i (1.40). It is now easy to combine all the terms and get the coefficients of the expansion of the numerical solution, that are called **elementary weights**

$$\Phi(t) = \sum_{i,j,k=1}^s b_i a_{ij} c_j^2 a_{ik} c_k^2.$$

The formal series expansion for the numerical solution is then

$$y_1 = y_0 + \sum_{t \in T} \frac{h^{r(t)}}{\sigma(t)} \Phi(t) F(t)(y_0)$$

and the order conditions are easily obtained by comparison with (1.39), obtaining the following

Theorem 1.6.1. The Runge-Kutta method (1.32) has order p if and only if

$$\Phi(t) = \frac{1}{\gamma(t)}$$

for each tree $t \in T$ such that $\rho(t) \leq p$.

As anticipated in the introduction to this Section, we found a result analogous to Theorem 1.6.1 for methods belonging to the family of General Linear Nyström methods for second order problems and it is Proposition 2.2.1.

1.7 Linear Stability of Numerical Integrators

Stability is a fundamental property of numerical methods. A method is stable if it is able to handle small errors without amplifying them. Small errors always occur in numerical procedures, due basically to the representation of machine numbers. Other errors are introduced by the numerical procedure, e.g. the LTE (see Section 1.4) in numerical integrators. A stable method is able to keep those perturbations under control in order to avoid them to affect the overall accuracy.

1.7.1 Introduction

In the numerical integration of initial value problems, stability is classically investigated in the linear sense.

Consider an IVP (1.4) and let y and z be solutions respectively corresponding to the initial values y_0 and z_0 ; let $\delta y := z - y$ be the difference between the solutions. We aim to find a relation connecting the initial values with the corresponding solutions. We derive z using the definition of δ

$$z' = y' + (\delta y)' = f(x, z) = f(x, y + \delta y), \quad (1.41)$$

and write the Taylor series expansion of $f(x, y + \delta y)$ based in (x, y) , then substitute in (1.41)

$$y' + (\delta y)' = f(x, y) + \frac{\partial f}{\partial y} \delta y + o(\|\delta y\|^2).$$

Truncating and using the definition of y we obtain

$$(\delta y)' = J \delta y + o(\|\delta y\|^2), \quad (1.42)$$

being $J = \frac{\partial f}{\partial y}$ the Jacobian of f .

For linear systems with constant coefficients [86]

$$y' = Ay$$

good stability properties are achieved when the real part of the eigenvalues of A are negative, since in such a case the corresponding solutions are decreasing. We found that the difference δ between two solutions of an IVP satisfies (1.42), i.e. a linear system with non-constant coefficients. It is useful anyway to consider as a test equation

$$y' = \lambda y, \lambda \in \mathbb{C} \quad (1.43)$$

or its vector homologous

$$y' = \Lambda y$$

since this allows us to take advantage of the connection between stability and the eigenvalues of Λ . This corresponds to assuming the Jacobian of f to be locally constant, but this is not always coherent with the actual problem.

Example 1.7.1. Consider the system $y' = A(x)y$, with

$$A = \begin{bmatrix} 0 & 1 \\ -\frac{1}{16x^2} & -\frac{1}{2x} \end{bmatrix}, x > 0.$$

A has the only eigenvalue: $\lambda = -\frac{1}{4x}$. If $x > 0$, λ is negative, so we expect the solutions of the system to be decreasing, but we see that

$$y = \begin{bmatrix} 4x^{\frac{1}{4}} \\ x^{-\frac{3}{4}} \end{bmatrix}$$

diverging with $x \rightarrow \infty$.

1.7.2 Linear Multistep Methods

Given a k step LMM (1.26), the global error satisfies the following difference equation

$$\sum_{j=0}^k [\alpha_j I - h\beta_j J] E_{n+j} = \phi, \quad (1.44)$$

being E_{n+j} the global error and ϕ the LTE in the grid-point x_{n+j} and J the Jacobian matrix of the system with respect to y . Based on the considerations made in the previous paragraphs, we assume J and ϕ to be constant. Equation (1.44) then becomes

$$\sum_{j=0}^k [\alpha_j - h\lambda\beta_j] E_{n+j} = \phi$$

whose characteristic polynomial

$$\pi(r, \bar{h}) = \sum_{j=0}^k [\alpha_j - \bar{h}\beta_j] r^j, \quad \bar{h} = h\lambda$$

is called *stability polynomial* of the method. Based on the considerations about the stability of difference equations made in Section 1.4.3 we give the following

Definition 1.7.1. A linear multistep method is said *absolutely stable* for \bar{h} if and only if all the roots of $\pi(r, \bar{h})$ are less or equal then one in norm and those of norm equal to one are simple. The set of all \bar{h} such that the method is absolutely stable is called *absolute stability region* of the method.

Definition 1.7.2. A LMM is *A-stable* if its absolute stability region embeds the left half plane of the complex numbers set.

1.7.3 Runge-Kutta methods

Applying the Runge-Kutta method (1.32) to the linear scalar test equation (1.43), we get

$$\begin{cases} Y_i = y_n + \hat{h} \sum_{j=1}^s a_{ij} Y_j, & i = 1, \dots, s, & \hat{h} = h\lambda, \\ y_{n+1} = y_n + \hat{h} \sum_{i=1}^s b_i Y_i. \end{cases} \quad (1.45)$$

We set

$$\mathbf{Y} = (Y_1, \dots, Y_s)^T \quad \mathbf{e} = (1, 1, \dots, 1) \in \mathbb{R}^s,$$

and (1.45) can be written as

$$\begin{cases} \mathbf{Y} = y_n \mathbf{e} + \hat{h} A \mathbf{Y}, & i = 1, \dots, s, \\ y_{n+1} = y_n + \hat{h} b^T \mathbf{Y}. \end{cases} \quad (1.46)$$

We derive a relation for the stages from the first equation in (1.46)

$$\mathbf{Y} = y_n \mathbf{e} \left(I - \hat{h} A \right)^{-1}$$

and, substituting it into the second, we obtain

$$y_{n+1} = y_n \left(1 + \hat{h}b^T \mathbf{e} \left(I - \hat{h}A \right)^{-1} \right).$$

The function

$$R(\hat{h}) = \left(1 + \hat{h}b^T \mathbf{e} \left(I - \hat{h}A \right)^{-1} \right)$$

is called *stability function* of the method.

The solution to the test equation provided by a Runge-Kutta method is then

$$y_{n+1} = R(\hat{h})y_n$$

going to zero when $|R(\hat{h})| < 1$.

Definition 1.7.3. A Runge-Kutta method is *absolutely stable* [11, 86] for \hat{h} if $|R(\hat{h})| < 1$. The set of all \hat{h} such that the method is absolutely stable is called *absolute stability region* of the method.

Analogously to the definition given for LMM, a RK method is called *A-stable* if and only if its absolute stability region embeds the left half plane of the complex numbers set.

1.8 Nonlinear stability analysis

The present section is devoted to the analysis on non linear stability of numerical integrators, that turns out to be fundamental in the treatment of problem with invariants [70, 86]. We introduce here the definition of contractivity for the solutions of a differential system and we will show how to extend it to the numerical ones.

Definition 1.8.1. Let $y(x)$ and $\tilde{y}(x)$ be solutions of the differential system $y'(x) = f(x, y(x))$, $x \in [x_0, X]$ corresponding to the initial values x_0 e \tilde{x}_0 respectively. Those solutions are said to be **contractive** in $[a, b]$ if and only if for each x_1, x_2 such that $a \leq t_1 \leq t_2 \leq b$, the following condition holds:

$$\|y(x_2) - \tilde{y}(x_2)\| \leq \|y(x_1) - \tilde{y}(x_1)\|. \quad (1.47)$$

Let $\{y_n\}, \{\tilde{y}_n\}$ be the numerical approximations of the solution provided by a k -step numerical method with different starting values. We define $\{Y_n\}, \{\tilde{Y}_n\} \in \mathbb{R}^{mk}$ as

$$\begin{aligned} Y_n &:= [y_{n+k-1}^T, \dots, y_n^T]^T, \\ \tilde{Y}_n &:= [\tilde{y}_{n+k-1}^T, \dots, \tilde{y}_n^T]^T. \end{aligned}$$

and give the following

Definition 1.8.2. The numerical approximations $\{y_n\}, \{\tilde{y}_n\}$ are contractive for $n \in [0, N]$ if and only if

$$\|Y_{n+1} - \tilde{Y}_{n+1}\| \leq \|Y_n - \tilde{Y}_n\|.$$

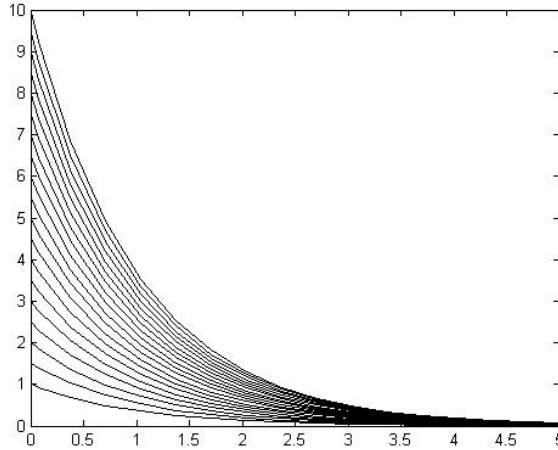


Figure 1.1: Contractivity of the solutions of $y' = -y$.

Under a geometric point of view, if we consider a one-dimensional system of one equation, we can say that if it has contractive solutions, then the solutions themselves tend to be closer and closer as the independent variable grows. We observe that contractivity is a more general property than the one analyzed in the case of linear stability, in fact it holds for a linear system $y' = Ay$ with A having eigenvalues with negative real part (fig. (1.1)). Significance of contractivity is also evident in the context of numerical stability, in fact, if a numerical method is able to preserve it, in the integration of a contractive ODE system the small perturbations introduced by round-off errors or inexact starting procedures do not cause the numerical solutions to vary too much from the exact one.

In order to give a characterization of systems with contractive solutions, we introduce the definition of *one-sided Lipschitz condition* in the Euclidean norm.

Definition 1.8.3. We say that a **one-sided Lipschitz condition** holds for the function $f(x, y)$ and for the problem $y' = f(x, y)$ if there exists a function $\nu(x)$ defined in $[x_0, X]$ such that

$$\langle f(x, y) - f(x, \tilde{y}), y - \tilde{y} \rangle_2 \leq \nu(x) \|y - \tilde{y}\|_2^2 \quad (1.48)$$

for each y, \tilde{y} belonging to a convex region M_x containing the exact solution and for each $x \in [x_0, X]$. The function $\nu(x)$ is called **one-sided Lipschitz constant**.

Remark 1.8.1. Condition (1.48) is more general of the usual Lipschitz condition, in fact, if f is Lipschitz with constant L , then (1.48) holds with $\nu(x) = \text{cost} = L$, due to the Schwartz inequality

$$\langle f(x, y) - f(x, \tilde{y}), y - \tilde{y} \rangle \leq \|f(x, y) - f(x, \tilde{y})\| \cdot \|y - \tilde{y}\| \leq L \|y - \tilde{y}\|^2.$$

Next is an example allowing us to make a few observations

Example 1.8.1. Consider the equations

1. $y' = y$,

$$2. \ y' = -y;$$

whose f functions are Lipschitz with $L = 1$ and let's compute their one-sided Lipschitz constants. For the first equation

$$\langle f(x, y) - f(x, \tilde{y}), y - \tilde{y} \rangle = \langle y - \tilde{y}, y - \tilde{y} \rangle = \|y - \tilde{y}\|^2,$$

then $\nu_1(x) = 1 = L$, while for the other

$$\langle f(x, y) - f(x, \tilde{y}), y - \tilde{y} \rangle = -\langle y - \tilde{y}, y - \tilde{y} \rangle = -\|y - \tilde{y}\|^2,$$

thus $\nu_2(x) = -1$.

We observe that in the case of the second equation we could have chosen $\nu_2(x) = 1 = L$, while this was not possible for the first. The relevant consideration here is that the first system has unbounded solutions, while the second's are decreasing, then contractive: we will show that the negativity of ν_2 is a condition for contractivity.

Theorem 1.8.1. If the IVP

$$\begin{cases} y' = f(x, y), & x \in [x_0, X] \\ y(x_0) = \eta_0 \end{cases} \quad (1.49)$$

has a negative one-sided Lipschitz constant then its solutions are contractive in $[x_0, X]$.

Proof. Let $y(x), \tilde{y}(x)$ be solutions of (1.49) corresponding to the initial values $\eta, \tilde{\eta}$. Consider the function

$$\Phi(x) = \|y(x) - \tilde{y}(x)\|^2.$$

Its derivative reads

$$\begin{aligned} \Phi'(x) &= \frac{d}{dx} \langle y(x) - \tilde{y}(x), y(x) - \tilde{y}(x) \rangle = 2 \langle y'(x) - \tilde{y}'(x), y(x) - \tilde{y}(x) \rangle = \\ &= 2 \langle f(x, y(x)) - f(x, \tilde{y}(x)), y(x) - \tilde{y}(x) \rangle \leq 2\nu(x)\Phi(x). \end{aligned}$$

Then

$$\Phi'(x) - 2\nu(x)\Phi(x) \leq 0. \quad (1.50)$$

Consider then the integrating factor $\eta(x) = e^{-2\int_0^x \nu(s)ds}$ and multiply it for both members of (1.50):

$$\Phi'(x)\eta(x) - 2\nu(x)\eta(x)\Phi(x) \leq 0,$$

thus $\Phi(x)\eta(x)$ is decreasing and

$$\Phi(x_2)\eta(x_2) \leq \Phi(x_1)\eta(x_1) \quad (1.51)$$

for each x_1, x_2 such that $x_0 \leq x_1 \leq x_2 \leq X$. From (1.51) and by hypothesis we obtain

$$\|y(x_2) - \tilde{y}(x_2)\|^2 \leq e^{\int_{x_1}^{x_2} \nu(s)ds} \|y(x_1) - \tilde{y}(x_1)\|^2 \leq \|y(x_1) - \tilde{y}(x_1)\|^2,$$

which proves the statement. \square

Theorem 1.8.1 holds in particular if $\nu(x) = 0$, then we give the following

Definition 1.8.4. System $y' = f(x, y)$ is **dissipative** in $[x_0, X]$ if

$$\langle f(x, y) - f(x, \tilde{y}), y - \tilde{y} \rangle \leq 0 \quad (1.52)$$

for each $y, \tilde{y} \in M_x$ and each $x \in [x_0, X]$.

1.8.1 Non-linear stability of implicit Runge-Kutta methods

In the remainder of this Section, we consider an s -stages Runge-Kutta method having as Butcher tableaux

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

Definition 1.8.5. A Runge-Kutta method is **B-stable** [11] if it provides contractive solutions whether applied to a dissipative autonomous system with any step-size. The method is called **BN-stable** if it provides contractive solutions whether applied to a dissipative non-autonomous system with any step-size.

Butcher [11] proved the following sufficient condition for the B-stability of a method. Let B and Q be the $s \times s$ matrices

$$B := \begin{pmatrix} b_1 & 0 & \cdots & 0 \\ 0 & b_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & b_s \end{pmatrix} \quad Q := BA^{-1} + A^{-T}B - A^{-T}bb^T A^{-1}, \quad (1.53)$$

If B and Q are non-negative definite, then the method is B-stable.

Example 1.8.2. For the Radau IA method

$$\begin{array}{c|cc} 0 & \frac{1}{4} & -\frac{1}{4} \\ \frac{2}{3} & \frac{1}{4} & \frac{5}{12} \\ \hline & \frac{1}{4} & \frac{3}{4} \end{array}$$

we have

$$B = \begin{pmatrix} \frac{1}{4} & 0 \\ 0 & \frac{3}{4} \end{pmatrix}$$

which is positive definite and

$$Q = \begin{pmatrix} 1 & -1.11e - 16 \\ -3.33e - 16 & 4.44e - 16 \end{pmatrix}$$

which is positive definite, having as eigenvalues

$$1, 4.44e - 16.$$

Thus the method is B-stable.

The Lobatto IIIC method

$$\begin{array}{c|cc} 0 & \frac{1}{2} & -\frac{1}{2} \\ 1 & \frac{1}{2} & \frac{1}{2} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

we have $B = bI$ and

$$Q = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

which is positive semi-definite, thus also Lobatto IIIC method is B-stable.

For methods whose A matrix is not invertible, as Radau II

$$\begin{array}{c|cc} \frac{1}{3} & \frac{1}{3} & 0 \\ 1 & 1 & 0 \\ \hline & \frac{3}{4} & \frac{1}{4} \end{array}$$

it is useful to give another definition, involving the B matrix as before and the matrix

$$M := BA + A^T B - bb^T.$$

Definition 1.8.6. A Runge-Kutta method is **algebraically stable** if $b_i > 0$ for $i = 1, \dots, s$ and the matrix M associated to the method is positive semi-definite.

The following Theorem states the connection between algebraic stability and B-stability

Theorem 1.8.2. If a Runge-Kutta method is algebraically stable, then it is BN-stable.

Example 1.8.3. Consider Radau II method

$$\begin{array}{c|cc} \frac{1}{3} & \frac{1}{3} & 0 \\ 1 & 1 & 0 \\ \hline & \frac{3}{4} & \frac{1}{4} \end{array}.$$

Matrices B and M assume the form

$$B = \begin{pmatrix} \frac{3}{4} & 0 \\ 0 & \frac{1}{4} \end{pmatrix}, M = \begin{pmatrix} -0.0625 & 0.0625 \\ 0.0625 & -0.0625 \end{pmatrix}$$

and M is negative semi-definite, having eigenvalues $-0, 125$ and 0 .

1.9 Symplectic Runge-Kutta Methods

We consider an IVP such that there exist a symmetric matrix Q (see Section 1.3.4) such that

$$y^T Q f(y) = 0$$

or, equivalently

$$y^T Q y = c, \tag{1.54}$$

being c a constant. Such problems are said to possess a *quadratic invariant*. We aim to find under which conditions an RK method preserves the invariant (1.54), so we impose that its numerical counterpart is preserved, that is $y_n^T Q y_n = c$. In order to achieve such a goal, we consider a RK method (1.32) and we write the expression of the method after one step

$$\begin{cases} y_1 = y_0 + h \sum_{i=1}^s b_i f(Y_i) \\ Y_i = y_0 + h \sum_{j=1}^s a_{ij} f(Y_j) \end{cases}.$$

From this expression it follows that

$$\begin{aligned} y_1^T Q y_1 &= y_1^T Q y_0 + h \sum_{i=1}^s b_i y_1^T Q f(Y_i) = y_0^T Q y_1 + h \sum_{i=1}^s b_i f(Y_i)^T Q y_1 = \\ &= y_0^T Q y_0 + 2h \sum_{i=1}^s b_i y_0^T Q f(Y_i) + h^2 \sum_{i,j=1}^s b_i b_j f(Y_i)^T Q f(Y_j). \end{aligned}$$

Defining a matrix M as

$$M := BA + A^T B - bb^T$$

and observing that

$$f(Y_i)^T Q y_0 + h \sum_{j=1}^s a_{ij} f(Y_i)^T Q f(Y_j) = 0,$$

we obtain

$$y_1^T Q y_1 = y_0^T Q y_0 - h^2 \sum_{i,j=1}^s m_{ij} f(Y_i)^T Q f(Y_j). \quad (1.55)$$

Equation (1.55) provides the preservation of the invariant(1.54) if $M = 0$. This motivates the following

Definition 1.9.1. A Runge-Kutta method with coefficients (A, b^T, c) is *symplectic* if and only if

$$M = \text{diag}(b)A + A^T \text{diag}(b) - bb^T \quad (1.56)$$

is the zero matrix. Symplectic RK methods are also often referred to as *canonical* methods.

Remark 1.9.1. An interesting link holds between symplecticity and non-linear stability of Runge-Kutta methods, in fact the matrix M defined in (1.56) is the so-called *algebraic stability matrix* of the method, arising while studying the application of RK methods to dissipative problems (see (1.8.6)).

An example of symplectic RK method is given by the family of Gauss-Legendre RK methods (1.33).

Chapter 2

General Linear Methods (GLMs)

The family of General Linear Methods (GLMs) or simply Multivalued methods was introduced in [10] with the aim of giving an unifying theoretical framework embedding all the existing methods. In the first part of this Chapter we will see how the family of multivalued methods is defined and how one can formulate the existing methods as GLMs. The topics of convergence and order are exploited and a linear stability theory is presented. The second part of the Chapter is devoted to the family of General Linear Methods for second order problems. Such methods have been introduced recently in [45] and furtherly studied in [50].

2.1 GLMs for first order problems

General Linear Methods are multistage-multivalued methods [10, 11, 70]. Denoting by s the number of stages and r the number of values that are carried out at each step, we introduce a formulation that makes use of an *abscissae vector* $\mathbf{c} = [c_1, c_2, \dots, c_s]$ and four coefficient matrices

$$\mathbf{A} \in \mathbb{R}^{s \times s}, \mathbf{U} \in \mathbb{R}^{s \times r}, \mathbf{B} \in \mathbb{R}^{r \times s}, \mathbf{V} \in \mathbb{R}^{r \times r},$$

collected in the $(s+r) \times (s+r)$ block matrix

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array} \right].$$

The component wise expression of a GLM $(\mathbf{c}, \mathbf{A}, \mathbf{U}, \mathbf{B}, \mathbf{V})$ is

$$\begin{cases} Y_i^{[n]} = \sum_{j=1}^s a_{ij} h F_j^{[n]} + \sum_{j=1}^r u_{ij} y_j^{[n]}, & i = 1, 2, \dots, s, \\ y_i^{[n+1]} = \sum_{j=1}^s b_{ij} h F_j^{[n]} + \sum_{j=1}^r v_{ij} y_j^{[n]}, & i = 1, 2, \dots, r, \end{cases} \quad (2.1)$$

where $Y_i^{[n]}$ are denoted as the *internal stages* of the method and, together with the other quantities appearing in (2.1), can be collected in three supervectors

$$y^{[n]} = \begin{bmatrix} y_1^{[n]} \\ y_2^{[n]} \\ \vdots \\ y_r^{[n]} \end{bmatrix} \in \mathbb{R}^{rd}, \quad Y^{[n]} = \begin{bmatrix} Y_1^{[n]} \\ Y_2^{[n]} \\ \vdots \\ Y_s^{[n]} \end{bmatrix} \in \mathbb{R}^{sd}, \quad F^{[n]} = \begin{bmatrix} f(x_n + c_1 h, Y_1^{[n]}) \\ f(x_n + c_2 h, Y_2^{[n]}) \\ \vdots \\ f(x_n + c_s h, Y_s^{[n]}) \end{bmatrix} \in \mathbb{R}^{sd}.$$

Method (2.1) can thus be formulated in a tensor form

$$\begin{cases} Y^{[n]} = h(\mathbf{A} \otimes \mathbf{I})F + (\mathbf{U} \otimes \mathbf{I})y^{[n]}, \\ y^{[n+1]} = h(\mathbf{B} \otimes \mathbf{I})F + (\mathbf{V} \otimes \mathbf{I})y^{[n]}, \end{cases}$$

being \mathbf{I} the identity matrix in $\mathbb{R}^{d \times d}$ and $A \otimes B$ the Kronecker tensor product:

$$A \otimes B = \begin{bmatrix} a_{11}B & a_{12}B & \cdots & a_{1s}B \\ a_{21}B & a_{22}B & \cdots & a_{2s}B \\ \vdots & \vdots & & \vdots \\ a_{s1}B & a_{s2}B & \cdots & a_{ss}B \end{bmatrix}.$$

Remark 2.1.1. As we will see more in detail in the following sections, the values that are carried out from step to step, namely the components of the $y[n]$ vector, can assume a very wide range of expressions related to the solution, including the solution itself, linear combinations of its derivatives, values of the solution in previous steps etc, while the internal stages provide an approximation to the solution in intra-step points given by $x_n + c_i h$. Usually, the values in the $y[n]$ vector are not provided by the IVP data and need to be computed by means of a starting procedure.

2.1.1 Classical methods as GLMs

An s stages Runge-Kutta method having the Butcher's tableaux

$$\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \\ \hline & \mathbf{b}^T \end{array} \quad (2.2)$$

can be written as a GLM with the same number of stages and $r = 1$, since only an approximation to the solution is carried out at each step. In particular, the matrix representation of (2.2) as a GLM [11] is

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array} \right] = \left[\begin{array}{c|c} A & \mathbf{e} \\ \hline b^T & 1 \end{array} \right], \quad (2.3)$$

being $\mathbf{e} = (1, \dots, 1)^T \in \mathbb{R}^s$. Formula (2.3) can be easily obtained comparing the componentwise expression of a RK (1.32) and a GLM (2.1).

A k -step Linear Multistep Method (1.26) can be formulated as a one-stage GLM having the following matrix representation

$$\left[\begin{array}{c|cccccccc} \beta_0 & \alpha_1 & \cdots & \alpha_{k-1} & \alpha_k & \beta_1 & \cdots & \beta_{k-1} & \beta_k \\ \beta_0 & \alpha_1 & \cdots & \alpha_{k-1} & \alpha_k & \beta_1 & \cdots & \beta_{k-1} & \beta_k \\ 0 & 1 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 & 0 & \cdots & 0 & 0 \\ 1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 1 & 0 \end{array} \right].$$

2.1.2 Convergence Issues

In this Section, we analyse the problem of convergence for GLMs and we give a few basic definitions concerning zero-stability and consistency. The first definition that we need is the classical *pre-consistency* definition given in [11, 82]

Definition 2.1.1. A GLM $(\mathbf{c}, \mathbf{A}, \mathbf{U}, \mathbf{B}, \mathbf{V})$ is said to be *preconsistent* if and only if there exist a vector $\mathbf{q}_0 \in \mathbb{R}^r$ called *preconsistency vector* such that

$$\mathbf{U}\mathbf{q}_0 = \mathbf{e}, \quad \mathbf{V}\mathbf{q}_0 = \mathbf{q}_0, \quad (2.4)$$

with $\mathbf{e} = [1, \dots, 1] \in \mathbb{R}^r$.

Definition 2.1.2. A preconsistent GLM $(\mathbf{c}, \mathbf{A}, \mathbf{U}, \mathbf{B}, \mathbf{V})$ is called *consistent* if and only if there exist a vector $\mathbf{q}_1 \in \mathbb{R}^r$ called *consistency vector* such that

$$\mathbf{B}\mathbf{e} + \mathbf{V}\mathbf{q}_1 = \mathbf{q}_0 + \mathbf{q}_1, \quad (2.5)$$

with $\mathbf{e} = [1, \dots, 1] \in \mathbb{R}^r$. The method is called *stage-consistent* if

$$\mathbf{A}\mathbf{e} + \mathbf{U}\mathbf{q}_1 = \mathbf{c}, \quad (2.6)$$

being $\mathbf{e} = [1, \dots, 1] \in \mathbb{R}^s$.

Formulas (2.4),(2.5) and (2.6) will find a rigorous justification in Section 2.2.1.

A crucial property of GLMs, as well as of all numerical integrators, is the property of zero-stability.

Definition 2.1.3. A GLM $(\mathbf{c}, \mathbf{A}, \mathbf{U}, \mathbf{B}, \mathbf{V})$ is *zero-stable* if and only if there exists a scalar C such that

$$\|\mathbf{V}^n\| \leq C,$$

for each $n \geq 0$.

Condition expressed in Definition 2.1.3 is equivalent to requiring that all the roots of the minimal polynomial of the matrix \mathbf{V} to have modulus less or equal to 1 and those of modulus 1 to be simple.

