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Multi-Value Numerical Modeling for Special Differential Problems

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Abstract

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 **??**) 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-multivalue 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 expres-

sion 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 multivalue 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 **??**. 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 multivalue 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.