Starting Procedures

As in the case of LMM, the definition of convergence is strictly related to the starting procedure used and also the order of a GLM is defined with respect to a given starting procedure, then it is worth spending a few words about the topic. Consider a GLM $(\mathbf{c}, \mathbf{A}, \mathbf{U}, \mathbf{B}, \mathbf{V})$ whose input vector is given by

$$y^{[n]} = \begin{bmatrix} y_1^{[n]} \\ y_2^{[n]} \\ \vdots \\ y_r^{[n]} \end{bmatrix}.$$

Since we want the quantities $y_i^{[n]}$ to be as general as possible, we consider for their approximation r generalized Runge-Kutta methods of the form

$$\begin{cases} Y_j^{(i)} = y_n^{(i)} + h \sum_{k=1}^s a_{jk}^{(i)} f(t_n + c_k^{(i)} h, Y_k^{(i)}), & j = 1, 2, \dots, s, \\ y_{n+1}^{(i)} = b_0^{(i)} y_n^{(i)} + h \sum_{j=1}^s b_j^{(i)} f(t_n + c_j^{(i)} h, Y_j^{(i)}), \end{cases}$$

represented by the Butcher tableau

$$S^{(i)} = \left(\begin{array}{c|c} c^{(i)} & A^{(i)} \\ \hline b_0^{(i)} & b^{(i)\top} \end{array} \right). \quad (2.7)$$

To our purposes, we will always assume that the starting method is *non-degenerate* (compare [11]), i.e. there exists an index i such that $b_0^{(i)} \neq 0$. A finishing procedure is then needed at the end of the integration process to rebuild the solution from the output of the method [70]. An example of starting procedure and technical details on its construction are given in Section 3.6.1.

Aiming to give a definition of convergence for GLMs, we assume that, for small values of the stepsize h , the starting method provides accurate approximations of

$$\begin{bmatrix} u_1 y(t_0) \\ u_2 y(t_0) \\ \vdots \\ u_r y(t_0) \end{bmatrix},$$

with \mathbf{u} being not zero in \mathbb{R}^r , and that the successive approximations converge to

$$\begin{bmatrix} u_1 y(\bar{t}) \\ u_2 y(\bar{t}) \\ \vdots \\ u_r y(\bar{t}) \end{bmatrix}. \quad (2.8)$$

Let $\mathbf{u}y(\bar{t})$ be the vector in (2.8), following [11, 82], we give the following

Definition 2.1.4. A GLM $(\mathbf{c}, \mathbf{A}, \mathbf{U}, \mathbf{B}, \mathbf{V})$ is **convergent** if and only if, for any IVP (1.4) whose f function is Lipschitz continuous with $\|f(y) - f(z)\| \leq L\|y - z\|$, there exist a non-zero vector $u \in \mathbb{R}^r$ and a starting procedure $\phi : (0, \infty) \rightarrow \mathbb{R}^r$ such that for any $i = 1, 2, \dots, r$, $\lim_{h \rightarrow 0} \phi_i(h) = u_i y(t_0)$, and such that for each $\bar{t} > t_0$, the sequence $y^{[n]}$, computed after n steps of size $h = (\bar{t} - t_0)/n$ and using $y^{[0]} = \phi(h)$, converges to $uy(\bar{t})$.

For GLMs, the Lax-Richtmyer Theorem holds, stating the equivalence between convergence and zero stability plus consistency.

The starting method has a remarkable influence also on the accuracy of the numerical approximation. Indeed, according to [11], we provide the following definition of order.

Definition 2.1.5. A GLM (A, U, B, V) has order p if, and only if, there exists a non-degenerate starting method S such that the numerical approximations obtained via the GLM with starting method S differ from those obtained applying S to the exact solution at the end of the same step by $O(h^{p+1})$.

Following [11], a GLM (2.1) has order p if

$$\begin{cases} \eta(t) = A\eta D(t) + U\xi(t), \\ E\xi(t) = B\eta D(t) + V\xi(t), \end{cases} \quad (2.9)$$

for any $t \in T$, with $\rho(t) \leq p$. As in [11], η represents the operator associated to the stages, ηD the one associated to the stage-derivatives, ξ is the starting method operator and E the exact solution one. The product of two operators is defined in [11], §386.

2.2 GLMs for Second Order Problems

The family of GLMs for second order problems, also referred to as the family of General Linear Nyström methods (GLNs) has been introduced in [45] by R. D'Ambrosio, E. Esposito and B. Paternoster for the numerical solution of the Hadamard well-posed special second order problem

$$\begin{cases} y''(t) = f(y(t)), & t \in [t_0, T], \\ y(t_0) = y_0 \in \mathbb{R}^d, \\ y'(t_0) = y'_0 \in \mathbb{R}^d. \end{cases} \quad (2.10)$$

These methods provide a natural generalization of GLMs (2.1) for first order problems. Their formulation involves three supervectors

$$y^{[n-1]} = \begin{bmatrix} y_1^{[n-1]} \\ y_2^{[n-1]} \\ \vdots \\ y_r^{[n-1]} \end{bmatrix} \in \mathbb{R}^{rd}, \quad y'^{[n-1]} = \begin{bmatrix} y'_1^{[n-1]} \\ y'_2^{[n-1]} \\ \vdots \\ y'_{r'}^{[n-1]} \end{bmatrix} \in \mathbb{R}^{r'd}, \quad Y^{[n]} = \begin{bmatrix} Y_1^{[n]} \\ Y_2^{[n]} \\ \vdots \\ Y_s^{[n]} \end{bmatrix} \in \mathbb{R}^{sd}$$

respectively denoted as input vector of the *external approximations*, input vector of the *first derivative approximations* and *internal stage vector*. The n -th step of a GLN method characterised by the coefficient matrices $\mathbf{A} \in \mathbb{R}^{s \times s}$, $\mathbf{P} \in \mathbb{R}^{s \times r'}$, $\mathbf{U} \in \mathbb{R}^{s \times r}$, $\mathbf{C} \in \mathbb{R}^{r' \times s}$, $\mathbf{R} \in \mathbb{R}^{r' \times r'}$, $\mathbf{W} \in \mathbb{R}^{r' \times r}$, $\mathbf{B} \in \mathbb{R}^{r \times s}$, $\mathbf{Q} \in \mathbb{R}^{r \times r'}$, $\mathbf{V} \in \mathbb{R}^{r \times r}$ is expressed as follows

$$\begin{aligned} Y_i^{[n]} &= h^2 \sum_{j=1}^s a_{ij} f(Y_j^{[n]}) + h \sum_{j=1}^{r'} p_{ij} y'_j{}^{[n-1]} + \sum_{j=1}^r u_{ij} y_j^{[n-1]}, & i = 1, \dots, s, \\ h y'_i{}^{[n]} &= h^2 \sum_{j=1}^s c_{ij} f(Y_j^{[n]}) + h \sum_{j=1}^{r'} r_{ij} y'_j{}^{[n-1]} + \sum_{j=1}^r w_{ij} y_j^{[n-1]}, & i = 1, \dots, r', \\ y_i^{[n]} &= h^2 \sum_{j=1}^s b_{ij} f(Y_j^{[n]}) + h \sum_{j=1}^{r'} q_{ij} y'_j{}^{[n-1]} + \sum_{j=1}^r v_{ij} y_j^{[n-1]}, & i = 1, \dots, r. \end{aligned} \quad (2.11)$$

The coefficient matrices involved in the formulation of the method can be collected in the following partitioned $(s + r' + r) \times (s + r' + r)$ matrix

$$\left[\begin{array}{c|c|c} \mathbf{A} & \mathbf{P} & \mathbf{U} \\ \hline \mathbf{C} & \mathbf{R} & \mathbf{W} \\ \hline \mathbf{B} & \mathbf{Q} & \mathbf{V} \end{array} \right], \quad (2.12)$$

denoted as the Butcher tableau of the GLM. Using these notations, a GLM for second order ODEs can then be expressed as follows:

$$\begin{aligned} Y^{[n]} &= h^2(\mathbf{A} \otimes \mathbf{I})F^{[n]} + h(\mathbf{P} \otimes \mathbf{I})y'^{[n-1]} + (\mathbf{U} \otimes \mathbf{I})y^{[n-1]}, \\ hy'^{[n]} &= h^2(\mathbf{C} \otimes \mathbf{I})F^{[n]} + h(\mathbf{R} \otimes \mathbf{I})y'^{[n-1]} + (\mathbf{W} \otimes \mathbf{I})y^{[n-1]}, \\ y^{[n]} &= h^2(\mathbf{B} \otimes \mathbf{I})F^{[n]} + h(\mathbf{Q} \otimes \mathbf{I})y'^{[n-1]} + (\mathbf{V} \otimes \mathbf{I})y^{[n-1]}, \end{aligned} \quad (2.13)$$

where \otimes denotes the usual Kronecker tensor product, \mathbf{I} is the identity matrix in $\mathbb{R}^{d \times d}$ and $F^{[n]} = [f(Y_1^{[n]}), f(Y_2^{[n]}), \dots, f(Y_s^{[n]})]^\top$. Analogously to the first order case, the vector $y^{[n-1]}$ of the external stages contains all the informations transferred advancing from the point t_{n-1} to the point t_n of the grid. It is important to observe that such a vector could also contain not only approximations to the solution of the problem in the grid points inherited from the previous steps, but also other informations computed in the past that we want to use in the integration process. The vector $y'^{[n-1]}$, instead, contains previous approximations to the first derivative of the solution computed in previous step points, while the values $Y_j^{[n-1]}$ provide an approximation to the solution in the internal points $t_{n-1} + c_j h$, $j = 1, 2, \dots, s$, where $\mathbf{c} = [c_1, c_2, \dots, c_s]$ is denoted as the *abscissae vector* of the method.

Remark 2.2.1. A more compact representation of methods (2.11) can be given embedding the first derivative-related quantities in the vector of external approximations. Such a simplification provides the reduced formula

$$\begin{aligned} Y^{[n]} &= h^2(\mathbf{A} \otimes \mathbf{I})F^{[n]} + (\mathbf{U} \otimes \mathbf{I})y^{[n-1]}, \\ y^{[n]} &= h^2(\mathbf{B} \otimes \mathbf{I})F^{[n]} + (\mathbf{V} \otimes \mathbf{I})y^{[n-1]}. \end{aligned} \quad (2.14)$$

A rigorous explanation of this procedure can be found in [45]. This simplified representation is often very useful in the process of construction of new methods and in the development of both order and stability conditions. In the following, we will use this formulation to construct examples of methods belonging to the family of GLNs.

2.2.1 Order Conditions

For second order equations, due to the presence of the derivative of the exact solution, we need a more general set of rooted trees, namely bi-coloured trees, defined as follows (compare [71])

$$NT = \{\bullet, \circ, \begin{array}{c} \bullet \\ | \\ \bullet \end{array}, \begin{array}{c} \circ \\ | \\ \bullet \end{array}, \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array}, \begin{array}{c} \circ \\ / \quad \backslash \\ \bullet \quad \bullet \end{array}, \begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \circ \end{array}, \begin{array}{c} \circ \\ / \quad \backslash \\ \bullet \quad \circ \end{array}, \begin{array}{c} \bullet \\ | \\ \bullet \\ | \\ \bullet \end{array}, \begin{array}{c} \circ \\ | \\ \bullet \\ | \\ \bullet \end{array}, \begin{array}{c} \bullet \\ | \\ \bullet \\ | \\ \bullet \end{array}, \dots\}.$$

The vertices $\tau_1 = \bullet$ and $\tau_2 = \circ$ are combined according to following the rules

1. the root of $t \in NT$ is always fat;
2. a meagre vertex has at most one son which has to be fat.

Following [27, 71], we adapt the theory of N-trees and of N-series introduced by Hairer and Wanner in [73] to the special problem

$$y''(x) = f(y(x)). \quad (2.15)$$

By calculating the derivatives of the exact solution of problem (2.15)

$$y''' = \frac{\partial f}{\partial y} y', \quad y^{(iv)} = \frac{\partial^2 f}{\partial y^2} y'^2 + \frac{\partial f}{\partial y} y'', \quad y^{(v)} = \frac{\partial^3 f}{\partial y^3} y'^3 + 3 \frac{\partial^2 f}{\partial y^2} y' f + \frac{\partial f}{\partial y} y''', \quad \dots$$

we observe that the terms including the derivative of f with respect to y' disappear, producing a smaller set of trees called Special N-trees (SNT) set [71]

$$SNT = \{ \bullet, \circ, \begin{array}{c} \bullet \\ | \\ \bullet \end{array}, \begin{array}{c} \bullet \bullet \\ | \\ \bullet \end{array}, \begin{array}{c} \bullet \bullet \\ | \\ \bullet \bullet \end{array}, \dots \}.$$

By combining the formalisms introduced in [27, 73], a composition rule of special Nyström trees is given according to the following scheme. We consider $t_1, \dots, t_k \in SNT$ and a new root τ_2 . Then,

1. if $t_i \neq \tau_1$, then its root is connected to a new meagre node, linked to the new root;
2. if $t_i = \tau_1$, then it is connected to the new root via a new branch.

The resulting SN-tree is denoted as $t = [t_1, \dots, t_k]$. Inversely, cutting the branches leaving from the root of a given $t \in SNT$, let u_1, u_2, \dots, u_k be the resulting subtrees. For any $u_i \neq \tau_1$, we cut off the branch leaving from its root τ_1 and denote the remaining part as t_i . For the remaining u_i , we set $t_i = \tau_1$. Then, the tree is decomposed as $t = [t_1, \dots, t_k]$.

Given these rules, we can extend the definition of elementary differential given in [11, 71] to the special problem (2.15). For a given $t = [t_1, \dots, t_k] \in SNT$, we recursively define the elementary differentials as follows

$$\begin{aligned} F(\bullet)(y, y') &= y', \\ F(\circ)(y, y') &= y'' = f, \\ F(t)(y, y') &= f^{(k)}(F(t_1)(y, y'), \dots, F(t_k)(y, y')). \end{aligned}$$

Moreover, for a given tree $t = [t_1^{\mu_1}, t_2^{\mu_2}, \dots, t_k^{\mu_k}]$, we recursively define the following useful functions ρ and α (compare [27, 73])

$$\begin{aligned} \rho(\bullet) &= 1, \quad \rho(\circ) = 2, \quad \rho(t) = 2 + \sum_{i=1}^k \mu_i \rho(t_i), \\ \alpha(\bullet) &= \alpha(\circ) = 1, \quad \alpha(t) = (\rho(t) - 2)! \prod_{i=1}^k \frac{1}{\mu_i!} \left(\frac{\alpha(t_i)}{\rho(t_i)} \right)^{\mu_i}. \end{aligned}$$









$\rho(t)$	t	$F(t)$	$\alpha(t)$
1		y'	1
2		f	1
3		$f'y'$	1
4		$f''(y', y')$	1
		$f'f$	1
5		$f'''(y', y', y')$	1
		$f''(y', f)$	3
		$f'f'y'$	1

Table 2.1: Special Nyström trees up to order 5 and associated elementary differentials

Following [73], we define a SN-series as

$$SN(a, y, y') = \sum_{t \in SNT} \frac{h^{\rho(t)}}{\rho(t)!} \alpha(t) a(t) F(t)(y, y'). \quad (2.16)$$

We observe that both the exact solution of (2.15) and its first derivative can be formally written as SN-series, whose coefficients are calculated in next sections. The following theorem, useful in the remainder of the paper, provides a representation form for the composition of a SN-series with the function f in (2.15) (compare [73]).

Theorem 2.2.1. For a given map $a : SNT \mapsto \mathbb{R}$ satisfying $a(\emptyset) = 1$, we have

$$f(SN(a, y, y')) = \sum_{t \in SNT} \frac{h^{\rho(t)-2}}{(\rho(t)-2)!} \alpha(t) a''(t) F(t)(y, y') \quad (2.17)$$

with

$$a''(t) = \begin{cases} 0, & \text{if } t = \emptyset, \tau_1, \\ 1, & \text{if } t = \tau_2, \\ a(t_1) \cdots a(t_k), & \text{if } t = [t_1, \dots, t_k]. \end{cases} \quad (2.18)$$

We now employ the theory of SN-series above recalled, to derive a general set of order conditions for the family of GLN methods (2.1). First of all, let us assume that the input vector is a SN-series of the form

$$y_i^{[0]} = \sum_{t \in SNT} \frac{h^{\rho(t)}}{\rho(t)!} \alpha(t) \xi_i(t) F(t)(y, y'), \quad (2.19)$$

and, analogously, that

$$Y_i^{[0]} = \sum_{t \in SNT} \frac{h^{\rho(t)}}{\rho(t)!} \alpha(t) \eta_i(t) F(t)(y, y'). \quad (2.20)$$

We need to establish how terms like $h^2 f(Y_i)$ and $h y_i'^{[0]}$ can be expressed as SN-series. Theorem 2.2.1 allows us to write $h^2 f(Y_i)$ as SN-series (2.16) of coefficients

$$\bar{\eta}_i(t) = \eta''_i(t) \cdot \rho(t) \cdot (\rho(t) - 1), \quad (2.21)$$

while, if $y_i'^{[0]}$ is a formal series of the form

$$y_i'^{[0]} = \sum_{t \in SNT} \frac{h^{\rho(t)-1}}{(\rho(t)-1)!} \alpha(t) \xi'_i(t) F(t)(y, y'), \quad (2.22)$$

$h y_i'^{[0]}$ is a SN-series (2.16) of coefficients

$$\delta_i(t) = \xi'_i(t) \cdot \rho(t)$$

With abuse of notation, we have denoted the coefficients of the SN-series (2.22) by $\xi'_i(t)$, even if they are not actually the first derivatives of $\xi_i(t)$ in (2.19).

We can now suitably extend the strategy proposed in [11], in order to develop an algebraic theory of order for GLNs. To this purpose, we insert the derived SN-series in the method formulation (2.13), obtaining

$$SN(\eta_i, y, y') = \sum_{j=1}^s a_{ij} SN(\bar{\eta}_j, y, y') + \sum_{j=1}^{r'} p_{ij} SN(\delta_j, y, y') + \sum_{j=1}^r u_{ij} SN(\xi_j, y, y'),$$

$i = 1, 2, \dots, s$, which leads to

$$SN(\eta_i, y, y') = SN \left(\sum_{j=1}^s a_{ij} \bar{\eta}_j + \sum_{j=1}^{r'} p_{ij} \delta_j + \sum_{j=1}^r u_{ij} \xi_j, y, y' \right), \quad i = 1, \dots, s.$$

Thus,

$$\eta_i(t) = \sum_{j=1}^s a_{ij} \bar{\eta}_j(t) + \sum_{j=1}^{r'} p_{ij} \delta_j(t) + \sum_{j=1}^r u_{ij} \xi_j(t), \quad i = 1, \dots, s. \quad (2.23)$$

In analogous way, we obtain the following equations for the external approximations

$$\widehat{\xi}_i(t) = \sum_{j=1}^s b_{ij} \bar{\eta}_j(t) + \sum_{j=1}^{r'} q_{ij} \delta_j(t) + \sum_{j=1}^r v_{ij} \xi_j(t), \quad i = 1, \dots, r, \quad (2.24)$$

$$\widehat{\delta}_i(t) = \sum_{j=1}^s c_{ij} \bar{\eta}_j(t) + \sum_{j=1}^{r'} r_{ij} \delta_j(t) + \sum_{j=1}^r w_{ij} \xi_j(t), \quad i = 1, \dots, r'. \quad (2.25)$$

Collecting the left-hand sides of (2.23), (2.24) and (2.25) in the vectors $\eta \in \mathbb{R}^s$, $\xi \in \mathbb{R}^r$ and $\delta \in \mathbb{R}^{r'}$, respectively, leads to the following matrix representation

$$\begin{cases} \eta = \mathbf{A}\bar{\eta} + \mathbf{P}\delta + \mathbf{U}\xi, \\ \widehat{\xi} = \mathbf{B}\bar{\eta} + \mathbf{Q}\delta + \mathbf{V}\xi, \\ \widehat{\delta} = \mathbf{C}\bar{\eta} + \mathbf{R}\delta + \mathbf{W}\xi. \end{cases} \quad (2.26)$$

As a consequence, the following result holds.

Proposition 2.2.1. If the operators $\widehat{\xi}$ and $\widehat{\delta}$ in (2.26) of a given GLN (2.1) are such that $\widehat{\xi}_i(t)$ and $\widehat{\delta}_i(t)$ coincide with the corresponding coefficients $E\xi_i(t)$ and $E\delta_i(t)$ in the Taylor series expansions of the exact values approximated by $y_i^{[n]}$ and $y_i'^{[n]}$ for any $t \in SNT$ of order $\rho(t) \leq p$ and $\rho(t) \leq p + 1$ respectively, then the method has order p , i.e.

$$\begin{cases} E\xi = \mathbf{B}\bar{\eta} + \mathbf{Q}\delta + \mathbf{V}\xi, & \rho(t) \leq p, \\ E\delta = \mathbf{C}\bar{\eta} + \mathbf{R}\delta + \mathbf{W}\xi, & \rho(t) \leq p + 1. \end{cases} \quad (2.27)$$

Moreover, the method has stage order q if the operators $\eta_i(t)$, $i = 1, \dots, s$, in (2.26) coincide with the coefficients $E\eta_i$ of the Taylor series expansion of $y(x_0 + c_i h)$, for any $t \in SNT$ of order $\rho(t) \leq q + 1$, i.e.

$$E\eta = \mathbf{A}\bar{\eta} + \mathbf{P}\delta + \mathbf{U}\xi. \quad (2.28)$$

t	$E\xi(t)$
\emptyset	ξ_0
\bullet	$\xi_0 + \xi_1$
\circ	$\xi_0 + 2\xi_1 + \xi_2$
\mathfrak{I}	$\xi_0 + 3\xi_1 + 3\xi_2 + \xi_3$
\vdots	\vdots
t	$T_{\rho(t)}\Xi_{\rho(t)}$

Table 2.2: Values of $E\xi(t)$ in (2.27)

Remark 2.2.2. The elements of the vector $E\xi(t)$ updated after one step only can be easily computed by means of series expansions arguments. Indeed, let us consider a specific component $y_i^{[n]}$ of the external stages vector and let us assume that it can be expanded in power series as follows:

$$y_i(x) = \xi_0 y_i(x) + h\xi_1 y_i'(x) + \frac{h^2}{2}\xi_2 y_i''(x) + \frac{h^3}{6}\xi_3 y_i'''(x) + \dots + \frac{h^k}{k!}\xi_k y_i^{(k)}(x) + \dots \quad (2.29)$$

Such an assumption is equivalent to considering a SN-series where all the coefficients of h^k have the same value. Expanding $y_i(x+h)$ in Taylor series, we get

$$y_i(x+h) = y_i(x) + hy_i'(x) + \frac{h^2}{2}y_i''(x) + \frac{h^3}{6}y_i'''(x) + \dots + \frac{h^k}{k!}y_i^{(k)}(x) + \dots \quad (2.30)$$

The values of $y_i^{(k)}(x)$ in (2.30) can be obtained from (2.29). Substituting such values in (2.30) and collecting the powers of h with the same exponent we obtain the values for $E\xi$ reported in Table 2.2, where T_k denotes the k -th row of the Tartaglia's triangle and Ξ_k a column vector whose components are ξ_0, \dots, ξ_{k-1} .

Exploiting Order Conditions for GLNs

By applying the result derived in Proposition 2.2.1, we derive the expressions of the operators (2.27) and (2.28) in correspondence of the trees up to order 4 for a GLN method (2.1). We observe that the algebraic conditions (2.27) and (2.28) in Proposition 2.2.1 have to be solved recursively by means of the decomposition rule given above, according to Theorem 2.2.1. We first consider (2.27) and (2.28) corresponding to the trees \emptyset , τ_1 and τ_2 , which provide the base case of the recursion, obtaining

$$\begin{aligned} \eta_i(\emptyset) &= \sum_{j=1}^r u_{ij} \xi_j(\emptyset), \quad i = 1, \dots, s, \\ E\delta_i(\emptyset) &= \sum_{j=1}^r w_{ij} \xi_j(\emptyset), \quad i = 1, \dots, r', \\ E\xi_i(\emptyset) &= \sum_{j=1}^r v_{ij} \xi_j(\emptyset), \quad i = 1, \dots, r, \end{aligned}$$

•

$$\begin{aligned}\eta_i(\bullet) &= \sum_{j=1}^{r'} p_{ij} \xi'_j(\bullet) + \sum_{j=1}^r u_{ij} \xi_j(\bullet), \quad i = 1, \dots, s, \\ E\delta_i(\bullet) &= \sum_{j=1}^{r'} r_{ij} \xi'_j(\bullet) + \sum_{j=1}^r w_{ij} \xi_j(\bullet), \quad i = 1, \dots, r', \\ E\xi_i(\bullet) &= \sum_{j=1}^{r'} q_{ij} \xi'_j(\bullet) + \sum_{j=1}^r v_{ij} \xi_j(\bullet), \quad i = 1, \dots, r,\end{aligned}$$

◦

$$\begin{aligned}\eta_i(\circ) &= 2 \sum_{j=1}^s a_{ij} \eta_j(\emptyset) + 2 \sum_{j=1}^{r'} p_{ij} \xi'_j(\circ) + \sum_{j=1}^r u_{ij} \xi_j(\circ), \quad i = 1, \dots, s, \\ E\delta_i(\circ) &= 2 \sum_{j=1}^s c_{ij} \eta_j(\emptyset) + 2 \sum_{j=1}^{r'} r_{ij} \xi'_j(\circ) + \sum_{j=1}^r w_{ij} \xi_j(\circ), \quad i = 1, \dots, r', \\ E\xi_i(\circ) &= 2 \sum_{j=1}^s b_{ij} \eta_j(\emptyset) + 2 \sum_{j=1}^{r'} q_{ij} \xi'_j(\circ) + \sum_{j=1}^r v_{ij} \xi_j(\circ), \quad i = 1, \dots, r.\end{aligned}$$

Once the base case is provided, the operators evaluated in the trees of order 2, 3 and 4 are recursively derived according to Theorem 2.2.1, leading to

‡

$$\begin{aligned}E\delta_i(\ddagger) &= 6 \sum_{j=1}^s c_{ij} \eta_j(\bullet) + 3 \sum_{j=1}^{r'} r_{ij} \xi'_j(\ddagger) + \sum_{j=1}^r w_{ij} \xi_j(\ddagger), \quad i = 1, \dots, r', \\ E\xi_i(\ddagger) &= 6 \sum_{j=1}^s b_{ij} \eta_j(\bullet) + 3 \sum_{j=1}^{r'} q_{ij} \xi'_j(\ddagger) + \sum_{j=1}^r v_{ij} \xi_j(\ddagger), \quad i = 1, \dots, r,\end{aligned}$$

♠

$$\begin{aligned}E\delta_i(\spadesuit) &= 12 \sum_{j=1}^s c_{ij} \eta_j(\bullet)^2 + 4 \sum_{j=1}^{r'} r_{ij} \xi'_j(\spadesuit) + \sum_{j=1}^r w_{ij} \xi_j(\spadesuit), \quad i = 1, \dots, r', \\ E\xi_i(\spadesuit) &= 12 \sum_{j=1}^s b_{ij} \eta_j(\bullet)^2 + 4 \sum_{j=1}^{r'} q_{ij} \xi'_j(\spadesuit) + \sum_{j=1}^r v_{ij} \xi_j(\spadesuit), \quad i = 1, \dots, r,\end{aligned}$$

⋄

$$\begin{aligned}E\delta_i(\diamond) &= 12 \sum_{j=1}^s c_{ij} \eta_j(\circ) + 4 \sum_{j=1}^{r'} r_{ij} \xi'_j(\diamond) + \sum_{j=1}^r w_{ij} \xi_j(\diamond), \quad i = 1, \dots, r', \\ E\xi_i(\diamond) &= 12 \sum_{j=1}^s b_{ij} \eta_j(\circ) + 4 \sum_{j=1}^{r'} q_{ij} \xi'_j(\diamond) + \sum_{j=1}^r v_{ij} \xi_j(\diamond), \quad i = 1, \dots, r,\end{aligned}$$

♣

$$\begin{aligned}E\delta_i(\clubsuit) &= 20 \sum_{j=1}^s c_{ij} \eta_j(\bullet)^3 + 5 \sum_{j=1}^{r'} r_{ij} \xi'_j(\clubsuit) + \sum_{j=1}^r w_{ij} \xi_j(\clubsuit), \quad i = 1, \dots, r', \\ E\xi_i(\clubsuit) &= 20 \sum_{j=1}^s b_{ij} \eta_j(\bullet)^3 + 5 \sum_{j=1}^{r'} q_{ij} \xi'_j(\clubsuit) + \sum_{j=1}^r v_{ij} \xi_j(\clubsuit), \quad i = 1, \dots, r,\end{aligned}$$



$$E\delta_i(\text{node}) = 20 \sum_{j=1}^s c_{ij} \eta_j(\bullet) \eta_j(\circ) + 5 \sum_{j=1}^{r'} r_{ij} \xi'_j(\text{node}) + \sum_{j=1}^r w_{ij} \xi_j(\text{node}), \quad i = 1, \dots, r',$$

$$E\xi_i(\text{node}) = 20 \sum_{j=1}^s b_{ij} \eta_j(\bullet) \eta_j(\circ) + 5 \sum_{j=1}^{r'} q_{ij} \xi'_j(\text{node}) + \sum_{j=1}^r v_{ij} \xi_j(\text{node}), \quad i = 1, \dots, r,$$



$$E\delta_i(\text{node}) = 20 \sum_{j=1}^s c_{ij} \eta_j(\text{node}) + 5 \sum_{j=1}^{r'} r_{ij} \xi'_j(\text{node}) + \sum_{j=1}^r w_{ij} \xi_j(\text{node}), \quad i = 1, \dots, r',$$

$$E\xi_i(\text{node}) = 20 \sum_{j=1}^s b_{ij} \eta_j(\text{node}) + 5 \sum_{j=1}^{r'} q_{ij} \xi'_j(\text{node}) + \sum_{j=1}^r v_{ij} \xi_j(\text{node}), \quad i = 1, \dots, r,$$

where $\eta_i(\text{node}) = 6 \sum_{j=1}^s a_{ij} \eta_j(\bullet) + 3 \sum_{j=1}^{r'} p_{ij} \xi'_j(\text{node}) + \sum_{j=1}^r u_{ij} \xi_j(\text{node}), \quad i = 1, \dots, s.$

2.2.2 Classical Methods as GLN and their Order Conditions

The family of GLN methods (2.1) properly contains many known classes of numerical methods for (1.4). Analogously, the order conditions above derived are general, hence it is possible to recover through them the order conditions of numerical methods already considered in the literature. To make this possible, we need to regard these methods as GLN methods and specialize the operators $E\delta$ and $E\xi$ on the case by case basis. This is clarified in the following examples.

RKN methods

Runge-Kutta-Nyström methods (see [71, 101])

$$Y_i = y_{n-1} + c_i h y'_{n-1} + h^2 \sum_{j=1}^s a_{ij} f(Y_j), \quad i = 1, \dots, s,$$

$$h y'_n = h y'_{n-1} + h^2 \sum_{j=1}^s b'_j f(Y_j), \tag{2.31}$$

$$y_n = y_{n-1} + h y'_{n-1} + h^2 \sum_{j=1}^s b_j f(Y_j),$$

can be recasted as GLN methods (2.1) with $r = r' = 1$, in correspondence to the tableau (2.12)

$$\left[\begin{array}{c|c|c} \mathbf{A} & \mathbf{P} & \mathbf{U} \\ \hline \mathbf{C} & \mathbf{R} & \mathbf{W} \\ \hline \mathbf{B} & \mathbf{Q} & \mathbf{V} \end{array} \right] = \left[\begin{array}{c|c|c} A & c & e \\ \hline b'^{\top} & 1 & 0 \\ \hline b^{\top} & 1 & 1 \end{array} \right],$$

where e is the unit vector in \mathbb{R}^s , and the input vectors $y^{[n-1]} = [y_{n-1}]$, $y'^{[n-1]} = [y'_{n-1}]$. Correspondingly, the set of order and stage order conditions (2.27)-(2.28) assumes the form

$$\begin{cases} E\eta = A\bar{\eta} + c\delta + e\xi, \\ E\delta = b^\top\bar{\eta} + \delta, \\ E\xi = b^\top\bar{\eta} + \delta + \xi. \end{cases} \quad (2.32)$$

The values of $E\eta$, $E\delta$ and $E\xi$ are reported in Table 2.3. We observe that these conditions match the classical ones (compare [73, 71]).

tree	$E\xi(t)$	$E\delta(t)$	$E\eta_i(t)$
\emptyset	1	0	1
\bullet	1	1	c_i
\circ	1	2	c_i^2
\bullet	1	3	c_i^3
\vdots	\vdots	\vdots	\vdots
t	1	$\rho(t)$	$c_i^{\rho(t)}$

Table 2.3: Values of $E\eta_i$, $E\delta$ and $E\xi$ for RKN methods regarded as GLN methods

Coleman hybrid methods

We now consider the following class of methods

$$Y_i = (1 + c_i)y_{n-1} - c_i y_{n-2} + h^2 \sum_{j=1}^s a_{ij} f(Y_j), \quad i = 1, \dots, s, \quad (2.33)$$

$$y_n = 2y_{n-1} - y_{n-2} + h^2 \sum_{j=1}^s b_j f(Y_j),$$

introduced by Coleman in [27] (also compare [46, 43, 44, 42]), which are denoted as two-step hybrid methods. Such methods (2.33) can be regarded as GLN methods corresponding to the reduced tableau

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array} \right] = \left[\begin{array}{c|cc} A & e + c & -c \\ \hline b^\top & 2 & -1 \\ 0 & 1 & 0 \end{array} \right]$$

obtained by assuming the remaining coefficient matrices in (2.12) equal to the zero matrix. Such methods are characterized by the the input vector $y^{[n-1]} = [y_{n-1} \ y_{n-2}]^\top$. The corresponding set of order and stage order conditions (2.27)-(2.28) takes the form

$$\begin{cases} E\eta = A\bar{\eta} + e + c\xi_1 - c\xi_2, \\ E\xi_1 = b^\top\bar{\eta} + 2\xi_1 - \xi_2, \\ E\xi_2 = \xi_1. \end{cases} \quad (2.34)$$

The coefficients for ξ_1, ξ_2 can be found in Table 2.4. We observe that the third equation in (2.34) is trivial by the definition of ξ_1 .

tree	$E\xi_1(t)$	$\xi_1(t)$	$\xi_2(t)$
\emptyset	1	1	1
\bullet	1	0	-1
\circ	1	0	1
\bullet	1	0	-1
\vdots	\vdots	\vdots	\vdots
t	1	0	$(-1)^{\rho(t)}$

Table 2.4: Values of $E\xi_1$, ξ_1 and ξ_2 for Coleman hybrid methods regarded as GLNs

Two-step Runge-Kutta-Nyström methods

Two-step Runge-Kutta-Nyström methods (TSRKN)

$$\begin{aligned}
Y_i^{[n-1]} &= y_{n-2} + hc_i y'_{n-2} + h^2 \sum_{j=1}^s a_{ij} f(Y_j^{[n-1]}), \quad i = 1, \dots, s, \\
Y_i^{[n]} &= y_{n-1} + hc_i y'_{n-1} + h^2 \sum_{j=1}^s a_{ij} f(Y_j^{[n]}), \quad i = 1, \dots, s, \\
hy'_n &= (1 - \theta)hy'_{n-1} + \theta hy'_{n-2} + h^2 v'_j f(Y_j^{[n-1]}) + h^2 w'_j f(Y_j^{[n]}), \\
y_n &= (1 - \theta)y_{n-1} + \theta y_{n-2} + h \sum_{j=1}^s v'_j y'_{n-2} + h \sum_{j=1}^s w'_j y'_{n-1} \\
&\quad + h^2 \sum_{j=1}^s v_j f(Y_j^{[n-1]}) + h^2 \sum_{j=1}^s w_j f(Y_j^{[n]}),
\end{aligned}$$

have been introduced and analyzed by Paternoster in [102, 104]. Such methods depend on two consecutive approximations to the solution and its first derivative in the grid points, but also on two consecutive approximations to the stage values, in line with the idea employed by Jackiewicz et al. (compare [14, 28, 31, 48, 40, 37, 39, 74, 82]) in the context of two-step Runge–Kutta methods for first order ODEs. TSRKN methods can be represented as GLNs (2.1) with $r = s + 2$ and $r' = 2$ through the tableau (2.12)

$$\left[\begin{array}{c|c|c} \mathbf{A} & \mathbf{P} & \mathbf{U} \\ \hline \mathbf{C} & \mathbf{R} & \mathbf{W} \\ \hline \mathbf{B} & \mathbf{Q} & \mathbf{V} \end{array} \right] = \left[\begin{array}{c|cc|ccc} A & c & 0 & e & 0 & 0 \\ \hline w'^{\top} & 1 - \theta & \theta & 0 & 0 & v'^{\top} \\ 0 & 1 & 0 & 0 & 0 & 0 \\ \hline w^{\top} & w'^{\top} e & v'^{\top} e & 1 - \theta & \theta & v^{\top} \\ 0 & 0 & 0 & 1 & 0 & 0 \\ I & 0 & 0 & 0 & 0 & 0 \end{array} \right],$$

in correspondence of the input vectors $y^{[n-1]} = [y_{n-1} \quad y_{n-2} \quad h^2 f(Y^{[n-1]})]^{\top}$, $y'^{[n-1]} =$

$[y'_{n-1} \quad y'_{n-2}]^\top$. The set of order conditions for these methods has the form

$$\left\{ \begin{array}{l} E\eta_i = \sum_{j=1}^s a_{ij}\bar{\eta}_j + c_i\delta_1 + \xi_1, \quad i = 1, \dots, s, \\ E\delta_1 = \sum_{j=1}^s w'_j\bar{\eta}_j + (1 - \theta)\delta_1 + \theta\delta_2 + \sum_{j=1}^s v'_j\xi_{3j}, \\ E\delta_2 = \delta_1, \\ E\xi_1 = \sum_{j=1}^s w_j\bar{\eta}_j + \sum_{j=1}^s w'_j\delta_1 + \sum_{j=1}^s v'_j\delta_2 + (1 - \theta)\xi_1 + \theta\xi_2 + \sum_{j=1}^s v_j\xi_{3j}, \\ E\xi_2 = \xi_1, \\ E\xi_{3i} = \bar{\eta}_i \quad i = 1, \dots, s, \end{array} \right. \quad (2.35)$$

whose coefficients $E\xi_1$, $E\delta_1$, ξ_1 , ξ_2 , δ_1 and δ_2 can be found in Table 2.5. We also observe that in the system (2.35) there are automatically satisfied conditions, i.e. the third, the fifth and the sixth.

tree	$E\xi_1(t)$	$E\delta_1(t)$	$\xi_1(t)$	$\xi_2(t)$	$\delta_1(t)$	$\delta_2(t)$
\emptyset	1	0	1	1	0	0
\bullet	1	1	0	-1	1	1
\circ	1	2	0	1	0	-1
\updownarrow	1	3	0	-1	0	1
\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots
t	1	$\rho(t)$	0	$(-1)^{\rho(t)}$	0	$(-1)^{\rho(t)-1}$

Table 2.5: Values of $E\xi_1$, $E\delta_1$, ξ_1 , ξ_2 , δ_1 and δ_2 for TSRKN methods regarded as GLNs

2.2.3 Construction Issues

The algebraic order theory we developed in Section 2.2.1 can be effectively used in the construction of new methods. In order to simplify the notations, without loss of generality, we consider the hybrid formulation (2.14) and we observe that Proposition 2.2.1 can be easily adapted to this case. To this purpose, we observe that the system (2.26) can be rewritten as

$$\left\{ \begin{array}{l} \eta = \mathbf{A}\bar{\eta} + \mathbf{U}\xi, \\ \hat{\xi} = \mathbf{B}\bar{\eta} + \mathbf{V}\xi, \end{array} \right. \quad (2.36)$$

where, using the same notation used in (2.26), we denote with η and ξ respectively the operators associated to the stages and to the quantities approximated by the method at each step. Due to the hybrid formulation, the approximations to the first derivative are now embedded in the solution vector, thus also the operator δ is now embedded in ξ . With this assumptions Proposition 2.2.1 assumes the form

Proposition 2.2.2. If the operator $\widehat{\xi}$ in (2.36) of a given GLN (2.14) is such that $\widehat{\xi}_i(t)$ coincide with the corresponding coefficients $E\xi_i(t)$ in the Taylor series expansions of the exact values approximated by $y_i^{[n]}$ for any $t \in SNT$ of order $\rho(t) \leq p+1$, then the method has order p , i.e.

$$E\xi = \mathbf{B}\bar{\eta} + \mathbf{V}\xi. \quad (2.37)$$

Moreover, the method has stage order q if the operators $\eta_i(t)$, $i = 1, \dots, s$, in (2.36) coincide with the coefficients $E\eta_i$ of the Taylor series expansion of $y(x_0 + c_i h)$, for any $t \in SNT$ of order less or equal to $q + 1$, i.e.

$$E\eta = \mathbf{A}\bar{\eta} + \mathbf{U}\xi. \quad (2.38)$$

We can use this result together with other basic conditions to construct new methods. As in the case of first order general linear methods, however, starting procedures are necessary (compare Section 3.6) and they are characterized by the operator ξ . We can treat this point in two ways: we can leave the values of ξ as free parameters and use them along the construction process but then we will need to construct and implement the starting procedures, or we can fix them at the beginning on known values and we will have less free parameters but a significant simplification in the implementation phase. In the present Section we show a construction process where we fix those values of the ξ operator that correspond to the solution, i.e. we consider as input vector

$$y^{[n]} \approx \begin{bmatrix} y(x_n) \\ y_2^{[n]}(x_n) \\ \vdots \\ y_r^{[n]}(x_n) \end{bmatrix}, \quad (2.39)$$

we fix the number of stages to $s = 1$ and the number of approximations to $r = 2$, then we write the operators ξ on the SN-trees up to order 5 (see Table 2.6) assuming that they assume the same value on all the trees of a fixed order (thus we can use Remark 2.2.2). Imposing order conditions up to the trees of order 4, we obtain the following example of one-stage explicit method of order 3.

$$\left[\begin{array}{c|cc} \mathbf{A} & \mathbf{U} \\ \mathbf{B} & \mathbf{V} \end{array} \right] = \left[\begin{array}{c|cc} 0 & 1 & 0 \\ \hline 1 & 1 & \frac{1}{2} \\ 2 & 0 & 1 \end{array} \right]. \quad (2.40)$$

To obtain a method of order 4, we consider a 2-stages, 3-values procedure and, as input vector, we consider

$$y^{[n]} \approx \begin{bmatrix} y(x_n) \\ h y'(x_n) \\ y_3^{[n]}(x_n) \end{bmatrix}, \quad (2.41)$$

thus inserting an approximation of the first derivative and leaving the third component as variable. In this case the coefficients used in the procedure are reported in Table 2.7, always assuming that they assume the same value on all the trees of a



$\rho(t)$	t	$\xi(t)$	$E\xi$
0	\emptyset	$(1, \xi_{02})$	$(1, \xi_{02})$
1	\bullet	$(1, \xi_{12})$	$(1, \xi_{02} + \xi_{12})$
2	\circ	$(0, \xi_{22})$	$(1, \xi_{02} + 2\xi_{12}\xi_{22})$
3		$(0, \xi_{32})$	$(1, \xi_{02} + 3\xi_{12} + 3 * \xi_{22} + \xi_{32})$
4		$(0, \xi_{42})$	$(1, \xi_{02} + 4\xi_{12} + 6\xi_{22} + 4\xi_{32} + \xi_{42})$

Table 2.6: Values assumed by the operators ξ and $E\xi$.




$\rho(t)$	t	$\xi(t)$	$E\xi$
0	\emptyset	$(1, 0, \xi_{03})$	$(1, 0, \xi_{03})$
1	\bullet	$(0, 1, \xi_{13})$	$(1, 1, \xi_{03} + \xi_{13})$
2	\circ	$(0, 0, \xi_{23})$	$(1, 2, \xi_{03} + 2\xi_{13} + \xi_{23})$
3		$(0, 0, \xi_{33})$	$(1, 3, \xi_{03} + 3\xi_{13} + 3\xi_{23} + \xi_{33})$
4		$(0, 0, \xi_{43})$	$(1, 4, \xi_{03} + 4\xi_{13} + 6 * \xi_{23} + 4\xi_{33} + \xi_{43})$
5		$(0, 0, \xi_{53})$	$(1, 5, \xi_{03} + 5\xi_{13} + 10 * \xi_{23} + 10\xi_{33} + 5\xi_{43} + \xi_{53})$

Table 2.7: Values assumed by the operators ξ and $E\xi$.

$$\begin{aligned}
\mathbf{A} &= \frac{\xi_{23}c_1^3 - \xi_{33}c_1^2 - 6a_12c_2\xi_{23} + 2a_12\xi_{33}}{6c_1\xi_{23} - 2\xi_{33}} \quad \mathbf{a12} \\
&\quad \frac{\xi_{23}c_2^3 - \xi_{33}c_2^2 - 6a_21c_1\xi_{23} + 2a_21\xi_{33}}{6c_2\xi_{23} - 2\xi_{33}} \\
\mathbf{U} &= \frac{6a_12\xi_{03}(c_1 - c_2) - 2c_1^3\xi_{03} + 3c_1\xi_{23} - \xi_{33}}{3c_1\xi_{23} - \xi_{33}} \quad \frac{6a_12\xi_{13}(c_1 - c_2) - c_1(2c_1^2\xi_{13} - 3c_1\xi_{23} + \xi_{33})}{2(-3a_12c_1 + 3a_12c_2 + c_1^3)} \\
&\quad \frac{6a_21\xi_{03}(c_1 - c_2) + 2c_2^3\xi_{03} - 3c_2\xi_{23} + \xi_{33}}{3c_2\xi_{23} - \xi_{33}} \quad \frac{6a_21\xi_{13}(c_2 - c_1) - c_2(2c_2^2\xi_{13} - 3c_2\xi_{23} + \xi_{33})}{2(3a_21(c_1 - c_2) + c_2^3)} \\
\mathbf{Col}_1(\mathbf{B}) &= \frac{-6c_2^2(\xi_{03}(\xi_{23} - \xi_{33}) + 3\xi_{13}\xi_{23} - 2\xi_{13}\xi_{33} + 3\xi_{23}^2) + 3c_2(\xi_{03}(\xi_{23} - \xi_{43}) + 4\xi_{13}\xi_{23} - 2\xi_{13}\xi_{43} + 6\xi_{23}^2 + 4\xi_{23}\xi_{33}) + \xi_{03}(\xi_{43} - \xi_{33}) - 4\xi_{13}\xi_{33} + 3\xi_{13}\xi_{43} - 6\xi_{23}\xi_{33} + 3\xi_{23}\xi_{43} - 4\xi_{33}^2}{6(c_1 - c_2)(6c_1c_2\xi_{23} - 2c_1\xi_{33} - 2c_2\xi_{33} + \xi_{43})} \\
&\quad \frac{6c_1^2(\xi_{23} - \xi_{33}) - 3c_1(\xi_{23} - \xi_{43}) + \xi_{33} - \xi_{43}}{6c_1^2(\xi_{23} - \xi_{33}) - 2c_1\xi_{33} - 2c_2\xi_{33} + \xi_{43}} \\
&\quad \frac{6(c_1 - c_2)(6c_1c_2\xi_{23} - 2c_1\xi_{33} - 2c_2\xi_{33} + \xi_{43})}{6(c_1 - c_2)(6c_1c_2\xi_{23} - 2c_1\xi_{33} - 2c_2\xi_{33} + \xi_{43})} \\
\mathbf{Col}_2(\mathbf{B}) &= \frac{6(c_1 - c_2)(6c_1c_2\xi_{23} - 2c_1\xi_{33} - 2c_2\xi_{33} + \xi_{43})}{6c_1^2(3\xi_{23} - 2\xi_{33}) + 6c_1(\xi_{43} - 2\xi_{23}) + 4\xi_{33} - 3\xi_{43}} \\
&\quad \frac{6(c_1 - c_2)(6c_1c_2\xi_{23} - 2c_1\xi_{33} - 2c_2\xi_{33} + \xi_{43})}{6(c_1 - c_2)(6c_1c_2\xi_{23} - 2c_1\xi_{33} - 2c_2\xi_{33} + \xi_{43})} \\
\mathbf{Col}_1(\mathbf{V}) &= \frac{1 - \frac{\xi_{03}(c_1(6c_2 - 2) - 2c_2 + 1)}{6c_1c_2\xi_{23} - 2c_1\xi_{33} - 2c_2\xi_{33} + \xi_{43}}}{2\xi_{03}(c_1(6c_2 - 3) - 3c_2 + 2)} \\
&\quad \frac{6c_1c_2\xi_{23} - 2c_1\xi_{33} - 2c_2\xi_{33} + \xi_{43}}{6c_1c_2\xi_{23} - 2c_1\xi_{33} - 3c_1 - 3c_2 + 2} - 6c_1\xi_{23} - 6c_2\xi_{23} + 6\xi_{23} + 4\xi_{33}) \\
\mathbf{Col}_2(\mathbf{V}) &= \frac{1 - \frac{\xi_{13}(c_1(6c_2 - 2) - 2c_2 + 1)}{6c_1c_2\xi_{23} - 2c_1\xi_{33} - 2c_2\xi_{33} + \xi_{43}}}{2\xi_{13}(c_1(6c_2 - 3) - 3c_2 + 2)} \\
&\quad \frac{\xi_{03}(\xi_{13}(c_1(2 - 6c_2) + 2c_2 - 1) + 6c_1c_2\xi_{23} - 2c_1\xi_{33} - 2c_2\xi_{33} + \xi_{43}) + 2\xi_{13}(\xi_{13}(c_1(3 - 6c_2) + 3c_2 - 2) + 3\xi_{23}(c_1 + c_2 - 1) - 2\xi_{33})}{6c_1c_2\xi_{23} - 2c_1\xi_{33} - 2c_2\xi_{33} + \xi_{43}} \\
\mathbf{Col}_3(\mathbf{V}) &= \frac{\xi_{03}(c_1(6c_2 - 2) - 2c_2 + 1) + 2\xi_{13}(6c_1c_2 - 3c_1 - 3c_2 + 2) + 6c_1c_2\xi_{23} - 6c_1\xi_{33} - 6c_2\xi_{23} - 2c_2\xi_{33} + 6\xi_{23} + 4\xi_{33} + \xi_{43}}{6c_1c_2\xi_{23} - 2c_1\xi_{33} - 2c_2\xi_{33} + \xi_{43}}
\end{aligned}$$

Table 2.8: General form of a method of order 3.

fixed order. Applying the order conditions up to the trees of order 4, we obtain the structure for a method of order 3 reported in Table 2.8 The eigenvalues of the \mathbf{V} matrix are

$$\left\{ 1, 1, \frac{6c_1c_2\xi_{23} - 6c_1\xi_{23} - 2c_1\xi_{33} - 6c_2\xi_{23} - 2c_2\xi_{33} + 6\xi_{23} + 4\xi_{33} + \xi_{43}}{6c_1c_2\xi_{23} - 2c_1\xi_{33} - 2c_2\xi_{33} + \xi_{43}} \right\}$$

and the abscissae are still not assigned. We have to impose order 4 and zero-stability, i.e. the third eigenvalue of \mathbf{V} being strictly less than 1 in modulus, that are 4 conditions and we have 10 free parameters left. We can use the remaining free parameters to impose, for example, a structure to matrix \mathbf{A} and a particular expression for the abscissae. Imposing order 4 we find that the abscissae must satisfy

$$c_1 = \frac{30c_2^2 - \sqrt{6}\sqrt{50c_2^4 - 100c_2^3 + 64c_2^2 - 14c_2 + 1} - 32c_2 + 6}{10(6c_2^2 - 6c_2 + 1)}$$

and imposing $0 < c_1 < c_2 < 1$ we find that c_2 is allowed to vary in the interval $[\frac{6+\sqrt{6}}{10}, 1]$. Choosing $c_2 = 1$, we find $c_1 = \frac{4-\sqrt{6}}{10}$. Before applying the other conditions for order 4 we want to find the simplest possible expression for matrix \mathbf{A} . It can be first reduced to a diagonal matrix imposing $a_{12} = a_{21} = 0$ and then we can impose $a_{11} = 0$ and find that $\xi_{23} = \frac{10(4\sqrt{6}\xi_{33} - 11\xi_{33})}{27\sqrt{6} - 68}$, but this condition results to be not compatible with the zero-stability. Imposing only the conditions for \mathbf{A} to be a diagonal matrix, we find that \mathbf{V} has automatically two eigenvalues equal to 1 and zero-stability is given by reducing the third eigenvalue to be between -1 and 1 in modulus. Combining this condition with the remaining equations for order 4 we obtain the family of methods whose coefficient matrices are reported in Table 2.9 with the above given abscissae and the condition

$$\xi_{23} > 0 \wedge \frac{21849\sqrt{6}\xi_{23} - 53648\xi_{23}}{11230\sqrt{6} - 27464} < \xi_{33} < \frac{24351\sqrt{6}\xi_{23} - 59874\xi_{23}}{25020\sqrt{6} - 62260}.$$

Since we have no bounds on the values of ξ_{03} and ξ_{13} we choose them as zero and we also fix the values of ξ_{23} and ξ_{33} respectively to 1 and 0 obtaining the method

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \mathbf{B} & \mathbf{V} \end{array} \right] = \left[\begin{array}{cc|cc} \frac{1}{600}(-4 + \sqrt{6})^2 & 0 & 1 & \frac{1}{10}(4 - \sqrt{6}) & \frac{1}{150}(-4 + \sqrt{6})^2 \\ 0 & \frac{1}{6} & 1 & 1 & \frac{2}{3} \\ \hline \frac{65}{144-21\sqrt{6}} & \frac{1}{603}(3 + 13\sqrt{6}) & 1 & 1 & \frac{1}{67}(-3 - 13\sqrt{6}) \\ \frac{45}{48-7\sqrt{6}} & \frac{1}{67}(11 + 3\sqrt{6}) & 0 & 1 & \frac{1}{67}(-32 - 27\sqrt{6}) \\ \frac{1}{402}(48 + 7\sqrt{6}) & \frac{1}{201}(93 + \sqrt{6}) & 0 & 0 & \frac{1}{-11+3\sqrt{6}} \end{array} \right].$$

The final values for the third component of the operator ξ related to such method are

$$\left(0, 0, 1, 0, -\frac{1}{5}, \frac{2}{5} \right).$$

A less general but easier construction technique leading to a very highly stable method is shown in Section 2.2.6.

$$\begin{aligned}
\mathbf{A} &= \begin{bmatrix} \frac{(\sqrt{6}-4)^2((\sqrt{6}-4)\xi_{23}+10\xi_{33})}{200(3(\sqrt{6}-4)\xi_{23}+10\xi_{33})} & 0 \\ \frac{\xi_{23}-\xi_{33}}{6\xi_{23}-2\xi_{33}} & \end{bmatrix} \\
\mathbf{U} &= \begin{bmatrix} \frac{(68-27\sqrt{6})\xi_{03}+25(3(\sqrt{6}-4)\xi_{23}+10\xi_{33})}{25(3(\sqrt{6}-4)\xi_{23}+10\xi_{33})-\frac{3\xi_{23}-\xi_{33}}{2\xi_{03}-3\xi_{23}+\xi_{33}}} & \frac{(\sqrt{6}-4)((8\sqrt{6}-22)\xi_{13}-15(\sqrt{6}-4)\xi_{23}-50\xi_{33})}{50(3(\sqrt{6}-4)\xi_{23}+10\xi_{33})-\frac{3\xi_{23}-\xi_{33}}{2\xi_{13}-3\xi_{23}+\xi_{33}}} \\ \frac{105\xi_{33}-65\xi_{23}}{3((7\sqrt{6}-48)\xi_{23}+6(11+\sqrt{6})\xi_{33})-\frac{3\xi_{23}-\xi_{33}}{5(27\xi_{23}-34\xi_{33})}} & \frac{50(3(\sqrt{6}-4)\xi_{23}+10\xi_{33})}{3\xi_{23}-\xi_{33}} \\ \frac{3((7\sqrt{6}-48)\xi_{23}+6(11+\sqrt{6})\xi_{33})}{5(13\xi_{03}\xi_{23}-21\xi_{03}\xi_{33}+27\xi_{13}\xi_{23}-34\xi_{13}\xi_{33}+3\xi_{23}^2-36\xi_{23}\xi_{33}+20\xi_{33}^2)} & \frac{50(3(\sqrt{6}-4)\xi_{23}+10\xi_{33})}{3\xi_{23}-\xi_{33}} \end{bmatrix} \\
\mathbf{Col}_1(\mathbf{B}) &= \begin{bmatrix} \frac{3((7\sqrt{6}-48)\xi_{23}+6(11+\sqrt{6})\xi_{33})}{(3\sqrt{6}-2)(\xi_{23}-3\xi_{33})} \\ \frac{3((7\sqrt{6}-48)\xi_{23}+6(11+\sqrt{6})\xi_{33})}{2(14+9\sqrt{6})\xi_{33}-3(6+\sqrt{6})\xi_{23}} \\ \frac{3((7\sqrt{6}-48)\xi_{23}+6(11+\sqrt{6})\xi_{33})}{2(14+9\sqrt{6})\xi_{33}-3(6+\sqrt{6})\xi_{23}} \\ \frac{3((7\sqrt{6}-48)\xi_{23}+6(11+\sqrt{6})\xi_{33})}{3((7\sqrt{6}-48)\xi_{23}+6(11+\sqrt{6})\xi_{33})} \end{bmatrix} \\
\mathbf{Col}_2(\mathbf{B}) &= \begin{bmatrix} \frac{3((7\sqrt{6}-48)\xi_{23}+6(11+\sqrt{6})\xi_{33})}{2(14+9\sqrt{6})\xi_{33}-3(6+\sqrt{6})\xi_{23}} \\ \frac{3((7\sqrt{6}-48)\xi_{23}+6(11+\sqrt{6})\xi_{33})}{2(14+9\sqrt{6})\xi_{33}-3(6+\sqrt{6})\xi_{23}} \\ \frac{3((7\sqrt{6}-48)\xi_{23}+6(11+\sqrt{6})\xi_{33})}{2(14+9\sqrt{6})\xi_{33}-3(6+\sqrt{6})\xi_{23}} \\ \frac{3((7\sqrt{6}-48)\xi_{23}+6(11+\sqrt{6})\xi_{33})}{3((7\sqrt{6}-48)\xi_{23}+6(11+\sqrt{6})\xi_{33})} \end{bmatrix} \\
\mathbf{Col}_1(\mathbf{V}) &= \begin{bmatrix} \frac{(3\sqrt{6}-11)\xi_{23}-(\sqrt{6}-12)\xi_{33}}{(3\sqrt{6}-11)\xi_{23}-(\sqrt{6}-12)\xi_{33}} \\ \frac{(3\sqrt{6}-11)\xi_{23}-(\sqrt{6}-12)\xi_{33}}{(2-3\sqrt{6})\xi_{03}} \\ \frac{(3\sqrt{6}-11)\xi_{23}-(\sqrt{6}-12)\xi_{33}}{(3\sqrt{6}-11)\xi_{23}-(\sqrt{6}-12)\xi_{33}} \\ \frac{(3\sqrt{6}-11)\xi_{23}-(\sqrt{6}-12)\xi_{33}}{(3-2\sqrt{6})\xi_{13}+(3\sqrt{6}-11)\xi_{23}-(\sqrt{6}-12)\xi_{33}} \end{bmatrix} \\
\mathbf{Col}_2(\mathbf{V}) &= \begin{bmatrix} \frac{(3\sqrt{6}-11)\xi_{23}-(\sqrt{6}-12)\xi_{33}}{(3-2\sqrt{6})\xi_{13}+(3\sqrt{6}-11)\xi_{23}-(\sqrt{6}-12)\xi_{33}} \\ \frac{(3\sqrt{6}-11)\xi_{23}-(\sqrt{6}-12)\xi_{33}}{(2-3\sqrt{6})\xi_{13}+(3\sqrt{6}-11)\xi_{23}-(\sqrt{6}-12)\xi_{33}} \\ \frac{(3\sqrt{6}-11)\xi_{23}-(\sqrt{6}-12)\xi_{33}}{(3\sqrt{6}-11)\xi_{23}-(\sqrt{6}-12)\xi_{33}} \\ \frac{(3\sqrt{6}-11)\xi_{23}-(\sqrt{6}-12)\xi_{33}}{(3-2\sqrt{6})\xi_{13}+(3\sqrt{6}-11)\xi_{23}-(\sqrt{6}-12)\xi_{33}} \end{bmatrix} \\
\mathbf{Col}_3(\mathbf{V}) &= \begin{bmatrix} \frac{3-2\sqrt{6}}{(11-3\sqrt{6})\xi_{23}+(\sqrt{6}-12)\xi_{33}} \\ \frac{3-2\sqrt{6}}{(11-3\sqrt{6})\xi_{23}+(\sqrt{6}-12)\xi_{33}} \\ \frac{(3-2\sqrt{6})\xi_{03}+(2-3\sqrt{6})\xi_{13}-\xi_{23}+\sqrt{6}\xi_{33}+8\xi_{33}}{(11-3\sqrt{6})\xi_{23}+(\sqrt{6}-12)\xi_{33}} \end{bmatrix}
\end{aligned}$$

Table 2.9: General form of a method of order 4.

$E\xi(\emptyset)$	$E\xi(\bullet)$	$E\xi(\circ)$	\dots	$E\xi(t)$
1	1	1	\dots	1
0	1	2	\dots	$\rho(t)$
0	0	2	\dots	$\rho(t)(\rho(t) - 1)$
0	0	0	\dots	$\rho(t)(\rho(t) - 1)(\rho(t) - 2)$
\vdots	\vdots	\vdots	\vdots	\vdots
0	0	0	\dots	$\rho(t)!$

Table 2.10: Values of $E\xi(t)$ in (2.27) for Nordsieck methods

2.2.4 GLNs in Nordsieck Form

This Section is focused on the family of hybrid GLN methods (2.14) in Nordsieck form, i.e. such that the vector of external approximations satisfies

$$y^{[n]} \approx \begin{bmatrix} y(x_n) \\ hy'(x_n) \\ h^2y''(x_n) \\ \vdots \\ h^r y^{(r)}(x_n) \end{bmatrix}, \quad (2.42)$$

that is an approximation to the Nordsieck vector [20, 71, 82, 99]. The motivation behind such a choice is that in such a way we don't need a starting procedure for our methods. Moreover, as we will see in detail, for the Nordsieck vector order conditions are simplified.

For GLN methods (2.14) depending on input vectors of the form (2.42), the values of the entries of $\xi(t)$ can be easily computed as follows

$$\xi_i(t) = \rho(t)! \delta_{\rho(t), i-1}, \quad i = 1, \dots, r, \quad (2.43)$$

being $t \in SNT$ and $\delta_{i,j}$ the usual Kronecker delta. This formula can be obtained by SN -series arguments: indeed, looking for a SN -representation of the input vector

$$y_i^{[n-1]} = SN(\xi_i, y, y'),$$

and taking into account that $y_i^{[n-1]} \approx h^{i-1}y^{(i-1)}(x_{n-1})$, we have

$$\begin{aligned} h^{i-1}y^{(i-1)}(x_{n-1}) &= SN(\xi_i, y, y') \\ &= 0 \cdot y(x_{n-1}) + 0 \cdot hy'(x_{n-1}) + \dots + \frac{h^{i-1}}{(i-1)!} \xi_i y^{(i-1)}(x_{n-1}) + \dots \end{aligned}$$

Thus, by comparison of the left and right-hand sides, we get (2.43).

The values of $E\xi(t)$ can be again computed by means of Taylor series expansion and are reported in Table 2.10. Such values are useful in order to provide order conditions specialized to the Nordsieck case [20, 71, 82, 99], i.e.

$$\mathbf{e}_1 + 3\mathbf{e}_2 + 6\mathbf{e}_3 + 6\mathbf{e}_4 = 6(\mathbf{Bc} + \mathbf{Ve}_4)$$

for order 2,

$$\mathbf{e}_1 + 4\mathbf{e}_2 + 12\mathbf{e}_3 + 24\mathbf{e}_4 + 24\mathbf{e}_5 = 12(\mathbf{B}\eta(\circ) + 2\mathbf{V}\mathbf{e}_5)$$

for order 3,

$$\mathbf{e}_1 + 5\mathbf{e}_2 + 20\mathbf{e}_3 + 60\mathbf{e}_4 + 120\mathbf{e}_5 + 120\mathbf{e}_6 = 20(\mathbf{B}\eta(\mathfrak{I}) + 6\mathbf{V}\mathbf{e}_6)$$

for order 4, with

$$\begin{aligned}\eta(\circ) &= 2(\mathbf{A}\mathbf{e} + \mathbf{U}\mathbf{e}_3), \\ \eta(\mathfrak{I}) &= 6(\mathbf{A}\mathbf{c} + \mathbf{U}\mathbf{e}_4),\end{aligned}$$

being \mathbf{e} the vector of ones in \mathbb{R}^s .

The notions of consistency for GLN methods (2.14) can be given in terms of operators of rooted trees.

Definition 2.2.1. A GLN method (2.1) is *consistent* if

$$\begin{aligned}\mathbf{U}\xi(\emptyset) &= \mathbf{e}, & \mathbf{V}\xi(\emptyset) &= E\xi(\emptyset), \\ \mathbf{U}\xi(\bullet) &= \mathbf{c}, & \mathbf{V}\xi(\bullet) &= E\xi(\bullet), \\ 2\mathbf{B}\mathbf{e} + \mathbf{V}\xi(\circ) &= E\xi(\circ).\end{aligned}\tag{2.44}$$

2.2.5 Error Analysis for GLNs in Nordsieck Form

Following the lines drawn in [21, 22, 11, 82] for the first order case, we now analyze the local discretization error associated to GLN methods (2.14), whose vector of external stages is given by the Nordsieck vector (2.42). Correspondingly, denoted by $\mathbf{e}_j = [e_{i,j}]_{i=1}^r$, $j = 1, \dots, r$, the vectors of the canonical basis in \mathbb{R}^r . Since we are approximating the Nordsieck at each step, we define the vectors $\tilde{\mathbf{y}}^{[n-1]}, \tilde{\mathbf{y}}^{[n]} \in \mathbb{R}^{rd}$ of the local solutions by

$$\begin{aligned}\tilde{\mathbf{y}}_i^{[n-1]} &= e_{i,0}y(x_{n-1}) + e_{i,1}hy'(x_{n-1}) + \dots + e_{i,p}h^p y^{(p)}(x_{n-1}), \\ \tilde{\mathbf{y}}_i^{[n]} &= e_{i,0}y(x_n) + e_{i,1}hy'(x_n) + \dots + e_{i,p}h^p y^{(p)}(x_n).\end{aligned}$$

Thus, the local discretization error associated to the i -th external stage of (2.14) is given by

$$le_i(x_n) = \tilde{\mathbf{y}}_i^{[n]} - h^2 \sum_{j=1}^s b_{ij} f(\tilde{\mathbf{Y}}_j^{[n]}) - \sum_{j=1}^r v_{ij} \tilde{\mathbf{y}}_j^{[n-1]}, i = 1, 2, \dots, r,\tag{2.45}$$

being

$$\tilde{\mathbf{Y}}_i^{[n]} = h^2 \sum_{j=1}^s a_{ij} f(\tilde{\mathbf{Y}}_j^{[n]}) - \sum_{j=1}^r u_{ij} \tilde{\mathbf{y}}_j^{[n-1]}, i = 1, 2, \dots, s.\tag{2.46}$$

The following result holds.

Theorem 2.2.2. For the numerical solution of the (2.10), with f globally Lipschitz, consider a GLN method (2.1) of order p and stage order q . Denoted by \mathbf{I} the identity matrix in $\mathbb{R}^{r \times r}$, the local truncation error associated to the grid point x_n is given by

$$le(x_n) = (\phi_p \otimes \mathbf{I})h^{p+1}y^{(p+1)}(x_{n-1}) + O(h^{p+2}), \quad (2.47)$$

if $q = p$ or $q = p - 1$ where

$$\phi_p = \sum_{k=1}^{p+1} \frac{\mathbf{e}_{p+1-k}}{k!} - \frac{\mathbf{B}\mathbf{c}^{p-1}}{(p-1)!}.$$

Proof. We observe that, due to the fact that the method (2.1) has stage order q ,

$$y(x_{n-1} + c_i h) = h^2 \sum_{j=1}^s a_{ij} f(y(x_{n-1} + c_j h)) + \sum_{j=1}^r u_{ij} \tilde{y}_j^{[n-1]} + \zeta_i(h), \quad (2.48)$$

where

$$\zeta_i(h) = \begin{cases} O(h^{p+1}), & \text{if } q = p, \\ O(h^p), & \text{if } q = p - 1. \end{cases} \quad (2.49)$$

Subtracting (2.48) from (2.46), we obtain

$$\tilde{Y}_i^{[n]} - y(x_{n-1} + c_i h) = h^2 \sum_{j=1}^s a_{ij} \left(f(\tilde{Y}_i^{[n]}) - f(y(x_{n-1} + c_j h)) \right) - \zeta_i(h), \quad i = 1, \dots, s.$$

Supposing that $L > 0$ is the Lipschitz constant of f , we have

$$\left\| \tilde{Y}^{[n]} - y(x_{n-1} + \mathbf{c}h) \right\| \leq h^2 L \|\mathbf{A}\| \left\| \tilde{Y}^{[n]} - y(x_{n-1} + \mathbf{c}h) \right\| + \|\zeta(h)\|,$$

i.e.

$$(1 - h^2 L \|\mathbf{A}\|) \left\| \tilde{Y}^{[n]} - y(x_{n-1} + \mathbf{c}h) \right\| \leq \|\zeta(h)\|,$$

where $y(x_{n-1} + \mathbf{c}h) = [y(x_{n-1} + c_i h)]_{i=1}^s$. We assume that h_0 is a real number such that

$$h_0 L \|\mathbf{A}\| < 1.$$

Hence, for any $h^2 \leq h_0$,

$$\left\| \tilde{Y}^{[n]} - y(x_{n-1} + \mathbf{c}h) \right\| \leq \frac{\|\zeta(h)\|}{1 - h_0 L \|\mathbf{A}\|}.$$

Consequently, for (2.49),

$$\left\| \tilde{Y}^{[n]} - y(x_{n-1} + \mathbf{c}h) \right\| = \begin{cases} O(h^{p+1}), & \text{if } q = p, \\ O(h^p), & \text{if } q = p - 1. \end{cases}$$

In the case $q = p$, inserting $\tilde{Y}^{[n]} = y(x_{n-1} + c_i h) + O(h^{p+1})$ into (2.45), we obtain

$$\sum_{k=0}^p e_{i,k} h^k y^{(k)}(x_n) = h^2 \sum_{j=1}^s b_{ij} y''(x_{n-1} + c_j h) + \sum_{j=1}^r \sum_{k=0}^p v_{ij} e_{jk} h^k y^{(k)}(x_{n-1}) - le_i(x_n).$$

Expanding $y^{(k)}(x_n)$ and $y''(x_{n-1} + c_j h)$ in Taylor series around x_{n-1} and collecting in powers of h , we get

$$\begin{aligned} \sum_{k=0}^p \left(\sum_{l=0}^k \frac{k!}{l!} e_{i,k-l} - \sum_{j=1}^s (k(k-1)) b_{ij} c_j^{k-2} - \sum_{j=1}^r k! v_{ij} e_{jk} \right) \frac{h^k}{k!} y^{(k)}(x_{n-1}) + \\ + \left(\sum_{l=1}^{p+1} \frac{e_{i,p+1-l}}{l!} - \sum_{j=1}^s \frac{b_{ij} c_j^{p-1}}{(p-1)!} \right) h^{p+1} y^{(p+1)}(x_{n-1}) = l e_i(x_n) + O(h^{p+2}). \end{aligned}$$

If $q = p$ or $q = p - 1$, all the terms up to order $O(h^p)$ vanish (compare [49]), and the local truncation error takes the form

$$l e_i(x_n) = \left(\sum_{l=1}^{p+1} \frac{e_{i,p+1-l}}{l!} - \sum_{j=1}^s \frac{b_{ij} c_j^{p-1}}{(p-1)!} \right) h^{p+1} y^{(p+1)}(x_{n-1}) + O(h^{p+2}),$$

that is equivalent to (2.47). \square

An alternative proof of Theorem 2.2.2 can be given using SN series (2.16) and is reported here

Proof. The expression of $l e(x_n)$ given in (2.45) is equivalent to (compare Theorem 2.2.1)

$$l e(x_n) = \tilde{y}(x_n) - y^{[n]} = SN(E\xi, y, y') - SN(\mathbf{B}\bar{\eta} + \mathbf{V}\xi, y, y') = SN(E\xi - \mathbf{B}\bar{\eta} - \mathbf{V}\xi, y, y').$$

Exploiting the series expression we obtain

$$l e(x_n) = \sum_{t \in SNT} \frac{h^{\rho(t)}}{\rho(t)!} \alpha(t) (E\xi(t) - \mathbf{B}\bar{\eta}(t) - \mathbf{V}\xi(t)) F(t)(y, y')$$

and due to the hypothesis of order p , all the terms corresponding to the trees of order less or equal to p disappear, providing

$$l e(x_n) = \sum_{\rho(t)=p+1} \frac{h^{\rho(t)}}{\rho(t)!} \alpha(t) (E\xi(t) - \mathbf{B}\bar{\eta}(t) - \mathbf{V}\xi(t)) F(t)(y, y') + O(h^{p+2}). \quad (2.50)$$

The coefficients $E(\xi)(t)$ and $\xi(t)$ depend only on $\rho(t) = p + 1$ and not on the specific considered tree (compare (2.43) and Table 2.10). We observe that also $\bar{\eta}(t)$ enjoy this property, since, assuming that $t = [t_1, t_2, \dots, t_k]$ (see [51])

$$\bar{\eta}(t) = \rho(t)(\rho(t) - 1)\eta(t_1)\eta(t_2) \dots, \eta(t_k),$$

and being $\rho(t_j) \leq p - 1, j = 1, \dots, k$, due to the high stage order hypothesis we have

$$\bar{\eta}(t) = \rho(t)(\rho(t) - 1)\mathbf{c}^{\rho(t_1)}\mathbf{c}^{\rho(t_2)} \dots, \mathbf{c}^{\rho(t_k)} = p(p+1)\mathbf{c}^{p-1}.$$

Substituting this expression in (2.50) we obtain

$$l e(x_n) = \frac{h^{p+1}}{(p+1)!} (E\xi(t_{p+1}) - \mathbf{B}p(p+1)\mathbf{c}^{p-1} - (p+1)!\mathbf{V}\mathbf{e}_{p+1}) \\ \sum_{\rho(t)=p+1} \alpha(t) F(t)(y, y') + O(h^{p+2})$$

which is equivalent to the thesis if $r = p + 1$. \square

2.2.6 Highly-stable GLNs

In [49], the authors constructed an example of P-stable GLN method of order 3 and stage-order 2 with a reduced computational cost with respect to the corresponding traditional methods, proving the efficacy of this numerical schemes and their usefulness not only as a general theoretical framework, but also in the practical solution of problems. P-stable methods can be effectively used in the numerical approach to periodic-stiff problems (see [49] and references therein), that are characterized by periodic solutions with low short and large frequencies requiring a very small integration stepsize if approached with generic integrators. P-stable methods, by their definition, are able to overcome this limitation, since the choice of the stepsize is independent from the values of the frequencies, but it only depends on the desired accuracy.

We recall here the definition of P-stability (see [49]), also if in the following we won't directly apply it, but we will use a strategy to overcome it. In order to provide the definition of P-stability, we need to introduce the basic concepts of linear stability analysis, starting from the stability matrix

$$\mathbf{M}(z^2) = \mathbf{V} - z^2 \mathbf{B} \mathbf{A} \mathbf{U}, \quad (2.51)$$

with $\mathbf{\Lambda} = (\mathbf{I} + z^2 \mathbf{A})^{-1}$, which is obtained following the canonical procedure, i.e. applying the GLN method (2.14) to the scalar linear test equation (compare [87])

$$y'' = -\lambda^2 y.$$

We also consider the characteristic polynomial $p(\omega, z^2)$ of (2.51) also referred to as the stability polynomial of (2.14).

We get to the definition of P-stable GLN through a few steps

Definition 2.2.2. $(0, \beta^2)$ is a **stability interval** for the GLN (2.14) if, $\forall z^2 \in (0, \beta^2)$, the spectral radius $\rho(M(z^2))$ of the matrix $M(z^2)$ satisfies

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

Definition 2.2.3. A GLN is A - stable if $(0, \beta^2) = (0, +\infty)$.

If the eigenvalues of the stability matrix (or, equivalently, 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 2.2.4. $(0, H_0^2)$ is a periodicity interval for the method (2.14) if, $\forall z^2 \in (0, H_0^2)$, the stability polynomial $p(\omega, z^2)$ has two complex conjugate roots of modulus 1, while all the others have modulus less than 1.

Definition 2.2.5. A GLN is P - stable if its periodicity interval is $(0, +\infty)$.

We introduce the method whose matrices of coefficients are

$$\left[\begin{array}{c|cccc} \mathbf{A} & \mathbf{U} \\ \mathbf{B} & \mathbf{V} \end{array} \right] = \left[\begin{array}{c|cccc} \frac{1}{4} & 1 & \frac{2-\sqrt{2}}{2} & \frac{1-\sqrt{2}}{2} & \frac{1-\sqrt{2}}{6} \\ \frac{3+2\sqrt{2}}{6} & 1 & 1 & -\frac{\sqrt{2}}{3} & -\frac{\sqrt{12}}{12} \\ \frac{5+3\sqrt{2}}{6} & 0 & 1 & \frac{1-3\sqrt{2}}{6} & \frac{2-\sqrt{2}}{12} \\ \frac{2+2\sqrt{2}}{2} & 0 & 0 & -\frac{\sqrt{2}}{2} & \frac{1}{2} \\ 1 & 0 & 0 & -1 & \frac{\sqrt{2}}{2} \end{array} \right], \quad (2.52)$$

with $c = \frac{2-\sqrt{2}}{2}$ and we briefly review here the technique used for its construction. The first step is to show the general form of a convergent hybrid GLN method (2.14) in Nordsieck form. To this purpose, we recall the definition of zero-stability given in [45]

Definition 2.2.6. A GLN method (2.1) is zero-stable if the roots of the minimal polynomial of the \mathbf{V} matrix lie on or within the unit circle and the multiplicity of the zeros on the unit circle is at most two.

The following convergence result holds.

Theorem 2.2.3. A GLN method (2.14) with input vector $y^{[n]}$ defined as in (2.42) is convergent if it has the form

$$\left[\begin{array}{c|ccc} \mathbf{A} & \mathbf{e} & \mathbf{c} & \frac{c^2}{2} - \mathbf{A}\mathbf{e} & \tilde{U} \\ \hline \mathbf{B} & \mathbf{e}_1 & \mathbf{e}_1 + \mathbf{e}_2 & \frac{\mathbf{e}_1}{2} + \mathbf{e}_2 + \mathbf{e}_3 - \mathbf{B}\mathbf{e} & \tilde{V} \end{array} \right] \quad (2.53)$$

with $\tilde{U} \in \mathbb{R}^{s \times (r-3)}$, $\tilde{V} \in \mathbb{R}^{r \times (r-3)}$ and all the eigenvalues of \bar{V} have modulus strictly less than 1, where \bar{V} is obtained by the matrix \mathbf{V} removing its first two rows and columns.

Proof. We are allowed to study the convergence of GLN methods by consistency and zero-stability analysis (compare [45]). Due to the nature (2.42) of the input vectors, we have

$$\xi(\emptyset) = \mathbf{e}_1, \quad \xi(\bullet) = \mathbf{e}_2, \quad \xi(\circ) = 2\mathbf{e}_3,$$

where $\mathbf{e}_1, \mathbf{e}_2$ and \mathbf{e}_3 are the first three vectors of the canonical basis in \mathbb{R}^r . The vectors $E\xi(\emptyset), E\xi(\bullet)$ and $E\xi(\circ)$ respectively assume the form $\mathbf{e}_1, \mathbf{e}_1 + \mathbf{e}_2, \mathbf{e}_1 + 2\mathbf{e}_2 + 2\mathbf{e}_3$. Taking into account these expressions of the mentioned vectors, the consistency conditions (2.44) give the expression (2.53) of the Butcher tableau. Correspondingly, the matrix \mathbf{V} assumes the form

$$\mathbf{V} = \left[\begin{array}{cc|cc} 1 & 1 & \frac{1}{2} - \sum_{i=1}^s b_{1i} & \tilde{v}_1 \\ 0 & 1 & 1 - \sum_{i=1}^s b_{2i} & \tilde{v}_2 \\ \hline \emptyset & \emptyset & & \\ \vdots & \vdots & \bar{V} & \\ 0 & 0 & & \end{array} \right],$$

where \tilde{v}_1 and \tilde{v}_2 are the first two rows of the matrix \tilde{V} . Hence, the matrix \mathbf{V} is block upper triangular, with a 2×2 block having eigenvalues 1 with multiplicity 2. As a consequence, the method is zero-stable if the eigenvalues of \bar{V} have moduli strictly less than 1, which completes the proof. \square

Theorem 2.2.3 gives us a starting framework to construct convergent methods in Nordsieck form. The further steps that are necessary to obtain method (2.52) are

- to impose the order and stage-order conditions up to order 3 and 2 respectively;

- to require the method being P-stable.

We consider the stability polynomial of the RK Nyström one-stage collocation method of Gauss-Legendre, that is

$$q(\omega, z^2) = \omega^2 + \frac{-8 + 2z^2}{4 + z^2}\omega + 1$$

and, being p the stability polynomial of the GLN we introduced above, we impose that

$$p(\omega, z^2) = q(\omega, z^2) * r(\omega, z^2)$$

in such a way that p has the same roots of q plus the roots of r . Requiring the roots of r to be strictly less than 1 in modulus, we achieve the desired property.

2.3 A note on the Parallel Solution of the Radial Schrödinger Equation

This Section deals with the parallel implementation of a family of methods, namely the family of Constant Piecewise (CP) methods, specifically designed for the numerical solution of the radial Schrödinger equation (1.11)

$$y'' + (E - V(x))y = 0.$$

These methods have been introduced by L. Gr. Ixaru (compare [79, 80, 81]) and further studied by V. Ledoux, M. Van Daele and G. Vanden Berghe (see [91, 92, 92, 94]). The idea behind CP methods is to use the perturbation technique to construct the numerical approximation of the solution of (1.11), whose importance in modern physics has already been discussed.

The novelty we propose in this Section is a parallel implementation of such methods. Parallel computing is an established and important reality in modern science, allowing to solve computationally expensive problems in shorter time, thus also saving the money needed to keep the supercomputers working. In recent times, this research stream obtained new lymph with the advent of multicore technology, which proved to be cheaper and more efficient than traditional parallel computing environments.

2.3.1 Methods Review

We focus our attention on the initial value problem for the radial Schrödinger equation

$$\begin{cases} y''(x) + (E - V(x))y(x) = 0, & x \in [a, b] \\ y(a) = y_0 \\ y'(a) = y'_0. \end{cases} \quad (2.54)$$

The function V is called *potential* of the problem, while the constant value E is known as the *energy*.

For the numerical solution of (2.54), we consider a partition of the interval $[a, b]$, namely we fix K grid-points

$$x_0 = a, < x_1 < x_2 < \dots < x_K = b$$

and denote with I_k the sub-interval $[x_{k-1}, x_k]$. Following [79, 80], in the generic subinterval, which we will denote with $I = [X, X + h]$, we advance the solution by means of the so-called *propagation matrix algorithm*

$$\begin{bmatrix} y(X + h) \\ y'(X + h) \end{bmatrix} = \begin{bmatrix} u(h) & v(h) \\ u'(h) & v'(h) \end{bmatrix} \begin{bmatrix} y(X) \\ y'(X) \end{bmatrix} \quad (2.55)$$

where the functions u and v are the solutions of the local problem

$$y''(\delta) + (E - V(\delta))y(\delta) = 0$$

respectively with initial values $y(0) = 1, y'(0) = 0$ and $y(0) = 0, y'(0) = 1$.

The perturbation technique plays its role in the approximation of the u and v functions, since we approximate the original potential V as

$$V(X + \delta) = \bar{V} + \Delta V(\delta)$$

where

$$\bar{V} = \frac{1}{h} \int_0^h V(X + \delta) d\delta \quad (2.56)$$

and

$$\Delta V(\delta) = V(X + \delta) - \bar{V}.$$

At this step, we consider \bar{V} , that is a constant, as the reference potential and $\Delta V(\delta)$ as a perturbation. We show the construction of the approximations of the u function with this technique, since it is analogous for v . We aim to write u as a perturbation series

$$u(\delta) = u_0(\delta) + u_1(\delta) + u_2(\delta) + \dots$$

where u_0 is the solution of

$$u''(\delta) + (E - \bar{V})u(\delta) = 0 \quad (2.57)$$

with initial values $u(0) = 1, u'(0) = 0$ and the so-called *correction terms* $u_i, i = 1, 2, \dots$ are obtained as the solution of the refined problem

$$u_i''(\delta) + (E - \bar{V})u_i(\delta) + \Delta V(\delta)u_{i-1} = 0, \quad u_i(0) = u_i'(0) = 0 \quad (2.58)$$

In practice each term is the solution to a perturbed problem that is closer and closer to the original one. Problems (2.57) and (2.58) can be solved analytically (compare [79, 80, 91]) but are found to depend on repeated integrals of the potential V evaluated in $X + \delta$. At this step, in order to simplify the calculations, we approximate the potential with an opportunely truncated series of shifted Legendre polynomials $P_n^*(\frac{\delta}{h})$, namely

$$V(X + h) = \sum_{n=0} V_n h^n P_n^*\left(\frac{\delta}{h}\right) \quad (2.59)$$

being $V_0 = \bar{V}$ and

$$V_i = 2(i + 1)h \int_0^h V(X + \delta) P_i^*\left(\frac{\delta}{h}\right) d\delta \quad i = 1, 2, \dots \quad (2.60)$$

The terms are then recombined to construct the approximation of the u and v functions and the (2.55) formula is used to advance the solution.

2.3.2 Parallel Implementation of the CP method

We report an algorithmic scheme for CP methods

- the integrals (2.59) and (2.60) are computed on each subinterval I_k by means of a Gauss quadrature formula;
- the integrals are then combined in order to obtain the approximations of u and v (compare [79, 92]);
- the matrix propagation algorithm (2.55) is used to advance the solution.

In practice, the huge part of the calculations is the computation of the integrals (2.59) and (2.60) that must be done on each interval, but it has only to be done at the beginning of the integration process, since each value is independent from the others and depends only on the potential and the Legendre polynomials, that are known. This part can be easily parallelized by opportunely splitting the work between various workers and, for example, we implemented such a strategy both in CUDA and OPENMP.

Chapter 3

Geometric Integration of First Order Problems

This Chapter deals with the numerical integration of ODEs which possess invariants and other geometric properties, such as symplecticity of the flow and symmetry. This topic attracted many researchers in recent times and a large amount of literature has been produced. In the early works of Cooper, Lasagni, Suris and Sanz-Serna [33, 88, 110, 113] a connection between the non-linear stability of Runge-Kutta methods and their ability to preserve quadratic invariants of ODEs has been found and the definition of symplectic RK method was given. Such methods found as a natural field of application the integration of Hamiltonian systems (1.13) and recently Sanz-Serna [111] found some new and interesting applications to other fields of Applied Mathematics. This Chapter begins with a brief introduction on some test problems, then the concept of G-symplecticity is introduced and applied to the construction of new and efficient GLMs. The last Section presents numerical results and comparison with existing methods.

3.1 A short collection of test problems

The main category of problems that are addressed in this Chapter is that of Hamiltonian systems, already introduced in Section 1.3. For the reader's ease, we report here the general form of an Hamiltonian problem

$$\begin{aligned}\dot{p}(t) &= -\frac{\partial}{\partial q}\mathcal{H}(p(t), q(t)), \\ \dot{q}(t) &= \frac{\partial}{\partial p}\mathcal{H}(p(t), q(t)),\end{aligned}\tag{3.1}$$

where $\mathcal{H} : \mathbb{R}^{2d} \rightarrow \mathbb{R}$ is the Hamiltonian of the system, $p(t), q(t) \in \mathbb{R}^d$ are generalized momenta and coordinates, respectively. In this Section we report a short collection of test problems that will be useful throughout the Chapter, both for examples and for numerical experiments.

- the simple pendulum problem

$$\begin{cases} \dot{p}(t) = -\sin q(t), & t \in [0, 50] \\ \dot{q}(t) = p(t), \\ p(0) = 0, & q(0) = 2.3, \end{cases} \quad (3.2)$$

whose Hamiltonian exhibits the form

$$H(p(t), q(t)) = \frac{p^2(t)}{2} - \cos q(t);$$

- the Kepler problem [70]

$$\begin{cases} \dot{p}_1(t) = -\frac{q_1(t)}{(q_1^2(t) + q_2^2(t))^{\frac{3}{2}}}, \\ \dot{p}_2(t) = -\frac{q_2(t)}{(q_1^2(t) + q_2^2(t))^{\frac{3}{2}}}, \\ \dot{q}_i(t) = p_i(t), & i = 1, 2, \\ p_1(0) = 0, & p_2(0) = \sqrt{\frac{1+e}{1-e}}, & q_1(0) = 1 - e, & q_2(0) = 0, \end{cases} \quad (3.3)$$

where the value of the eccentricity $e \in [0, 1[$ is fixed to $\frac{1}{2}$. The Hamiltonian of this problem is

$$\mathcal{H}(p(t), q(t)) = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}};$$

- the Hènon-Heiles Problem [70]

$$\begin{cases} \dot{p}_1(t) = -q_1(t)(1 + 2q_2(t)), & t \in [0, 50] \\ \dot{p}_2(t) = -(q_2(t) + q_1^2(t) - q_2^2(t)), \\ \dot{q}_i(t) = p_i(t), & i = 1, 2, \\ p_1(0) = \sqrt{0.3185}, & p_2(0) = q_1(0) = q_2(0) = 0, \end{cases} \quad (3.4)$$

with Hamiltonian

$$H(p(t), q(t)) = \frac{1}{2}(p_1^2 + p_2^2 + q_1^2 + q_2^2) + q_1^2 q_2 - \frac{1}{3} q_2^3.$$

;

- the planar three-body problem

$$\begin{cases} \dot{p}_i(t) = \sum_{j \neq i} \frac{q_i - q_j}{r_{ij}^3}, & i = 1, 2, 3, \\ \dot{q}_i(t) = p_i(t), & i = 1, 2, 3, \end{cases} \quad (3.5)$$

with $r_{ij} = \|q_i - q_j\|_2$, describing the motion of three coplanar bodies having unitary mass under a Newtonian gravitational force field. The Hamiltonian of this problem assumes the form

$$\mathcal{H}(p(t), q(t)) = \sum_{i=1}^3 \frac{1}{2} p_i^\top p_i - \sum_{i < j} \frac{1}{r_{ij}}.$$

We consider the initial conditions computed by Carles Simó (compare [25])

$$\begin{aligned} p_1(0) &= [0.46620368, 0.43236573]^\top, & q_1(0) &= [0.97000436, -0.24308753]^\top, \\ p_2(0) &= [0.46620368, 0.43236573]^\top, & q_2(0) &= [-0.97000436, 0.24308753]^\top, \\ p_3(0) &= [-0.93240737, -0.86473146]^\top, & q_3(0) &= [0, 0]^\top, \end{aligned}$$

which provides a figure-of-eight orbit;

- the non-separable problem whose Hamiltonian is given by

$$\mathcal{H}(p(t), q(t)) = \frac{p^2}{2(1 + U'(q)^2)} + U(q), \quad U(q) = 0.1(q(q-2))^2 + 0.008q^3, \quad (3.6)$$

with initial values

$$p(0) = 0.49, \quad q(0) = 0,$$

describing the path of a particle of unit mass moving on a wire of shape $U(q)$ [3];

- the non-reversible problem [58]

$$\begin{cases} \dot{p}(t) = -\frac{q(t)^5}{5} - q(t)^3 + q(t)^2, \\ \dot{q}(t) = p(t)^2 - \frac{1}{2}, \\ p(0) = 1, \quad q(0) = 0, \end{cases} \quad (3.7)$$

whose Hamiltonian function is

$$\mathcal{H}(p(t), q(t)) = \frac{p(t)^3}{3} - \frac{p(t)}{2} + \frac{q(t)^6}{30} + \frac{q(t)^4}{4} - \frac{q(t)^3}{3} + \frac{1}{6}.$$

3.2 G-symplecticity

Canonical methods are designed to preserve quadratic invariants exactly up to the round-off error, but this nice property is a privilege of RK methods: in fact Butcher and Hewitt [13] proved that if a GLM is symplectic, than it can be reduced to a canonical RK method (see also [114] for LMM). In order to analyze the geometric properties of GLMs, a weaker condition of preservation needs to be considered. The following definition was introduced by Hairer (see for example the monograph [70])

Definition 3.2.1. A GLM $(\mathbf{c}, \mathbf{A}, \mathbf{U}, \mathbf{B}, \mathbf{V})$ is **G-symplectic** if and only if there exist a symmetric semi-positive definite $r \times r$ matrix \mathbf{G} and a diagonal $s \times s$ matrix \mathbf{D} such that

$$\begin{cases} \mathbf{G} = \mathbf{V}^T \mathbf{G} \mathbf{V} \\ \mathbf{D} \mathbf{U} = \mathbf{B}^T \mathbf{G} \mathbf{V} \\ \mathbf{D} \mathbf{A} + \mathbf{A}^T \mathbf{D} = \mathbf{B}^T \mathbf{G} \mathbf{B}. \end{cases} \quad (3.8)$$

This definition is motivated by the following [67]

Theorem 3.2.1. A G-symplectic GLM satisfies

$$\|y^{[n]}\|_G = \|y^{[n-1]}\|_G + 2h \sum_{i=1}^s d_i \langle Y_i, F_i \rangle \quad (3.9)$$

where the norm in (3.9) is defined as

$$\|y\|_G^2 = \sum_{i=1}^r \sum_{j=1}^r g_{ij} y_i^T y_j. \quad (3.10)$$

Proof. We prove that, for a G-symplectic method

$$\langle y^{[n]}, y^{[n]} \rangle_G - \langle y^{[n-1]}, y^{[n-1]} \rangle_G - 2h \sum_{i=1}^s d_i \langle Y_i, F_i \rangle = 0. \quad (3.11)$$

Considering the expressions of $y^{[n]}$ and $y^{[n-1]}$ given by a GLM, (3.11) becomes

$$\begin{aligned} & \sum_{i,j=1}^r g_{ij} \langle \mathbf{B}hF_i + \mathbf{V}y_i^{[n-1]}, \mathbf{B}hF_j + \mathbf{V}y_j^{[n-1]} \rangle - \\ & \quad - \sum_{i,j=1}^r g_{ij} \langle y_i^{[n-1]}, y_j^{[n-1]} \rangle - \\ & \quad - 2h \sum_{i=1}^s d_i \langle \mathbf{A}hF_i + \mathbf{U}y_i^{[n-1]}, F_i \rangle \end{aligned}$$

and using the properties of the scalar product

$$\begin{aligned} & - [\mathbf{G} - \mathbf{V}^T \mathbf{G} \mathbf{V}] \langle y_i^{[n-1]}, y_j^{[n-1]} \rangle - \\ & - [\mathbf{D} \mathbf{U} - \mathbf{B}^T \mathbf{G} \mathbf{V}] \langle y_i^{[n-1]}, hF_j \rangle - \\ & - [\mathbf{D} \mathbf{A} + \mathbf{A}^T \mathbf{D} - \mathbf{B}^T \mathbf{G} \mathbf{B}] \langle hF_i, hF_j \rangle \end{aligned}$$

that is zero. □

This Theorem provides that a G-symplectic GLM preserves the invariants of a problem in the G-norm, in fact if we consider a problem such that

$$\langle y, f(y) \rangle = 0,$$

(3.9) provides

$$\|y^{[n]}\|_G = \|y^{[n-1]}\|_G.$$

Remark 3.2.1. We observe that, as shown in [11], the G-symplecticity conditions given above are obtained considering the algebraic stability matrix of the GLM and imposing it to be zero, imitating the profile revealed while studying the geometric properties of RK methods introduced in Section 1.9.

An example of G-symplectic method was given in [11]

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \mathbf{B} & \mathbf{V} \end{array} \right] = \left[\begin{array}{cc|cc} \frac{3+\sqrt{3}}{6} & 0 & 1 & -\frac{3+2\sqrt{3}}{3} \\ -\frac{\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} & 1 & \frac{3+2\sqrt{3}}{3} \\ \hline \frac{1}{2} & \frac{1}{2} & 1 & 0 \\ \frac{1}{2} & -\frac{1}{2} & 0 & -1 \end{array} \right] \quad (3.12)$$

that is G-symplectic with

$$G = \begin{pmatrix} 1 & 0 \\ 10 & 1 + \frac{2}{3}\sqrt{3} \end{pmatrix}, \quad D = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}.$$

3.2.1 Parasitism

It is known from the literature (compare [12, 70]) that the long-term behaviour of multistep and/or multivalued methods is corrupted by parasitic components introduced in the numerical solution. The presence of these components is mainly due to the fact that such methods are notoriously not self-starting, thus they require the employ of starting procedures to recover the missing initial values.

Hairer et al. (compare [70] and references therein) analyzed this phenomenon for multistep methods. This study subsequently led them to retain that the numerical solution of a GLM admits the representation (compare [70], §XV.8.3)

$$y^{[n]} = \tilde{y}(t_n) + \sum_{\ell \in I^*} \zeta_\ell^n z_\ell(t_n),$$

where $\tilde{y}(t)$, $z(t)$ are smooth functions and I^* is an index set (see [69]). In this representation, the numerical solution is expressed as summation of two terms: the first summand is the exact solution of the associated modified equation (compare [68, 69]), while the second one is the actual parasitic part of the numerical solution. Such a parasitic part is equal to zero for canonical Runge–Kutta methods, while it does not annihilate for non-symplectic methods and it is responsible of their non-conservative behaviour. Maintaining such parasitic terms bounded is then the first necessary task for the derivation of multistep or multivalued methods with a reliable long-term behaviour (compare [12, 36, 67, 70]).

Butcher (compare [12] and references therein) proposes two different approaches for the control of the parasitic components. The first one, for GLMs with $r = 2$ and $V = \text{diag}(1, -1)$, assures the boundedness of the parasitic components by imposing an algebraic constraint on the coefficients of the method, i.e. $\mu = (BU)_{22} = 0$. In the second approach, a reduction of the effects of parasitism is obtained by composing two G-symplectic methods N and P, both having $\mu \neq 0$: the numerical scheme computes m steps of the method N and one single step of P, in such a way that, after $m + 1$ steps, the sum of the scaled values of μ is exactly cancelled.

We now extend the result reported in [12] (also compare [67]), connected to the first approach by Butcher above discussed, by providing a general algebraic

constraint on the coefficients of a GLM in order to make the parasitic components in the numerical approximation bounded. In the following, we will always denote by \dot{X} , the matrix obtained by removing the first row and the first column of X .

Theorem 3.2.2. The parasitic components of a GLM (2.1) are bounded if \dot{V} is power-bounded and $\dot{B}\dot{U}$ is the zero matrix.

Proof. We assume, without loss of generality, that the first component of the vector $y^{[n]}$ is an approximation to $y(t_n)$. Then, we introduce on the external approximation $y_i^{[n]}$, $i = 2, \dots, r$, the perturbation $(-1)^n \lambda_i^{[n]}$ and analyze how it propagates along the overall numerical scheme.

We first analyze the influence of the propagations on the internal stages

$$Y_i + \delta Y_i = h \sum_{j=1}^s a_{ij} F_j^{[n]} + u_{i1} y_1^{[n]} + \sum_{j=2}^r u_{ij} \left(y_j^{[n]} + (-1)^n \lambda_j^{[n]} \right),$$

obtaining

$$\delta Y_i = (-1)^n \sum_{j=2}^r u_{ij} \lambda_j^{[n]}.$$

Similarly, for the stage derivatives F_i

$$F_i + \delta F_i = f(Y_i + \delta Y_i) \approx f(Y_i) + \delta Y_i \frac{\partial f}{\partial y},$$

we obtain

$$\delta F_i = \delta Y_i \frac{\partial f}{\partial y} = (-1)^n \sum_{j=2}^r u_{ij} \lambda_j^{[n]} \frac{\partial f}{\partial y}.$$

Thus, we get from (2.1) the difference equation

$$\lambda^{[n+1]} = -\dot{V} \lambda^{[n]} + h \dot{B}\dot{U} \frac{\partial f}{\partial y} \lambda^{[n]}, \quad (3.13)$$

where $\lambda = [\lambda_2, \dots, \lambda_r]^\top$. Due to the hypothesis, the solution of (3.13) is bounded and the result is given. \square \square

As a consequence, GLMs (2.1) with $r = 2$ produce bounded parasitic components if they satisfy the further constraint

$$\mu = \sum_{i=1}^2 b_{2i} u_{i2} = 0, \quad (3.14)$$

that recovers the result obtained in [12, 67].

3.3 Near conservation of invariants by B-series methods

One natural question that arises when studying geometric integration is the following: up to which accuracy does a non canonical method preserve geometric properties of ODEs? This Section gives a partial answer.

Let us consider the set of forests (compare [23] and references therein)

$$\mathcal{F} = \{\emptyset, \bullet, \bullet\bullet, \mathbf{!}, \bullet\bullet\bullet, \mathbf{!}\bullet, \mathbf{V}, \mathbf{!}, \dots\},$$

where a forest $u = t_1 \cdots t_n \in \mathcal{F}$ is given by the commutative juxtaposition of the rooted trees t_1, \dots, t_n .

Definition 3.3.1. Given a forest $u \in \mathcal{F}$ and denoted with \mathcal{D} the set $C^\infty(\mathbb{R}^n, \mathbb{R}^m)$, we define the following differential operator

$$\begin{aligned} X(u) : \mathcal{D} &\rightarrow \mathcal{D}, \\ g &\mapsto X(u)[g] = g^{(k)}(F(t_1), \dots, F(t_k)). \end{aligned}$$

The role of the operator X is crucial in the theorem contained in the following section, together with the composition rule (compare [23])

$$g \circ B(a, y) = \sum_{u \in \mathcal{F}} \frac{h^{\rho(u)}}{\sigma(u)} \alpha(u) X(u)[g],$$

where $g \in \mathcal{D}$, and

$$\alpha(\emptyset) = 1, \quad \alpha(t_1 \cdots t_n) = \prod_{i=1}^n a(t_i).$$

3.3.1 Accuracy of invariant conservation by non-parasitic B-series methods

The following theorem clarifies the role of the order of accuracy in the numerical conservation of the Hamiltonian of (3.1) by a B-series method with annihilated parasitic components, which is the case of Runge-Kutta methods. In the remainder of this section, with a slight abuse of notation, we denote the Hamiltonian of (3.1) by $\mathcal{H}(y(t))$, where

$$y(t) = \begin{bmatrix} p(t) \\ q(t) \end{bmatrix}.$$

Theorem 3.3.1. Consider an Hamiltonian problem (3.1) whose Hamiltonian function \mathcal{H} belongs to $C^\infty(\mathbb{R}^{2d}, \mathbb{R})$ and a B-series method of order p , with coefficients $b(t)$ and annihilated parasitic components. Then,

$$\mathcal{H}(y_1) = \mathcal{H}(y(t_0)) + O(h^{p+1}).$$

Proof. We consider the action of the map \mathcal{H} on the B-series of the exact solution $y(t_1)$ and the numerical one y_1 , i.e.

$$\mathcal{H}(y(t_1)) = \mathcal{H}(y(t_0)) + \sum_{\rho(u) \geq 1} \frac{h^{\rho(u)}}{\sigma(u)} \alpha(u) X(u) [\mathcal{H}], \quad (3.15)$$

$$\mathcal{H}(y_1) = \mathcal{H}(y(t_0)) + \sum_{\rho(u) \geq 1} \frac{h^{\rho(u)}}{\sigma(u)} \beta(u) X(u) [\mathcal{H}]. \quad (3.16)$$

In (3.15), since the Hamiltonian is constant along the exact solution of (3.1), we have

$$\sum_{\rho(u) \geq 1} \frac{h^{\rho(u)}}{\sigma(u)} \alpha(u) X(u) [\mathcal{H}] = 0.$$

Hence,

$$\sum_{1 \leq \rho(u) \leq p} \frac{h^{\rho(u)}}{\sigma(u)} \alpha(u) X(u) [\mathcal{H}] = - \sum_{\rho(u) > p} \frac{h^{\rho(u)}}{\sigma(u)} \alpha(u) X(u) [\mathcal{H}]. \quad (3.17)$$

The method has order p , so $\alpha(u) = \beta(u)$ for all forests u such that $\rho(u) \leq p$. Then, combining (3.16), (3.17) and the hypothesis of parasitism absence, we obtain

$$\begin{aligned} \mathcal{H}(y_1) - \mathcal{H}(y(t_0)) &= \sum_{1 \leq \rho(u) \leq p} \frac{h^{\rho(u)}}{\sigma(u)} \beta(u) X(u) [\mathcal{H}] + \sum_{\rho(u) > p} \frac{h^{\rho(u)}}{\sigma(u)} \beta(u) X(u) [\mathcal{H}] \\ &= - \sum_{\rho(u) > p} \frac{h^{\rho(u)}}{\sigma(u)} \alpha(u) X(u) [\mathcal{H}] + \sum_{\rho(u) > p} \frac{h^{\rho(u)}}{\sigma(u)} \beta(u) X(u) [\mathcal{H}] \\ &= O(h^{p+1}), \end{aligned} \quad (3.18)$$

that proves the statement. \square

Remark 3.3.1. We observe that the hypothesis of being the method non-parasitic is crucial in the proof of Theorem 3.3.1, because we notice in (3.18) the absence of further terms corrupting the accuracy of the Hamiltonian conservation. In other words, if a B-series method has order p and its parasitic components are annihilated, then the Hamiltonian is preserved up to order p .

3.3.2 The case of GLMs with bounded parasitic components

Section 3.3.1 deals with the ideal case of B-series methods free from parasitism, which is actually not the case of GLMs with bounded parasitic components. We now aim to check up to which order the Hamiltonian of problem (3.1) is preserved by a GLM of order p with bounded parasitic components, i.e. we are interested in determining the integer value α such that

$$\|e_n^{\mathcal{H}}\| = O(h^\alpha), \quad (3.19)$$

where

$$e_n^{\mathcal{H}} = \mathcal{H}(p_n, q_n) - \mathcal{H}(p_0, q_0) \quad (3.20)$$

is the Hamiltonian deviation observed in the n -th step point.

In order to address this issue, we derive the following three-stage symmetric and non G-symplectic GLM (2.1) of order 4

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array} \right] = \left[\begin{array}{ccc|cc} -\frac{41}{150} & \frac{19}{50} & -\frac{11}{25} & 1 & \frac{1}{12} \\ \frac{83}{1100} & \frac{11}{25} & -\frac{17}{1100} & 1 & \frac{1}{12} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{3} & 1 & \frac{1}{12} \\ \hline \frac{11}{600} & \frac{289}{300} & \frac{11}{600} & 1 & \frac{1}{6} \\ \frac{1}{2} & -1 & \frac{1}{2} & 0 & -1 \end{array} \right] \quad (3.21)$$

with abscissa vector $c = \left[-\frac{1}{3}, \frac{1}{2}, \frac{4}{3} \right]^T$ and having bounded parasitic components, because it satisfies the hypothesis of Theorem 3.2.2. We report in Tables 3.1 and 3.2 the numerical evidence obtained by comparing the observed values of α for the two-stage Gauss RK method (1.33) (which is a symplectic and symmetric (see Section 3.5) method of order 4), the three-stage Lobatto IIIA method (which is a symmetric method of order 4, but non-symplectic) and the GLM (3.21), when applied to the simple pendulum problem (3.2) and the Hènon-Heiles Problem (3.4)

Table 3.1: Observed values of α in (3.19) for the simple pendulum problem (3.2)

	Gauss	Lobatto IIIA	Symmetric GLM
$h = 1/2^3$			
$h = 1/2^4$	4.0016	4.0015	3.2903
$h = 1/2^5$	4.0004	4.0004	3.0328
$h = 1/2^6$	4.0001	4.0001	2.9843
$h = 1/2^7$	4.0025	3.9991	2.9843
$h = 1/2^8$	4.0124	4.0414	2.9905

Table 3.2: Observed values of α in (3.19) for the Hènon-Heiles problem (3.4)

	Gauss	Lobatto IIIA	Symmetric GLM
$h = 1/2^3$			
$h = 1/2^4$	3.9978	3.9978	4.3132
$h = 1/2^5$	3.9995	3.9995	3.8951
$h = 1/2^6$	3.9998	3.9998	3.5158
$h = 1/2^7$	3.9996	4.0008	3.2666
$h = 1/2^8$	4.0033	4.0067	3.1322

The result stated in Theorem 3.3.1 is confirmed by the numerical evidence in the case of Runge-Kutta methods, that are non-parasitic, i.e. α is equal to the order p of convergence of the methods. In the case of GLM (3.21), we notice that the observed value of α is no more equal to the order of convergence of the method, but it reduces to $\alpha = p - 1$, due to the fact that the parasitic components in the numerical solution are bounded but not completely removed, as suggested by Theorem 3.2.2.

3.4 Construction of G-symplectic GLMs

In this Section, a first experiment of construction of G-symplectic GLMs is reported. The methods constructed here present the advantage of not needing a starting procedure, since exact starting values can be computed by hand starting from the initial data provided by the problem. Together with minimal requirements of accuracy and stability, we enforce our methods to attain a certain order of convergence. In order to achieve this goal, we review the order conditions for GLMs (2.1) reported in [82], that provide a great simplification with respect to the order conditions depending

on trees given in (2.9), but have stronger requirements. We consider a GLM (2.1), whose input vector at the n -th step satisfies the condition

$$y_i^{[n]} = \sum_{k=0}^p q_{ik} h^k y^{(k)}(t_n) + O(h^{p+1}), \quad i = 1, 2, \dots, r, \quad (3.22)$$

being q_{ik} real parameters, $i = 1, 2, \dots, r$, $k = 0, 1, \dots, p$. Then, we also require the internal stages $Y_i^{[n]}$ to be approximations of order $q \geq p - 1$ of the solution in the points $t_n + c_i h$, i.e.

$$Y_i^{[n]} = y(t_n + c_i h) + O(h^{q+1}), \quad i = 1, 2, \dots, r. \quad (3.23)$$

We impose a condition similar to (3.22) also to the output approximations

$$y_i^{[n+1]} = \sum_{k=0}^p q_{ik} h^k y^{(k)}(t_{n+1}) + O(h^{p+1}), \quad i = 1, 2, \dots, r, \quad (3.24)$$

so that the integers p and q are respectively the order and stage-order of the method (compare Section 2.2.1). We denote by

$$\mathbf{q}_k = [q_{1k} \quad q_{2k} \quad \cdots \quad q_{rk}]^T \in \mathbb{R}^r, \quad k = 0, 1, \dots, p,$$

the vectors containing all the parameters q_{ik} appearing in (3.22) and (3.24). The following theorem holds (compare [82]).

Theorem 3.4.1. The GLM $(\mathbf{c}, \mathbf{A}, \mathbf{U}, \mathbf{B}, \mathbf{V})$ whose input vectors $y_i^{[n]}$ satisfy (3.22) has order p and stage-order $q = p$ if and only if

$$\sum_{l=0}^k \frac{\mathbf{q}_{k-l}}{l!} - \frac{\mathbf{B}c^{k-1}}{(k-1)!} - \mathbf{V}\mathbf{q}_k = 0, \quad k = 0, 1, \dots, p, \quad (3.25)$$

and

$$\frac{c^k}{k!} - \frac{\mathbf{A}c^{k-1}}{(k-1)!} - \mathbf{U}\mathbf{q}_k = 0, \quad k = 0, 1, \dots, q. \quad (3.26)$$

We observe that, for $k = 0, 1$, we recover conditions of preconsistency, consistency and stage-consistency. It is also easy to verify that these conditions can be recovered from (2.9) with the hypotheses that were made in this Section.

Remark 3.4.1. A similar result can be proved (compare [82]) also when the stage order is equal to $q = p - 1$: indeed, GLMs of order p and stage-order $q = p - 1$ satisfy the set of algebraic conditions

$$\begin{aligned} \sum_{l=0}^k \frac{\mathbf{q}_{k-l}}{l!} - \frac{\mathbf{B}c^{k-1}}{(k-1)!} - \mathbf{V}\mathbf{q}_k &= 0, \quad k = 0, 1, \dots, p, \\ \frac{c^k}{k!} - \frac{\mathbf{A}c^{k-1}}{(k-1)!} - \mathbf{U}\mathbf{q}_k &= 0, \quad k = 0, 1, \dots, p-1. \end{aligned}$$

High stage order is a desirable property since it avoids the effects of the order reduction phenomenon which typically arises in the numerical treatment of stiff problems via Runge-Kutta methods [11].

Remark 3.4.2. For a cheap solution of the nonlinear system in the internal stages to be computed at each step, we derive here methods with lower triangular or diagonal coefficient matrix \mathbf{A} . In fact (compare, for instance, [11, 72] and references therein), the integration of a d -dimensional system (1.4) via an implicit s stage GLM (2.1) requires the solution of a nonlinear system of equations of dimension sd at each time step. A lower triangular matrix allows to split the sd -dimensional nonlinear system in s successive subsystems of dimension d . Moreover, if all the elements on the diagonal are equal, in solving the nonlinear systems by means of Newton-type iterations, the stored LU factorization of the Jacobian can repeatedly be used.

We neglect the case $s = r = 2$ since, as proved in [67], such methods cannot be free from parasitism. So, we consider the case $s = 3$, $r = 2$ and assume that the external stage vector $y^{[n]}$ is an approximation to the Nordsieck vector (2.42)

$$\begin{bmatrix} y(t_n) \\ hy'(t_n) \end{bmatrix}.$$

Correspondingly, the preconsistency and consistency vectors \mathbf{q}_0 and \mathbf{q}_1 assume the forms

$$\mathbf{q}_0 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \mathbf{q}_1 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

Under these assumptions, the preconsistency conditions (2.4) imply that the matrices \mathbf{U} and \mathbf{V} have the form

$$\mathbf{U} = \begin{bmatrix} 1 & u_{12} \\ 1 & u_{22} \end{bmatrix}, \quad \mathbf{V} = \begin{bmatrix} 1 & v_{12} \\ 0 & v_{22} \end{bmatrix}.$$

We observe that the matrix \mathbf{V} satisfies the zero-stability requirement if and only if $-1 \leq v_{22} < 1$.

In the remainder, without loss of generality, we assume $g_{11} = 1$: this choice is consequence of the fact that the above form of the matrix \mathbf{V} makes the first condition in (3.8) a linear system of two equations in three unknowns. Thus, its vector solution depends on a free parameter and, in order to avoid affecting the positive definiteness, we choose g_{11} as parameter and fix its value to 1.

We next solve the first G-symplecticity condition in (3.8) with respect to g_{12} and g_{22} , obtaining

$$g_{12} = -\frac{v_{12}}{-1 + v_{22}}, \quad g_{22} = \frac{v_{12}^2}{(1 - v_{22})^2}.$$

We next consider the second condition in (3.8): by comparing the first column of the matrix \mathbf{DU} with that of the matrix $\mathbf{B}^T \mathbf{G} \mathbf{V}$ we obtain the following values for the entries of the matrix \mathbf{D}

$$d_{11} = \frac{(b_{11} + b_{21}v_{12} - b_{11}v_{22})}{(1 - v_{22})}, \quad d_{22} = \frac{(b_{12} + b_{22}v_{12} - b_{12}v_{22})}{(1 - v_{22})},$$

$$d_{33} = \frac{(b_{13} + b_{23}v_{12} - b_{13}v_{22})}{(1 - v_{22})},$$

and solving the remaining three equations with respect to b_{21} , v_{12} and b_{13} we get

$$b_{13} = -b_{23}u_{22}, \quad b_{21} = \frac{b_{11}(-1 + v_{22})}{v_{12}}, \quad v_{12} = u_{22}(-1 + v_{22}).$$

By solving the first equation in (2.5), we find the following values of b_{11} and b_{22}

$$b_{11} = 1 - b_{12} - u_{22} + b_{23}u_{22} + u_{22}v_{22}, \quad b_{22} = -\frac{-1 + b_{12}}{u_{22}},$$

while parasitism is removed by solving condition (3.14) with respect to v_{22} , obtaining

$$v_{22} = 1 - b_{12} + b_{23}u_{32} + (-1 + b_{12} - u_{22}(-1 + b_{23} + v_{22})) \frac{u_{12}}{u_{22}}.$$

By imposing the second consistency condition (2.5) we get

$$u_{12} = c_1 - a_{11}, \quad u_{22} = c_2 - a_{22} - a_{21}, \quad u_{32} = c_3 - a_{31} - a_{32} - a_{33},$$

while the last condition in (3.8) provides

$$a_{21} = 0, \quad a_{22} = \frac{1}{2}.$$

Imposing order and stage-order 2 we finally come to the matrices

$$\mathbf{A} = \begin{bmatrix} \frac{c_1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ \frac{c_3(-2a_{33} + c_3)}{2c_1} & a_{32} & a_{33} \end{bmatrix}, \quad \mathbf{U} = \begin{bmatrix} 1 & \frac{c_1}{2} \\ 1 & -\frac{1}{2} \\ 1 & \frac{c_3}{2} \end{bmatrix}$$

$$\mathbf{B} = \begin{bmatrix} \frac{1 - b_{23}c_3}{2c_1} & \frac{3}{2} & \frac{b_{23}}{2} \\ \frac{1 - b_{23}c_3}{c_1} & 1 & b_{23} \end{bmatrix}, \quad \mathbf{V} = \begin{bmatrix} 1 & -\frac{1 + c_1 + b_{23}c_1 - b_{23}c_3}{2c_1} \\ 0 & \frac{-1 - b_{23}c_1 + b_{23}c_3}{c_1} \end{bmatrix}.$$

We choose $a_{33} = \frac{c_3}{2}$ and $a_{32} = 0$ to enforce the diagonal structure of the matrix \mathbf{A} and, in correspondence of the values $c_1 = -\frac{1}{2}$, $c_3 = \frac{1}{2}$, $b_{23} = \frac{4}{3}$ we obtain the method

$$\left[\begin{array}{ccc|cc} \mathbf{A} & \mathbf{U} & & & \\ \mathbf{B} & \mathbf{V} & & & \end{array} \right] = \left[\begin{array}{ccc|cc} -\frac{1}{4} & 0 & 0 & 1 & -\frac{1}{4} \\ 0 & \frac{1}{2} & 0 & 1 & -\frac{1}{2} \\ 0 & 0 & \frac{1}{4} & 1 & \frac{1}{4} \\ \hline -\frac{1}{3} & \frac{3}{2} & \frac{2}{3} & 1 & -\frac{5}{6} \\ -\frac{2}{3} & 1 & \frac{4}{3} & 0 & -\frac{2}{3} \end{array} \right] \quad (3.27)$$

with abscissa vector

$$\mathbf{c}^T = \left[-\frac{1}{2} \quad 0 \quad \frac{1}{2} \right]$$

and

$$\mathbf{G} = \begin{bmatrix} 1 & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{4} \end{bmatrix}, \quad \mathbf{D} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

Performing an analogous construction by assuming

$$y^{[n]} \approx \begin{bmatrix} y(t_n) \\ h^2 y''(t_n) \end{bmatrix}$$

and imposing order 2 and stage order 2 of convergence, we get the diagonally implicit GLM

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \mathbf{B} & \mathbf{V} \end{array} \right] = \left[\begin{array}{ccc|cc} \frac{1}{6} & 0 & 0 & 1 & -\frac{1}{24} \\ \frac{1}{3} & \frac{1}{6} & 0 & 1 & -\frac{1}{24} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{6} & 1 & -\frac{1}{24} \\ \hline -\frac{1}{4} & \frac{5}{4} & 0 & 1 & -\frac{1}{12} \\ -14 & 22 & -8 & 0 & -1 \end{array} \right] \quad (3.28)$$

with abscissa vector

$$\mathbf{c}^T = \left[\frac{1}{6}, \frac{1}{2}, \frac{5}{6} \right]$$

and

$$\mathbf{G} = \begin{bmatrix} 1 & -\frac{1}{24} \\ -\frac{1}{24} & \frac{1}{576} \end{bmatrix}, \quad \mathbf{D} = \begin{bmatrix} \frac{1}{3} & 0 & 0 \\ 0 & \frac{1}{3} & 0 \\ 0 & 0 & \frac{1}{3} \end{bmatrix}.$$

3.4.1 Numerical Experiments

We now show the numerical results arising from the comparison of the derived GLMs (3.27) and (3.28) with the G-symplectic method (3.12) [11] of order 4 and stage order 2. The computations have been done on a node with CPU Intel Xeon 6 core X5690 3,46GHz, belonging to the E4 multi-GPU cluster of Mathematics Department of Salerno University.

Concerning the problem (3.2), we observe from Fig. 3.1 that, even if the method (3.12) is G-symplectic, it does not provide an accurate numerical conservation of the Hamiltonian: this is due to the presence of parasitic components in the numerical solution which destroy the overall accuracy. Such a behaviour is not advisable on our methods (3.27) and (3.28), as shown in Fig. 3.2 and 3.3, since they are free from parasitism, i.e. they satisfy the condition for the removal of the parasitic components in the numerical solution. Hence, we advise an accurate numerical conservation of the Hamiltonian for one million step points. A similar analysis can be carried out for problem (3.3), as reported in Fig. 3.4, 3.5, and 3.6: also in this case, method (3.12) fails in accurately preserving the numerical Hamiltonian, while our methods are able conserving it over one million points.

Figures 3.2 - 3.3 and 3.5 - 3.6 reveal the presence of a threshold on the accuracy gained in the numerical conservation of the Hamiltonian by G-symplectic methods (3.27) and (3.28).

For the simple pendulum problem (3.2), the constant α (3.19) assumes the form

$$\alpha = \left\| |p(t_n)| + |\sin(q(t_n))| \right\|_{\infty}$$

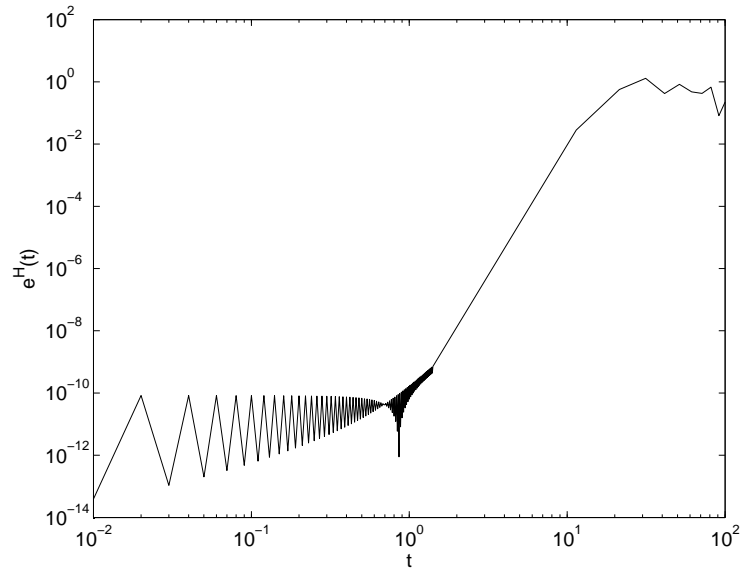


Figure 3.1: Hamiltonian deviation $e^H(t)$ associated to method (3.12) applied to problem (3.2) with stepsize 10^{-2}

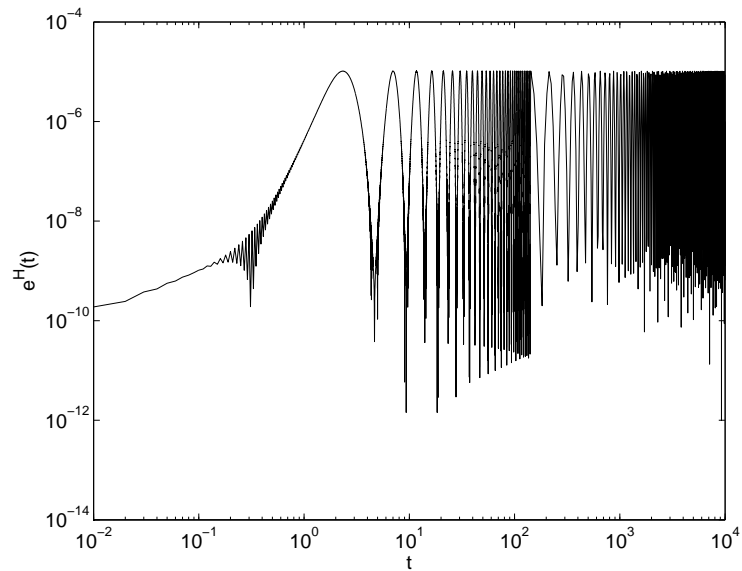


Figure 3.2: Hamiltonian deviation $e^H(t)$ associated to method (3.28) applied to problem (3.2) with stepsize 10^{-2}

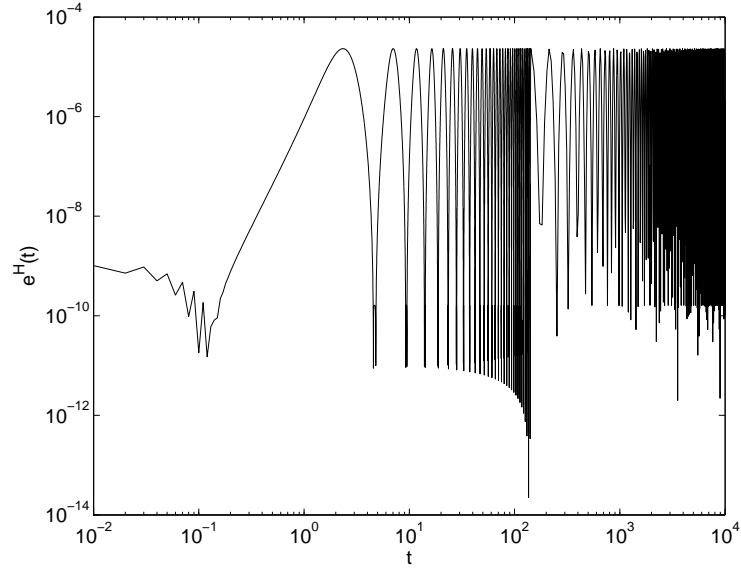


Figure 3.3: Hamiltonian deviation $e^H(t)$ associated to method (3.27) applied to problem (3.2) with stepsize 10^{-2}

and its observed values in correspondence of methods (3.27) and (3.28) are both 2.39. In the case of Kepler problem (3.3), α takes the form

$$\alpha = \left\| \left\| p(t_n) \right\|_1 + \frac{\|q(t_n)\|_1}{\|q(t_n)\|_2^3} \right\|_\infty$$

and the numerically observed values for methods (3.27) and (3.28) are 6.37 and 5.69, respectively.

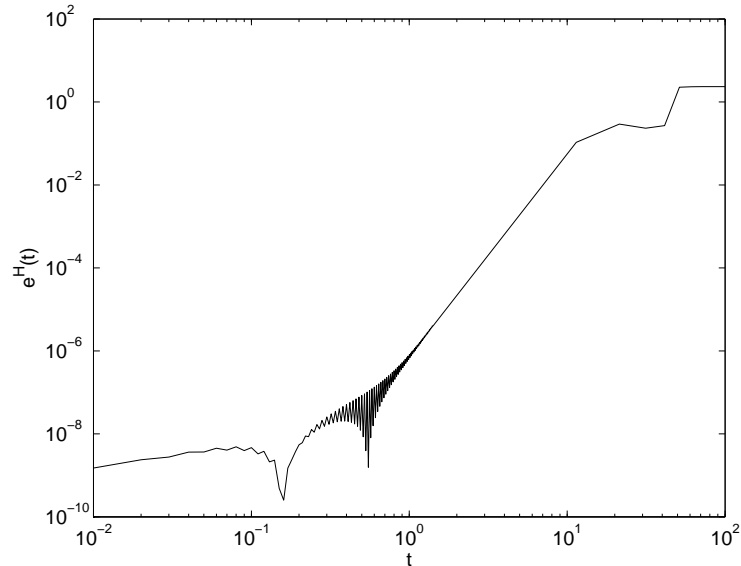


Figure 3.4: Hamiltonian deviation $e^H(t)$ associated to method (3.12) applied to problem (3.3) with stepsize 10^{-2}

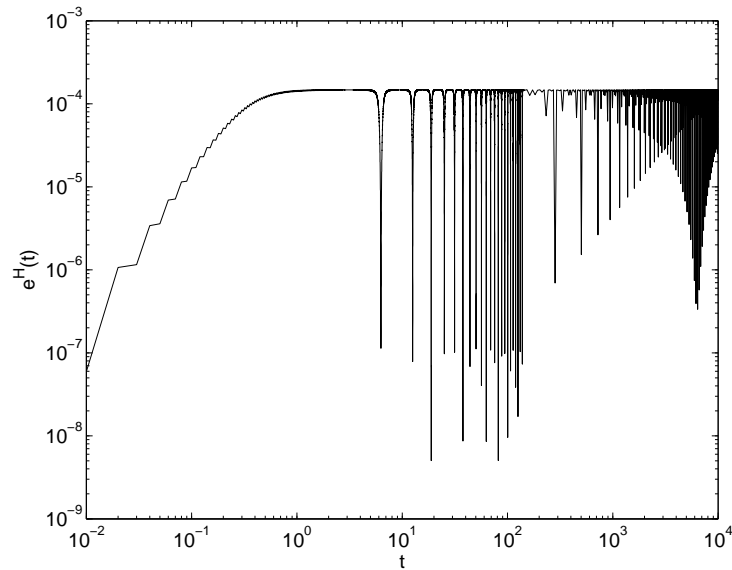


Figure 3.5: Hamiltonian deviation $e^H(t)$ associated to method (3.28) applied to problem (3.3) with stepsize 10^{-2}

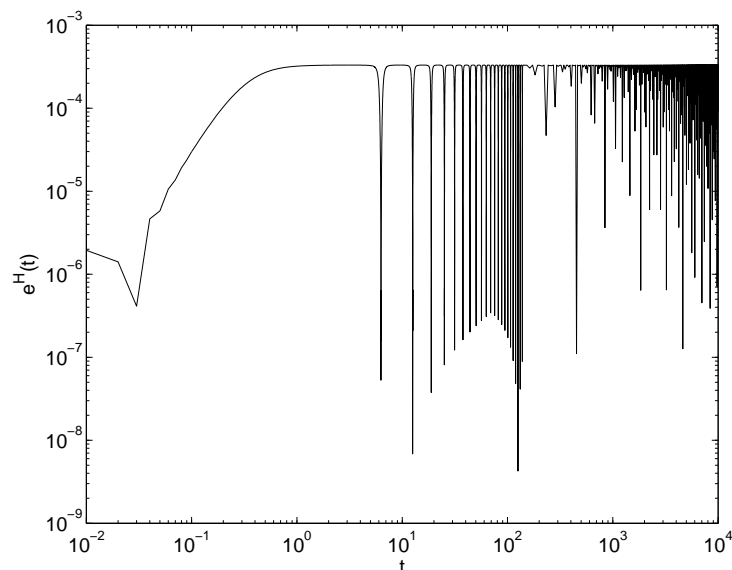


Figure 3.6: Hamiltonian deviation $e^H(t)$ associated to method (3.27) applied to problem (3.3) with stepsize 10^{-2}

3.5 Symmetric Integration

For conservative mechanical systems and, in particular, Hamiltonian systems, a property of time reversibility holds: in practice, this means that inverting the direction of the velocity for a fixed initial point does not change the trajectory of the motion, but only its direction. In particular, by reversing the direction of the flow, the invariants are still preserved. Thus, a desirable property for numerical methods applied to such problems is that of providing a reversible numerical flow. In the context of RK methods, this property is related to that of symmetry, i.e. that of coincidence between the numerical method and its adjoint [70]. We briefly recall

here these concepts. It is useful at this point to recall the definition of *flow* of a differential system

Definition 3.5.1. Given an ODE $y' = f(x, y)$, we define its *flow* [70] over point x as the operator which associates at each initial value y_0 the solution of the ODE evaluated in x . Denoting the flow with ϕ_x , we have

$$\phi_x(y_0) = y(x)$$

being y the solution of the IVP associated to the given ODE and the initial value y_0 .

Many properties of ODE systems can be studied by means of their flow, thus it is useful to define a numerical counterpart of this operator. In particular, we define the *numerical flow* [70] of a method as the h -dependent operator

$$\Phi_h : y_n \mapsto y_{n+1}$$

advancing the solution from step to step by means of the method's formula. In practice it is equivalent to talk about methods and their associated flow. Time reversal symmetry can be formulated in terms of flow, namely the flow of an autonomous system always satisfy

$$\phi_{-x} = \phi_x^{-1}$$

or, equivalently

$$\phi_{-x}^{-1} = \phi_x.$$

In general, this property is not shared by numerical integrators, the following definition introduces a crucial operator

Definition 3.5.2. The *adjoint method* of a method Φ_h is the inverse map of the original method with step $-h$, i.e.

$$\Phi_h^* := \Phi_{-h}^{-1}.$$

A numerical method is *symmetric* if it coincides with its adjoint.

In practice, to obtain the adjoint of a method it suffices to invert, when possible, the expression of the method itself with step $-h$. We will see an example of this procedure in the Section 3.5.1. A fundamental result concerning adjoint methods is summarized in the following Theorem (compare [70])

Theorem 3.5.1. Let Φ_h be a one-step method of order p satisfying

$$\Phi_h(y_0) = \phi_h(y_0) + C(y_0)h^{p+1} + O(h^{p+2}),$$

then its adjoint satisfies

$$\Phi_h^*(y_0) = \phi_h(y_0) + (-1)^p C(y_0)h^{p+1} + O(h^{p+2}).$$

If the method is symmetric, then its maximal order is even.

As shown in [70], the methods belonging to the family of Gauss-Legendre Runge-Kutta methods are symmetric. A concept of symmetry for GLMs has been defined in [67, 70] as follows.

Theorem 3.5.2. Let $L \in \mathbb{R}^{r \times r}$ be an involution matrix and $P \in \mathbb{R}^{s \times s}$ a permutation matrix. If the method (2.1) satisfies

$$\begin{aligned} P^{-1}AP &= UV^{-1}B - A, & P^{-1}UL &= UV^{-1}, \\ L^{-1}BP &= B, & L^{-1}VL &= V^{-1}, \end{aligned} \quad (3.29)$$

then it is symmetric.

3.5.1 Symmetric GLNs

In this Section, we construct the adjoint of a GLN method (2.14) in the hybrid form. The same procedure can be applied in the general form with trivial variations. We assume the adjoint of method (2.14) to have the expression

$$\begin{aligned} \tilde{Y} &= h^2 \tilde{\mathbf{A}}f(\tilde{Y}) + \tilde{\mathbf{U}}\tilde{y}_n \\ \tilde{y}_{n-1} &= h^2 \tilde{\mathbf{B}}f(\tilde{Y}) + \tilde{\mathbf{V}}\tilde{y}_n. \end{aligned}$$

Assuming there exist a permutation matrix \mathbf{P} and an invertible matrix \mathbf{L} such that

$$\tilde{Y} = \mathbf{P}Y$$

$$\tilde{y} = \mathbf{L}y$$

the adjoint assumes the form

$$\begin{aligned} \mathbf{P}Y &= h^2 \tilde{\mathbf{A}}\mathbf{P}f(Y) + \tilde{\mathbf{U}}\mathbf{L}y_n \\ \mathbf{L}y_{n-1} &= h^2 \tilde{\mathbf{B}}\mathbf{P}f(Y) + \tilde{\mathbf{V}}\mathbf{L}y_n \end{aligned} \quad (3.30)$$

since $f(\mathbf{P}Y) = \mathbf{P}f(y)$.

We can obtain expressions for Y and y_{n-1} from (2.14)

$$\begin{aligned} Y &= h^2(\mathbf{A} - \mathbf{U}\mathbf{V}^{-1}\mathbf{B})F(Y) + \mathbf{U}\mathbf{V}^{-1}y_n \\ y_{n-1} &= -h^2\mathbf{V}^{-1}\mathbf{B}F(Y) + \mathbf{V}^{-1}y_n \end{aligned}$$

and substituting in (3.30)

$$\begin{aligned} \mathbf{P}Y &= h^2(\mathbf{P}\mathbf{A}\mathbf{P}^{-1} - \mathbf{P}\mathbf{U}\mathbf{V}^{-1}\mathbf{B}\mathbf{P}^{-1}) * \mathbf{P}F(Y) + \mathbf{P}\mathbf{U}\mathbf{V}^{-1}\mathbf{L}^{-1}\mathbf{L}y_n \\ \mathbf{L}y_{n-1} &= -h^2\mathbf{L}\mathbf{V}^{-1}\mathbf{B}\mathbf{P}^{-1}\mathbf{P}F(Y) + \mathbf{L}\mathbf{V}^{-1}\mathbf{L}^{-1}\mathbf{L}y_n \end{aligned}$$

we find the following expression for the matrices of the adjoint method.

$$\begin{aligned} \tilde{\mathbf{A}} &= \mathbf{P}\mathbf{A}\mathbf{P}^{-1} - \mathbf{P}\mathbf{U}\mathbf{V}^{-1}\mathbf{B}\mathbf{P}^{-1} \\ \tilde{\mathbf{U}} &= \mathbf{P}\mathbf{U}\mathbf{V}^{-1}\mathbf{L}^{-1} \\ \tilde{\mathbf{B}} &= -\mathbf{L}\mathbf{V}^{-1}\mathbf{B}\mathbf{P}^{-1} \\ \tilde{\mathbf{V}} &= \mathbf{L}\mathbf{V}^{-1}\mathbf{L}^{-1} \end{aligned}$$

Table 3.3: Values of $\xi_i(t)$ and $E\xi_i(t)$, $i = 1, 2$, up to order $p = 4$

	ξ_1	ξ_2	$E\xi_1$	$E\xi_2$
\emptyset	1	0	1	0
τ	0	θ_1	1	θ_1
$[\tau]$	0	θ_2	$\frac{1}{2}$	$\theta_1 + \theta_2$
$[\tau^2]$	0	θ_3	$\frac{1}{3}$	$\theta_1 + 2\theta_2 + \theta_3$
$[[\tau]]$	0	θ_4	$\frac{1}{6}$	$\frac{1}{2}\theta_1 + \theta_2 + \theta_4$
$[\tau^3]$	0	θ_5	$\frac{1}{4}$	$\theta_1 + 3\theta_2 + 3\theta_3 + \theta_5$
$[\tau[\tau]]$	0	θ_6	$\frac{1}{8}$	$\frac{1}{2}\theta_1 + \frac{3}{2}\theta_2 + \theta_3 + \theta_4 + \theta_6$
$[\tau[\tau^2]]$	0	θ_7	$\frac{1}{12}$	$\frac{1}{3}\theta_1 + \theta_2 + 2\theta_4 + \theta_7$
$[\tau^4]$	0	θ_8	$\frac{1}{24}$	$\frac{1}{6}\theta_1 + \frac{1}{2}\theta_2 + \theta_4 + \theta_8$

Theorem 3.5.3. Let \mathbf{P} be an $s \times s$ permutation matrix and \mathbf{L} an $r \times r$ invertible matrix. A GLN method (2.14) is symmetric if and only if its coefficient matrices are such that

$$\begin{aligned}\mathbf{A} &= \mathbf{PAP}^{-1} - \mathbf{PUV}^{-1}\mathbf{BP}^{-1} \\ \mathbf{U} &= \mathbf{PUV}^{-1}\mathbf{L}^{-1} \\ \mathbf{B} &= -\mathbf{LV}^{-1}\mathbf{BP}^{-1} \\ \mathbf{V} &= \mathbf{LV}^{-1}\mathbf{L}^{-1}.\end{aligned}$$

3.6 A Symmetric G-symplectic GLM

We derive a two-value and three-stage GLM (i.e. $r = 2$, $s = 3$), assuming that the first component of the numerical solution approximates the exact one, so we do not need any finishing method. The initial value for the second component is computed by means of a generalized 8-stage RK method with elementary weights

$$\{0, \theta_1, \theta_2, \theta_3, \theta_4, \theta_5, \theta_6, \theta_7, \theta_8\},$$

which are left as free parameters. The values of $\xi_i(t)$ and $E\xi_i(t)$, $i = 1, 2$, corresponding to trees up to order 4 and depending on such parameters are reported in Table 3.3.

To obtain a basic consistency condition, we solve the second equation in (2.9) for the empty tree, observing that $\eta D(\emptyset) = 0$ by definition. This leads to

$$\begin{cases} E\xi_1(\emptyset) = v_{11}\xi_1(\emptyset) + v_{12}\xi_2(\emptyset), \\ E\xi_2(\emptyset) = v_{21}\xi_1(\emptyset) + v_{22}\xi_2(\emptyset), \end{cases} \quad (3.31)$$

and, by taking into account the values in Table 3.3, we obtain

$$v_{11} = 1, \quad v_{21} = 0.$$

As a consequence, the matrix V of a preconsistent GLM (2.1) with $r = 2$ has always the form

$$V = \begin{bmatrix} 1 & v_{12} \\ 0 & v_{22} \end{bmatrix}. \quad (3.32)$$

At this point, it is worth assuming $v_{22} = -1$. In fact (compare [70], §XV.8.3), in order to limit as much as possible the effects of parasitism, the eigenvalues of the matrix V have to be the r -th roots of unity. Moreover, this choice automatically leads to zero-stable methods (compare [11, 82]).

The first vector equation in (2.9) with $t = \emptyset$, leads to

$$\begin{cases} \eta_1(\emptyset) = u_{11}, \\ \eta_2(\emptyset) = u_{21}, \\ \eta_3(\emptyset) = u_{31}, \end{cases} \quad (3.33)$$

and, since $\eta_i(\emptyset) = 1$, we get

$$u_{11} = 1, \quad u_{21} = 1, \quad u_{31} = 1.$$

Thus, by imposing preconsistency, G-symplecticity, symmetry and condition (3.14) to bound the parasitic components, we obtain the GLM

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array} \right] = \left[\begin{array}{ccc|cc} \frac{1}{2}\alpha & 0 & 0 & 1 & u_{32} \\ \alpha & \frac{1}{2}\beta & 0 & 1 & u_{32} \\ \alpha & \beta & \frac{1}{2}\alpha & 1 & u_{32} \\ \hline b_{13} & b_{12} & b_{13} & 1 & 2u_{32} \\ b_{23} & -2b_{23} & b_{23} & 0 & -1 \end{array} \right] \quad (3.34)$$

where $\alpha = b_{13} + b_{23}u_{32}$ and $\beta = b_{12} - 2b_{23}u_{32}$, and the system (2.9) assumes the form

$$\begin{cases} \eta_1(t) = \frac{1}{2}\alpha\eta_1 D(t) + \xi_1(t) + u_{32}\xi_2(t), \\ \eta_2(t) = \alpha\eta_1 D(t) + \frac{1}{2}\beta\eta_2 D(t) + \xi_1(t) + u_{32}\xi_2(t), \\ \eta_3(t) = \alpha\eta_1 D(t) + \beta\eta_2 D(t) + \frac{1}{2}\eta_3 D(t) + \xi_1(t) + u_{32}\xi_2(t), \\ E\xi_1(t) = b_{13}\eta_1 D(t) + b_{12}\eta_2 D(t) + b_{13}\eta_3 D(t) + \xi_1(t) + 2u_{32}\xi_2(t), \\ E\xi_2(t) = b_{23}\eta_1 D(t) - 2b_{23}\eta_2 D(t) + b_{23}\eta_3 D(t) - \xi_2(t). \end{cases} \quad (3.35)$$

Due to symmetry, we imposed order conditions associated to odd order trees only. This led to

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array} \right] = \left[\begin{array}{ccc|cc} \frac{1}{6}\gamma & 0 & 0 & 1 & \frac{1}{24} \\ \frac{1}{3}\gamma & -\frac{1}{6}\delta & 0 & 1 & \frac{1}{24} \\ \frac{1}{3}\gamma & \frac{1}{6}\delta & \frac{1}{6}\gamma & 1 & \frac{1}{24} \\ \hline \frac{1}{6}\varphi & -\frac{1}{4} - \frac{2\sqrt[3]{2}}{3} - \frac{\sqrt[3]{4}}{3} & \frac{1}{6}\varphi & 1 & \frac{1}{12} \\ 1 & -2 & 1 & 0 & -1 \end{array} \right], \quad (3.36)$$

Table 3.4: Elementary weights of the starting procedure for the computation of $y_2^{[0]}$

θ_1	θ_2	θ_3	θ_4	θ_5	θ_6	θ_7	θ_8
0	0	$\frac{1}{24}(2 - \sqrt[3]{2})$	$-\frac{1}{24}(\sqrt[3]{2} + \sqrt[3]{4})$	0	0	0	0

being $\gamma = 2 + \frac{\sqrt[3]{4}}{2} + \sqrt[3]{2}$, $\delta = (1 + \sqrt[3]{2})^2$, $\varphi = \frac{15}{4} + 2\sqrt[3]{2} + \sqrt[3]{4}$, and with abscissa vector

$$c = \left[\frac{1}{6}\gamma, \quad \frac{1}{2}, \quad -\frac{1}{12}(\sqrt[3]{2} - 2)(4 + \sqrt[3]{2}) \right]^T.$$

This method is G -symplectic with respect to the matrices

$$G = \begin{bmatrix} 1 & \frac{1}{24} \\ \frac{1}{24} & \frac{1}{576} \end{bmatrix}, \quad D = \begin{bmatrix} \frac{1}{3}\gamma & 0 & 0 \\ 0 & -\frac{1}{3}\delta & 0 \\ 0 & 0 & \frac{1}{3}\gamma \end{bmatrix},$$

and symmetric with $L = I$ and

$$P = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}.$$

3.6.1 Starting procedure

As announced, we derive as starting method for the initial value of the second external approximation $y_2^{[0]}$ the generalized Runge-Kutta method with elementary weights $0, \theta_1, \dots, \theta_8$ given in Table 3.4.

We introduce the following eight-stage generalized RK method with

$$A = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{6} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{4} & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{5}{6} & -\frac{8}{3} & \frac{5}{2} & 0 & 0 & 0 & 0 & 0 \\ -\frac{8}{5} & \frac{3}{5} & 1 & \frac{1}{5} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{4} & \frac{1}{2} & -\frac{1}{4} & 0 & 0 & 0 \\ -1 & 0 & 1 & -\frac{1}{6} & \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{5} & \frac{3}{5} & 0 & 0 & 0 & \frac{2}{5} & 0 \end{bmatrix},$$

$$c = \begin{bmatrix} 0 \\ \frac{1}{6} \\ -\frac{1}{4} \\ \frac{2}{3} \\ \frac{1}{5} \\ \frac{1}{2} \\ \frac{1}{3} \\ \frac{4}{5} \end{bmatrix},$$

and weights obtained by solving the linear system

$$\begin{cases} b_1 + b_2 + b_3 + b_4 + b_5 + b_6 + b_7 + b_8 = 0 \\ 10b_2 - 15b_3 + 40b_4 + 12b_5 + 30b_6 + 20b_7 + 48b_8 = 0 \\ \frac{b_2}{36} + \frac{b_3}{16} + \frac{4b_4}{9} + \frac{b_5}{25} + \frac{b_6}{4} + \frac{b_7}{9} + \frac{16b_8}{25} + \frac{1}{24}(-2 + \sqrt[3]{2}) = 0 \\ -60b_3 - 770b_4 - 12b_5 + 159b_6 - 188b_7 - 36b_8 + 30(\sqrt[3]{2} + \sqrt[3]{4}) = 0 \\ \frac{b_2}{216} - \frac{b_3}{64} + \frac{8b_4}{27} + \frac{b_5}{125} + \frac{b_6}{8} + \frac{b_7}{27} + \frac{64b_8}{125} = 0 \\ 450b_3 - 15400b_4 - 72b_5 + 2385b_6 - 1880b_7 - 864b_8 = 0 \\ -600b_3 + 3550b_4 + 7260b_5 + 9843b_6 + 364b_7 + 3300b_8 = 0 \\ -2250b_4 - 3210b_5 - 5955b_6 + 935b_7 - 1668b_8 = 0 \end{cases}$$

Remark 3.6.1. The linearity of this system is due to the fact that the number of employed internal stages in the starting procedure (eight) equals the number of order conditions to impose to gain order 4 in the approximation of the starting value $y_2^{[0]}$.

3.6.2 Minimizing the Error Constant

For a method of order p , it is easy to extract the leading term of the error

$$\sum_{\rho(t)=p+1} \frac{h^{\rho(t)}}{\sigma(t)} \hat{\xi}(t) F(t)(y(x_0)) = h^{p+1} \sum_{\rho(t)=p+1} \frac{1}{\sigma(t)} (B\eta D(t) + V\xi(t)) F(t)(y(x_0)), \quad (3.37)$$

which we will next aim to minimize.

We consider as a starting point method (3.36). We consider the quantities $\hat{\xi}(t)$ appearing in (3.37) for $t \in T$, $\rho(t) = 5$ and we minimize the sum of their absolute values by employing the **Mathematica** intrinsic routine **Minimize**. We perform a constrained minimization process depending on the following constraints

$$0 < u_{32} < \frac{1}{4} \quad 0 < b_{23} \leq 1,$$

and achieve $u_{32} = \frac{1}{8}$ and $b_{23} = \frac{1}{2}$. These values lead to the following coefficient

matrices

$$A = \begin{bmatrix} \frac{1}{6} \left(2 + \frac{1}{\sqrt[3]{2}} + \sqrt[3]{2} \right) & 0 & 0 \\ \frac{1}{3} \left(2 + \frac{1}{\sqrt[3]{2}} + \sqrt[3]{2} \right) & -\frac{1}{6} (1 + \sqrt[3]{2})^2 & 0 \\ \frac{1}{3} \left(2 + \frac{1}{\sqrt[3]{2}} + \sqrt[3]{2} \right) & -\frac{1}{3} (1 + \sqrt[3]{2})^2 & \frac{1}{6} \left(2 + \frac{1}{\sqrt[3]{2}} + \sqrt[3]{2} \right) \end{bmatrix},$$

$$B = \begin{bmatrix} \frac{1}{6} \left(\frac{29}{8} + 2\sqrt[3]{2} + 2^{2/3} \right) & \frac{1}{24} (-5 - 16\sqrt[3]{2} - 8 \cdot 2^{2/3}) & \frac{1}{6} \left(\frac{29}{8} + 2\sqrt[3]{2} + 2^{2/3} \right) \\ & \frac{1}{2} & \\ & & -1 \\ & & & \frac{1}{2} \end{bmatrix},$$

$$U = \begin{bmatrix} 1 & \frac{1}{8} \\ 1 & \frac{1}{8} \\ 1 & \frac{1}{8} \end{bmatrix}, \quad V = \begin{bmatrix} 1 & \frac{1}{4} \\ 0 & -1 \end{bmatrix}.$$

We also observe that, for such method, $\hat{\xi}(t)$ is zero for all trees of order 5 except $[[[\tau]]]$ (compare [11]), whose value is approximately equal to 0.17.

3.6.3 Numerical Experiments

We now provide some numerical experiments comparing the GLM (3.36) with the partitioned RK method [100, 107]

$$\begin{array}{c} \left| \frac{A}{b} \right. \\ \left| \frac{A}{b} \right. \end{array} = \begin{array}{c} \begin{array}{cccccc} 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{3} & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{3} & -\frac{1}{3} & 0 & 0 & 0 & 0 \\ \frac{1}{3} & -\frac{1}{3} & 1 & 0 & 0 & 0 \\ \frac{1}{3} & -\frac{1}{3} & 1 & -\frac{1}{3} & 0 & 0 \\ \frac{1}{3} & -\frac{1}{3} & 1 & -\frac{1}{3} & \frac{1}{3} & 0 \end{array} \\ \hline \begin{array}{cccccc} \frac{1}{3} & -\frac{1}{3} & 1 & -\frac{1}{3} & \frac{1}{3} & 0 \end{array} \\ \begin{array}{cccccc} \frac{7}{48} & 0 & 0 & 0 & 0 & 0 \\ \frac{7}{48} & \frac{3}{8} & 0 & 0 & 0 & 0 \\ \frac{7}{48} & \frac{3}{8} & -\frac{1}{48} & 0 & 0 & 0 \\ \frac{7}{48} & \frac{3}{8} & -\frac{1}{48} & -\frac{1}{48} & 0 & 0 \\ \frac{7}{48} & \frac{3}{8} & -\frac{1}{48} & -\frac{1}{48} & \frac{3}{8} & 0 \\ \frac{7}{48} & \frac{3}{8} & -\frac{1}{48} & -\frac{1}{48} & \frac{3}{8} & \frac{7}{48} \end{array} \\ \hline \begin{array}{cccccc} \frac{7}{48} & \frac{3}{8} & -\frac{1}{48} & -\frac{1}{48} & \frac{3}{8} & \frac{7}{48} \end{array} \end{array} \quad (3.38)$$

which originates by coupling a diagonally implicit method with an explicit one, thus leading to an overall explicit scheme in case of separable Hamiltonians. Such partitioned pairs are indeed of practical interest only for separable Hamiltonian problems (compare, for instance, [70] and references therein). Both methods, i.e. our GLM (3.36) and the partitioned RK (3.38) are symmetric and of order 4. Moreover,

Table 3.5: Numerical comparison of the partitioned RK method (3.38) with respect to the G-symplectic GLM (3.36)

	PRK	GLM
Simple pendulum	$\ e^{\mathcal{H}}\ _{\infty} = 9.51e - 14$ $fe = 12000000$	$\ e^{\mathcal{H}}\ _{\infty} = 1.28e - 13$ $fe = 10697133$
Kepler problem	$\ e^{\mathcal{H}}\ _{\infty} = 5.73e - 14$ $fe = 12000000$	$\ e^{\mathcal{H}}\ _{\infty} = 1.88e - 13$ $fe = 11017887$
Hènon-Heiles problem	$\ e^{\mathcal{H}}\ _{\infty} = 1.48e - 14$ $fe = 12000000$	$\ e^{\mathcal{H}}\ _{\infty} = 5.02e - 14$ $fe = 9088029$
3-body problem	$\ e^{\mathcal{H}}\ _{\infty} = 2.43e - 13$ $fe = 12000000$	$\ e^{\mathcal{H}}\ _{\infty} = 7.48e - 13$ $fe = 11988456$
Bead on wire	non-separable	$\ e^{\mathcal{H}}\ _{\infty} = 1.11e - 14$ $fe = 8999952$
Non-reversible problem	$\ e^{\mathcal{H}}\ _{\infty} = 3.64e - 14$ $fe = 12000000$	$\ e^{\mathcal{H}}\ _{\infty} = 4.59e - 013$ $fe = 8999871$

the GLM is G-symplectic with zero growth parameter for the parasitic components, while the RK method is symplectic.

The reported tests have been carried out on a node with CPU Intel Xeon 6 core X5690 3,46GHz, belonging to the E4 multi-GPU cluster of Mathematics Department of Salerno University. In particular, it is our aim to show the accuracy gained in the numerical conservation of the Hamiltonian of the following dynamical systems:

We perform one million steps of the mentioned numerical methods and compute the Hamiltonian deviation (3.20). The values of the observed Hamiltonian deviations and the number of function evaluations (fe in Table 3.5) required by the overall integration schemes are reported in Table 3.5. We observe that the accuracy gained in preserving the Hamiltonian of the above dynamical systems is essentially the same for both the RK method and the GLM. However the main novelty here is that the derived GLM requires a lower computational effort, due to the lower number of stages: each step of the GLM requires 3 internal stages, while the RK method involves 12 stages.

It is also worth observing that the hypothesis of bounded parasitic components is absolutely crucial: parasitic methods, such as the G-symplectic GLM presented in [11], fail in preserving the Hamiltonian over suitably long time intervals and, moreover, completely destroy the symplecticity of the phase space. This is also visible from the orbit patterns, reported in Figures 3.7, 3.8 and 3.9.

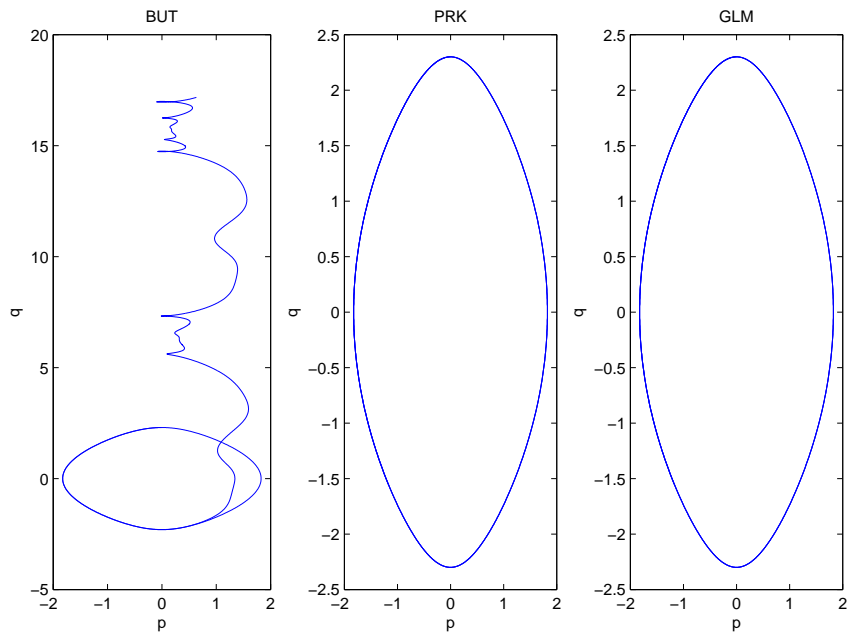


Figure 3.7: Orbit patterns for problem (3.2), gained by the G-symplectic method presented in [11] (BUT), the symplectic PRK method (3.38) and the GLM (3.36)

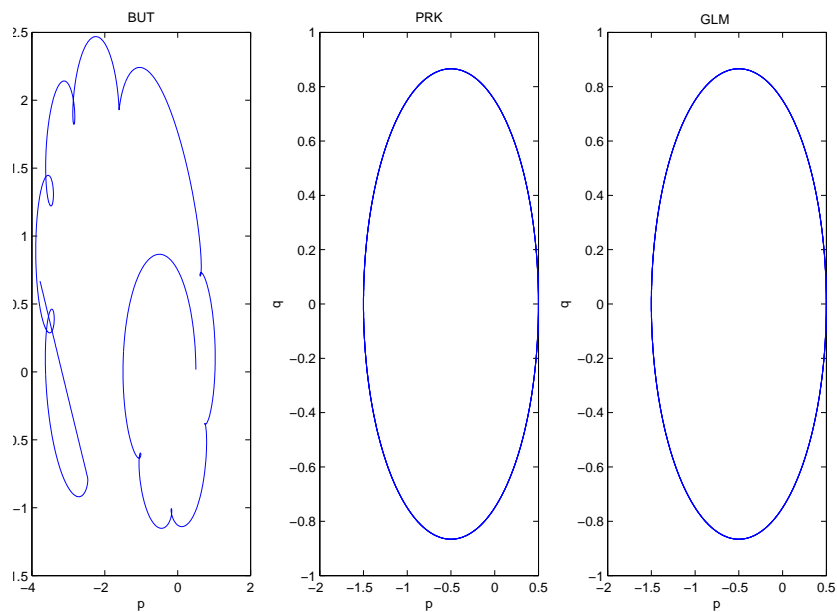


Figure 3.8: Orbit patterns for problem (3.3), gained by the G-symplectic method presented in [11] (BUT), the symplectic PRK method (3.38) and the GLM (3.36)

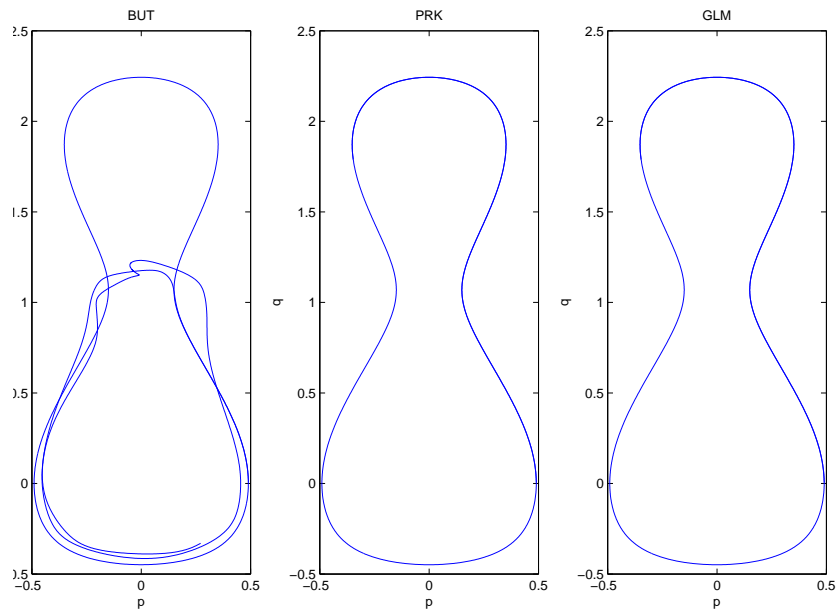


Figure 3.9: Orbit patterns for problem (3.6), gained by the G-symplectic method presented in [11] (BUT), the symplectic PRK method (3.38) and the GLM (3.36)

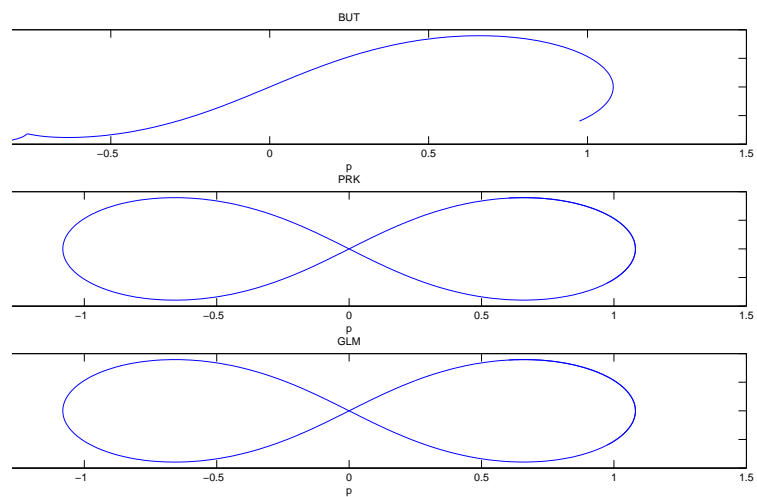


Figure 3.10: Orbit patterns for problem (3.5), gained by the G-symplectic method presented in [11] (BUT), the symplectic PRK method (3.38) and the GLM (3.36)

Part II

Chapter 4

Cardiac Tissue Structure Information from DTMRI Images

The topics described in this Chapter concern two periods of study the author spent at the departement of Computer Science at the Oxford University under the supervision of professor Kevin Burrage.

Diffusion Tensor Magnetic Resonance Imaging (DT-MRI) is an imaging technique finalized to the extraction of information about the living tissues. Such technique has been successfully used in the analysis of the human brain. In order to investigate on the structure of the heart, we analyzed a set of DT-MRI images of an ex-vivo rat heart by means of a recently proposed model.

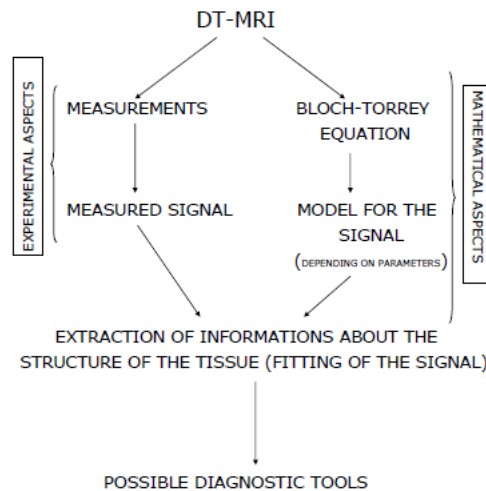


Figure 4.1: A scheme of the operations performed

4.1 Diffusion

The classical diffusion equation

$$\frac{\partial C}{\partial t} = k\Delta C \quad (4.1)$$

is used to describe the phenomenon of molecular diffusion, i.e. the transport of molecules in a given media. Here C represents the concentration of molecules and k is called diffusion coefficient. In this description of the phenomenon, it is implicitly assumed that molecules can diffuse in all the directions freely with the same coefficient k . In some media this is not realistic, as the structure of the media itself could affect the motion of the particles, and equation (4.1) has to be modified in order to take such informations into account. In particular, we consider the equation

$$\frac{\partial C}{\partial t} = \nabla \cdot (\mathbf{D} \nabla C) \quad (4.2)$$

where \mathbf{D} is a symmetric tensor called the **diffusion tensor**. The tensor \mathbf{D} can be used in many ways to extract information on the underlying media. In particular, \mathbf{D} can be diagonalized as

$$\mathbf{D} = Q^T \Lambda Q \quad (4.3)$$

where Q is an orthogonal matrix whose columns are the eigenvectors (v_1, v_2, v_3) of \mathbf{D} and Λ is a diagonal matrix whose diagonal elements $(\lambda_1, \lambda_2, \lambda_3)$ are the eigenvalues of \mathbf{D} . We can think to the v_i as being the principal directions of diffusion and to the λ_i as being weights relative to such directions. A very common measure of the anisotropy is given by the so-called **fractional anisotropy** (FA) coefficient, that is defined in terms of the λ_i as

$$FA = \frac{1}{\sqrt{2}} \frac{\sqrt{(\lambda_1 - \lambda_2)^2 + (\lambda_2 - \lambda_3)^2 + (\lambda_3 - \lambda_1)^2}}{\sqrt{\lambda_1^2 + \lambda_2^2 + \lambda_3^2}}. \quad (4.4)$$

4.2 Principles of Magnetic Resonance Imaging

Magnetic Resonance Imaging (MRI) is an imaging technique used in medicine. It is based on the fact that living tissues contain a big quantity of molecules of water. The tissue to scan is put in a strong (static) magnetic field, so that the spins of most of the hydrogen protons contained in water tend to align with the applied field. The magnetization vector M of a portion of tissue (defined as the sum of the magnetic moments of the atoms composing the portion) is measured at this step and gives a value M_0 . The tissue is then briefly exposed to a Radio Frequency (RF) current having the right frequency to flip the spins of the proton. After such impulse, the spins tend to recover the orientation given by the static magnetic field (relaxation) and such process is "recorded" by means of receiving coils that measure M in the plane perpendicular to the static magnetic field. The relaxation phase is characterized by two time constants:

1. T_1 is called the spin-lattice relaxation time, i.e. a quantity in relation with the component of the magnetization along the direction of the applied field;
2. T_2 is called the spin-spin relaxation time and is related to the interactions between the proton being analyzed and its neighbors.

This phenomenon can be described in mathematical terms with the **Bloch equations**

$$\frac{dM_x}{dt} = \gamma(M_y B_z - M_z B_y) - \frac{M_x}{T_2} \quad (4.5)$$

$$\frac{dM_y}{dt} = \gamma(M_z B_x - M_x B_z) - \frac{M_y}{T_2} \quad (4.6)$$

$$\frac{dM_z}{dt} = \gamma(M_x B_y - M_y B_x) - \frac{M_z - M_0}{T_1} \quad (4.7)$$

being M the magnetization or magnetic polarization, M_0 the initial magnetization, γ the gyromagnetic ratio of the water proton and B the applied gradient field.

4.2.1 dMRI

Diffusion MRI (dMRI), also referred as Diffusion Tensor MRI (DTMRI), is an evolved technique of MRI based on the observation that water molecules in living tissues are not static, but they are diffusing into the media. The measurement of such diffusion can be used to extract information on the structure of the tissues. For example, for the human brain, many studies have proved that the diffusion of water in white matter is different from diffusion in gray matter (see, for example, [62, 89, 90]). This is mainly due to the fact that white matter is composed of axons (see fig. 4.2) where the diffusion has a privileged direction, that is the direction of the myelin sheath. Those results can be very useful in the analysis of altered tissues.

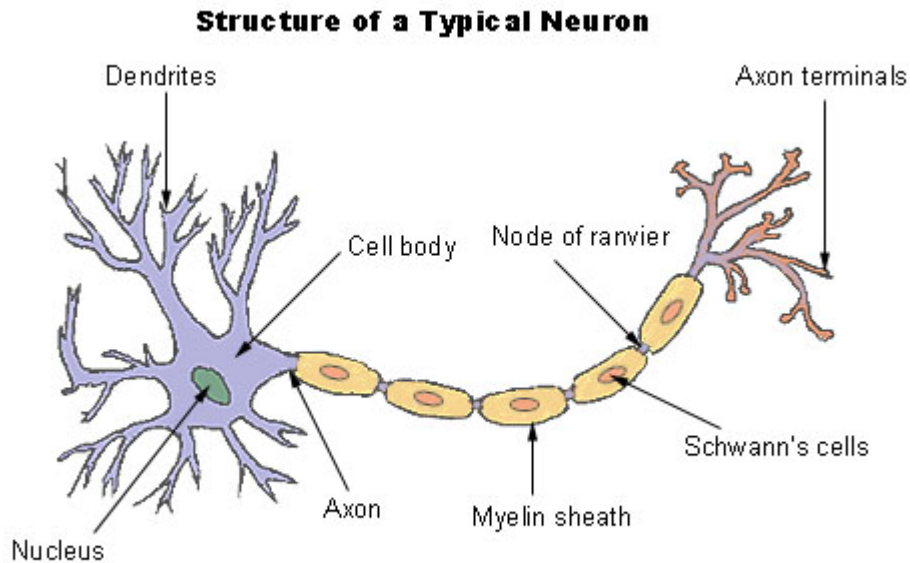


Figure 4.2: An Axon.

DT-MRI experiments can be modeled by means of the the so called **Bloch-Torrey equation**, that is obtained by the Bloch equations introducing the diffusion term introduced in (4.2)

$$\frac{d\mathbf{M}}{dt} = \gamma(\mathbf{M} \times \mathbf{B}) - \frac{M_x \mathbf{e}_1 + M_y \mathbf{e}_2}{T_2} - \frac{(M_z - M_0) \mathbf{e}_3}{T_1} + \nabla \cdot (\mathbf{D} \nabla \mathbf{M}). \quad (4.8)$$

Usually, both the Bloch-Torrey and the Bloch equations are simplified by neglecting the z component of the magnetization vector. This can be done because the applied field is directed in the z direction. In these cases, we only consider an equation for $M_{xy} = M_x + iM_y$, i.e. the transverse components of M , that can be easily obtained from (4.9) and has the form, using a complex notation and neglecting relaxation

$$\frac{\partial \mathbf{M}_{\mathbf{xy}}}{\partial t} = -i\gamma(\mathbf{r} \cdot \mathbf{G})\mathbf{M}_{\mathbf{xy}}(\mathbf{r}, t) + \nabla \cdot (\mathbf{D}\nabla \mathbf{M}_{\mathbf{xy}}(\mathbf{r}, t)). \quad (4.9)$$

Equation (4.9) can be used to derive a model for the attenuation of the signal, that is the quantity recorded during MRI experiments. In particular, we assume a solution for (4.9) in the form

$$\mathbf{M}_{\mathbf{xy}}(\mathbf{r}, t) = S_0 S(t) \exp\left(-i\gamma \mathbf{r} \cdot \int_0^t \mathbf{f}(s) ds\right) \quad (4.10)$$

where $\mathbf{f}(t)$ describes the applied gradient field and $S_0 = M_0$. The time derivative of this solution is

$$\frac{\partial \mathbf{M}_{\mathbf{xy}}}{\partial t} = S_0 S'(t) \exp\left(-i\gamma \mathbf{r} \cdot \int_0^t \mathbf{f}(s) ds\right) - i\gamma \mathbf{r} \frac{d \int_0^t \mathbf{f}(s) ds}{dt} \mathbf{M}_{\mathbf{xy}}$$

and substituting into equation (4.9) we obtain the following first order ODE for $S(t)$

$$S'(t) = -S(t) \left[\left(\int_0^t \mathbf{f}(s) ds \right) \cdot \mathbf{D} \cdot \left(\int_0^t \mathbf{f}(s) ds \right) \right] \quad (4.11)$$

that has solution

$$S(t) = \exp\left(- \left[\left(\int_0^t \mathbf{f}(s) ds \right) \cdot \mathbf{D} \cdot \left(\int_0^t \mathbf{f}(s) ds \right) \right] \right). \quad (4.12)$$

For the following particular choice of f , that has been proposed by Stejskal and Tanner

$$\mathbf{f}(t) = \begin{cases} 1 & 0 < t < \delta \\ -1 & \Delta < t < \delta + \Delta \\ 0 & \text{elsewhere} \end{cases} \quad (4.13)$$

it is easy to prove that the expression of the signal (4.12) simplifies to

$$S(t) = S_0 \exp\left(-(\gamma G \delta)^2 \left(\Delta - \frac{\delta}{3}\right) \mathbf{g}^T \mathbf{D} \mathbf{g}\right) \quad (4.14)$$

where G is the intensity of the applied gradient field and \mathbf{g} is its direction. The quantity $(\gamma G \delta)^2 \left(\Delta - \frac{\delta}{3}\right)$ is referred to as **b-value**, leading to the final expression of the attenuation

$$S(t) = S_0 \exp(-b \mathbf{g}^T \mathbf{D} \mathbf{g}). \quad (4.15)$$

It is worth observing that the signal is measured at a final time TE , often called **echo time**, that is the time elapsing between the starting of the RF pulse and the maximum value of the signal.

4.3 Estimation of the diffusion tensor

Given a set of measurements for the signal S and the initial measurement S_0 , equation (4.15) can be used to estimate the coefficients of the diffusion tensor (compare [98]). In particular, the usual approach consists in manipulating (4.15) in order to obtain an over-dimensional linear system that is solved by means of a least squares approximation. We consider a set of measurements $\{S_i\}_{i=1,\dots,m}$ obtained in correspondence to a set of directions $\{\mathbf{g}_i\}_{i=1,\dots,m}$ and b -values $\{b_i\}_{i=1,\dots,m}$ such that $m \geq 6$ and there are at least six different directions between the \mathbf{g}_i 's. These assumptions are necessary because, in order to estimate the diffusion tensor, we need to estimate six components (as the tensor is symmetric). In particular, denoting

$$\mathbf{D} = \begin{pmatrix} D_{xx} & D_{xy} & D_{xz} \\ D_{xy} & D_{yy} & D_{yz} \\ D_{xz} & D_{yz} & D_{zz} \end{pmatrix}$$

we obtain from (4.15)

$$\log \frac{S_i}{S_0} = -b_i \mathbf{g}_i^T \mathbf{D} \mathbf{g}_i \quad i = 1, \dots, m.$$

The explicit expression for $\mathbf{g}_i^T \mathbf{D} \mathbf{g}_i$ is the quadratic form

$$g_{ix}^2 D_{xx} + g_{iy}^2 D_{yy} + g_{iz}^2 D_{zz} + 2g_{ix}g_{iy}D_{xy} + 2g_{ix}g_{iz}D_{xz} + 2g_{iy}g_{iz}D_{yz}$$

that can be written as the product

$$\mathbf{k}_i \bar{\mathbf{D}}$$

where

$$\mathbf{k}_i = \left[g_{ix}^2 \quad g_{iy}^2 \quad g_{iz}^2 \quad 2g_{ix}g_{iy} \quad 2g_{ix}g_{iz} \quad 2g_{iy}g_{iz} \right], \quad \bar{\mathbf{D}} = \begin{bmatrix} D_{xx} \\ D_{yy} \\ D_{zz} \\ D_{xy} \\ D_{xz} \\ D_{yz} \end{bmatrix}$$

Denoted with \mathbf{K} the matrix whose rows are the vectors \mathbf{k}_i and with \mathbf{B} the vector whose elements are $\left(-\frac{\log \frac{S_i}{S_0}}{b_i} \right)$, we can estimate the coefficients of the diffusion tensor solving the $m \times 6$ linear system

$$\mathbf{K} \bar{\mathbf{D}} = \mathbf{B}.$$

4.4 The fractional approach

Living tissues on a microscopic scale are highly heterogeneous media, made of channels, membranes and areas of different viscosity. All these factors affect the diffusion of the water molecules into the tissues making it different from that predicted by the diffusion equations (4.1) and (4.2). It is easy to verify that a solution of (4.1) is the classical Gaussian PDF, so molecular diffusion in the standard case happens

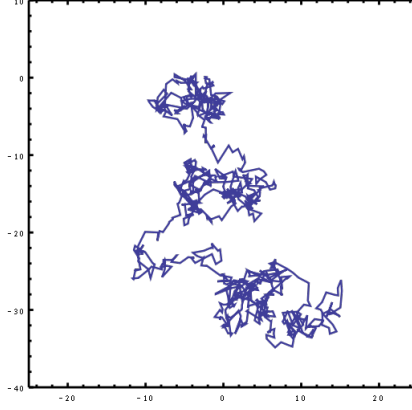


Figure 4.3: Example of trajectory of a random walker according to the laws of Brownian Motion.

according to the law of Brownian motion (fig 4.3). In particular, if we consider a 1D case, the mean squared distance traveled by a random walker can be described as

$$E[\Delta x^2] = 2kt$$

where k has the same meaning as (4.1). Such a law is generalized as

$$E[\Delta x^2] = 2kt^{2H},$$

and we talk of sub-diffusion if $H < \frac{1}{2}$ and of super-diffusion if $H > \frac{1}{2}$. This generalization is obtained introducing fractional derivatives with respect to time and/or space in the standard diffusion equation, providing

$$\frac{\partial^\alpha C}{\partial t^\alpha} = k' \Delta^{\frac{\beta}{2}} C. \quad (4.16)$$

where k' is a generalized diffusion coefficient with units modified to recover the identities and $0 < \alpha \leq 1$, $1 < \beta \leq 2$. Fractional derivatives can be defined in several ways. For space-fractional derivatives, we consider the Riesz formulation

$${}_{RZ}D^\beta f(x) = \Gamma(1 + \beta) \frac{\sin \frac{\pi\beta}{2}}{\pi} \int_0^\infty \frac{f(x+t) - 2f(x) + f(x-t)}{t^{\beta+1}} dt \quad (4.17)$$

while for time-fractional derivatives we introduce the Caputo definition

$${}_a^C D^\alpha f(t) = \frac{1}{\Gamma(1 - \alpha)} \int_a^t \frac{f(\tau) d\tau}{t - \tau^\alpha}. \quad (4.18)$$

It is worth observing that the stochastic description of the motion of a random walker generated by a space-fractional generalization of the diffusion equation by means of Riesz derivatives gives rise to a stochastic process that is called Lévy Flight, i.e. a process governed by heavy tailed distributions (fig. 4.4).

4.4.1 Fractional extensions of the Bloch-Torrey equation

Following [95], we present two possible fractional generalizations of the Bloch-Torrey equation, considering the simple case in which D is a scalar.

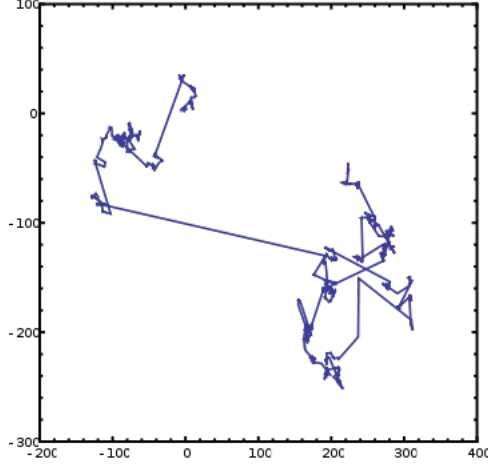


Figure 4.4: Example of trajectory of a random walker according to the laws of a Lévy Flight.

- A space-fractional generalization:

$$\frac{\partial \mathbf{M}_{\mathbf{xy}}}{\partial t} = -i\gamma(\mathbf{r} \cdot \mathbf{G})\mathbf{M}_{\mathbf{xy}}(\mathbf{r}, t) + D\mu^{2(\beta-1)}\Delta^{2\beta}(\mathbf{M}_{\mathbf{xy}}(\mathbf{r}, t)). \quad (4.19)$$

where $\frac{1}{2} < \beta \leq 1$ and being μ a parameter used to regularize the units. Performing for the signal an analysis similar to that made for (4.9), we obtain

$$S = S_0 \exp \left(-D\mu^{2(\beta-1)}(\gamma G \delta)^{2\beta} \left(\Delta - \delta \frac{2\beta - 1}{2\beta + 1} \right) \right).$$

- A time-fractional generalization:

$$\tau_0^{\alpha-1} {}_0^C D_\alpha^t \mathbf{M}_{\mathbf{xy}} = -i\gamma(\mathbf{r} \cdot \mathbf{G})\mathbf{M}_{\mathbf{xy}}(\mathbf{r}, t) + \nabla \cdot (\mathbf{D} \nabla \mathbf{M}_{\mathbf{xy}}(\mathbf{r}, t)). \quad (4.20)$$

leads, in the case of an applied gradient field of magnitude G in the z direction, to the following expression for the signal

$$S = S_0 E_\alpha(-i\gamma G z \tau (t/\tau)^\alpha) \exp(-B(t/\tau)^{3\alpha})$$

where E_α is the single parameter Mittag-Leffler function and B is defined as follows

$$B = \frac{2\Gamma(2-\alpha)D\gamma^2 G^2 \tau^3}{3\alpha^2 \Gamma(2\alpha+1)}.$$

A further generalization has been recently introduced in [62], considering a space fractional BT equation in the general case where \mathbf{D} is the diffusion tensor. Consider the decomposition of \mathbf{D} given in (4.3). Let $\{\mathbf{V}^\theta, \mathbf{V}^\phi, \mathbf{V}^\psi\}$ be the columns of \mathbf{Q} , i.e. the eigenvectors of \mathbf{D} ordered in the sense of increasing eigenvalues. The matrix \mathbf{Q} induces on the tridimensional space a coordinate change: let \mathbf{r}' , \mathbf{G}' be respectively the position vector and the applied gradient field in the new coordinate system. A fractional in space generalization of equation (4.9) can be written as

$$\frac{\partial \mathbf{M}_{\mathbf{xy}}}{\partial t} = -i\gamma(\mathbf{r}' \cdot \mathbf{G}')\mathbf{M}_{\mathbf{xy}}(\mathbf{r}, t) + \nabla \cdot (\mu^\beta \mathbf{D} \nabla \mathbf{M}_{\mathbf{xy}}(\mathbf{r}, t)), \quad (4.21)$$

where the gradient operator is now to be understood in the \mathbf{r}' coordinate system. Such an equation provides the following model for the signal

$$S = S_0 \exp \left(- \sum_{h=\theta, \phi, \psi} \mu_h^{2\beta_h - 2} \lambda_h |\gamma \delta \mathbf{G}^T \mathbf{V}^h|^{2\beta_h} \left(\Delta - \delta \frac{2\beta_h - 1}{2\beta_h + 1} \right) \right). \quad (4.22)$$

4.5 Numerical Experiments

We considered a set of MRI images of an ex-vivo rat heart. While, in the case of brain, images can be obtained in-vivo, with the heart it is more difficult due to the fact that the heart is moving and deforming. The dataset contained 514 images obtained by varying both the direction of the applied gradient field and the b -value plus a non-weighted image. The maximum applied gradient field was $99.3G/cm$ corresponding to a b -value of $4000s/mm^2$. The times δ and Δ were chosen as $3ms$ and $7ms$ respectively. Each image consists of a grid of resolution 96×96 points in the xy coordinates and of 22 slices in the axial direction. An example of non-

Table 4.1: Information on the dataset

	value	number of directions
1	160	6
2	320	12
3	480	8
4	640	6
5	800	24
6	960	24
7	1280	12
8	1440	30
9	1600	24
10	1760	24
11	1920	8
12	2080	24
13	2240	48
14	2560	6
15	2720	48
16	2880	36
17	3040	24
18	3200	24
19	3360	48
20	3520	24
21	3840	24
22	4000	30

weighted image for a slice is shown in figure 4.5, while figure 4.6 shows an acquisition for the same slice at a certain b -value and a certain direction. As it can be seen

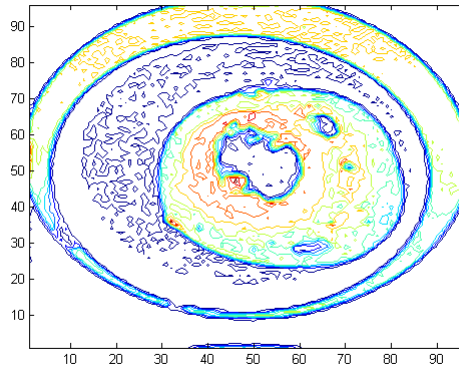


Figure 4.5: Non-weighted image

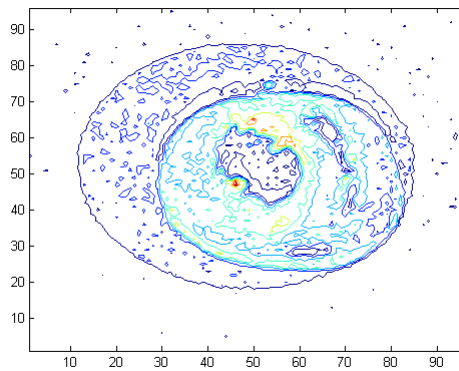


Figure 4.6: An example of signal acquisition

from figures, the images have to be preprocessed in order to remove those points where actually there is no tissue. Numerical experiments have been performed in order to fit the μ and the β parameters in the model (4.22). An estimation of such parameters can give us insights on the structure of the heart, opening the road to new possible diagnostic techniques. In order to do that, we followed two strategies, comparing the results.

- at first, we followed the same approach proposed in [62]: we considered a restricted set of measures, obtained in correspondence of a fixed b-value (in particular $b = 1440$) in order to estimate the coefficients of the diffusion tensor with model (4.15) and then we ran a minimization routine on the whole data-set. It is worth observing that that the procedure used to estimate the diffusion tensor coefficient is not the one described in Section 3, in fact, as observed also in [85], a better approach is that of setting the problem as a non linear minimization problem, i.e. by minimizing the squared norm of the residuals.
- An alternative approach consists in solving a minimization problem with the coefficients of the diffusion tensor as variables, in order to obtain a better fitting of the measured signal.

The minimization problem turned out in both cases to be very sensitive, in fact, the numerical results show an high dependance on the starting approximations provided to the routine. In particular, the first approach described above is very sensitive on the choice of the b-value subset used in the approximation of the diffusion tensor (compare Table 4.2). The results obtained following the first approach reflect those in [62], showing that the β coefficient in the direction of the third eigenvector of \mathbf{D} has a lower value compared to the other two (compare fig. 4.7). The second approach

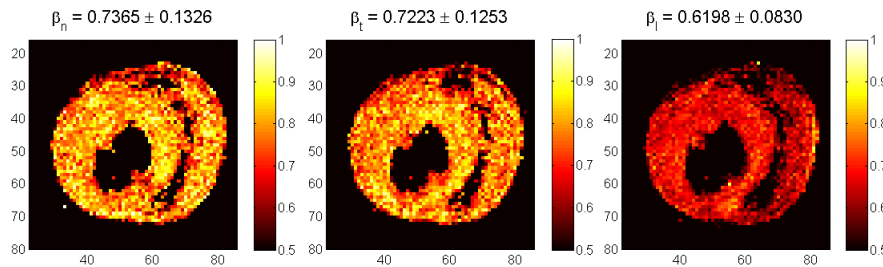


Figure 4.7: computed values of beta

turned out to be more effective in the approximation of the signal (compare figures 4.10 4.11 and 4.12). In order to provide good starting values for the minimization routine, which depends strongly on them, we ran the two approaches in sequence, i.e. we computed approximations to \mathbf{D} , μ and β with the first approach and then we used these values as starting approximations for the solution of the second minimization problem. The values for μ and β computed with such an approach are shown in fig. 4.8. The results are consistent with the ones shown in fig. 4.7, showing just a little reduction of the standard deviation. Fig. 4.9 shows a comparison between the fractional anisotropies computed with the two different approaches.

Table 4.2: Influence of the initial data on the results with the first approach

initial b -value	eigenvectors	eigenvalues
800	(0.5403 0.7881 -0.2949)	0.0010
	(-0.0525 0.3814 0.9229)	0.0012
	(0.8399 -0.4831 0.2474)	0.0017
960	(0.5945 0.6026 -0.5324)	0.0010
	(-0.0878 0.7068 0.7019)	0.0012
	(0.7993 -0.3705 0.4731)	0.0016
1440	(0.5673 0.4316 -0.7014)	0.0009
	(0.0485 -0.8677 -0.4947)	0.0011
	(-0.8221 0.2466 -0.5132)	0.0014
2240	(0.4891 0.6741 -0.5535)	0.0008
	(0.1576 -0.6924 -0.7041)	0.0010
	(-0.8579 0.2572 -0.4449)	0.0012
2720	(0.4911 0.8618 -0.1272)	0.0008
	(-0.5045 0.4004 0.7649)	0.0009
	(0.7101 -0.3115 0.6314)	0.0012
2880	(-0.2933 0.3691 0.8819)	0.0007
	(0.4177 0.8792 -0.2291)	0.0008
	(0.8600 -0.3012 0.4120)	0.0011
3360	(-0.3397 -0.8634 0.3732)	0.0006
	(-0.1886 0.4512 0.8723)	0.0008
	(0.9214 -0.2259 0.3161)	0.0009
4000	(0.1842 0.9581 0.2196)	0.0005
	(0.1587 -0.2494 0.9553)	0.0007
	(-0.9700 0.1411 0.1980)	0.0008

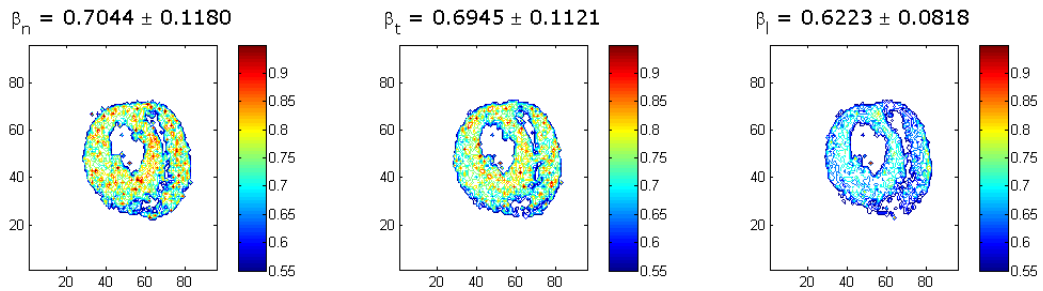


Figure 4.8: Computed values of beta with the second approach

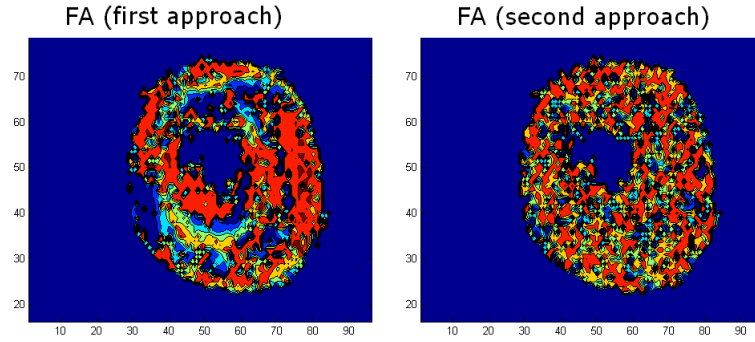


Figure 4.9: Comparison of Fractional Anisotropies

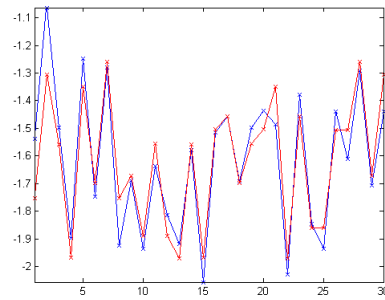


Figure 4.10: Numerical and measured signal for $b = 1440$ with the full-fractional model

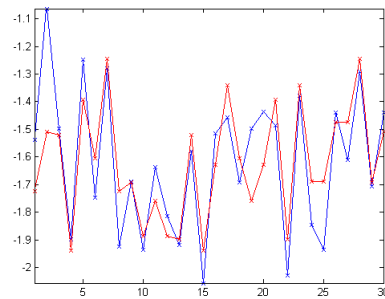


Figure 4.11: Numerical and measured signal for $b = 1440$ with the fractional model

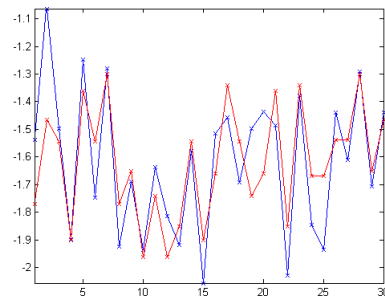


Figure 4.12: Numerical and measured signal for $b = 1440$ with the standard model

Conclusions and Future Perspectives

This thesis is based mainly on three topics

1. the analysis and development of new numerical schemes for second order Ordinary Differential Equations belonging to the family of General Linear Nyström methods, treated in the second part of Chapter 2;
2. the geometric integration of Hamiltonian systems of Ordinary Differential Equations, discussed in Chapter 3;
3. the analysis of Diffusion Tensor Magnetic Resonance heart images finalized to the extraction of structural tissue information, which is presented in Chapter 4.

Concerning the numerical integration of second order problems, we developed an algebraic theory of order for General Linear Nyström methods, which is extremely useful in the construction of new methods. We also gave a few examples of construction techniques, exploiting the effectiveness of our theory and shown how to produce starting methods for such algorithms. The theory of General Linear Nyström methods is very young and still much work can be done to expand it; in particular, in a future perspective, efforts must be put in the construction of highly stable methods, in order to improve the results presented in Section 2.2.6, that are highly encouraging, since the constructed method is much more effective than the corresponding RK scheme. Another possible direction in the future research on this topic regards the investigation of geometric properties of General Linear Nyström methods. In this view, we already developed time reversal symmetry conditions, presented in Section 3.5.1. The results above discussed are published in [51] and in another recently submitted paper.

Conversely, the theory of General Linear Methods for first order problems is solid and well established, but still much work can be done. In particular, the geometric properties of these methods can be investigated more in detail, since recent works show that the conditions of G-symplecticity can probably be weakened, thus opening the road to the research of new methods that are computationally less expensive than the ones presented here. For example, it would be of great interest to develop explicit G-symplectic methods. In this thesis, we dealt with the issues related to the construction of new G-symplectic General Linear Methods. The main issue, as it was widely discussed in Chapter 4, is that of parasitism, that have been successfully solved, thus allowing to construct four new methods with very good conservation

properties. We also investigated the relation between the order of a method and its ability to preserve invariants also if it does not possess particular geometric properties and finally we characterized the order of accuracy of the Hamiltonian deviation as a measure of the invariants preserving ability of a method. Another possible scenario for a future work on the subject of General Linear Methods for first order Ordinary Differential Equations is that of developing collocation based General Linear Methods, possessing high-stability properties and allowing to provide a continuous approximation of the solution. Our results on this topic are published in [36, 52] and a third paper has been recently submitted.

The work on the analysis of Diffusion Tensor Magnetic Resonance heart images is still in progress, it has wide possibilities for future developments and it is of great scientific relevance. It is crucial at this step to perform a statistical analysis on as many data sets as possible, in order to reinforce the conclusions shown here and also to deeply analyze all the possible implications of these results, in order to find new fields of application.

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