Abstract

The aim of this research is the construction and the analysis of new families of numerical methods for the integration of special second order Ordinary Differential Equations (ODEs). The modeling of continuous time dynamical systems using second order ODEs is widely used in many fields of applications, as celestial mechanics, seismology, molecular dynamics, or in the semidiscretisation of partial differential equations (which leads to high dimensional systems and stiffness). Although the numerical treatment of this problem has been widely discussed in the literature, the interest in this area is still vivid, because such equations generally exhibit typical problems (e.g. stiffness, metastability, periodicity, high oscillations), which must efficiently be overcome by using suitable numerical integrators. The purpose of this research is twofold: on the one hand to construct a general family of numerical methods for special second order ODEs of the type $y'' = f(y(t))$, in order to provide an unifying approach for the analysis of the properties of consistency, zero-stability and convergence; on the other hand to derive special purpose methods, that follow the oscillatory or periodic behaviour of the solution of the problem.

In this work we focus our attention on the initial value problems based on special second order ODEs

$$\begin{cases} y''(t) = f(y(t)), \quad t \in [t_0, T], \\ y(t_0) = y_0 \in \mathbb{R}^d, \\ y'(t_0) = y'_0 \in \mathbb{R}^d, \end{cases} \tag{1}$$

where the function $f : \mathbb{R}^d \to \mathbb{R}^d$ does not explicitly depend on y' and is supposed to be smooth enough in order to ensure that the corresponding problem (1) is Hadamard well-posed. Although the problem (1) could be transformed into a doubled dimensional system of first order ODEs and solved by standard formulae for first order differential systems, the development of numerical methods for its direct integration is more natural and efficient. We are concerned with General Linear Methods (GLMs) for second order

ODEs, with the aim to provide an unifying approach for the analysis of the basic properties of numerical methods for ODEs. This class of methods properly includes all the classical methods already considered in the literature, such as linear multistep methods, Runge-Kutta-Nyström methods, two-step hybrid methods and two-step Runge-Kutta-Nyström methods as special cases. The family of methods that we consider is wider and more general with respect to the ones already considered in the literature: in fact, our new methods depend on more parameters which can be exploited, for instance, in order to provide a better balance between order of convergence and stability properties.

A systematic theory concerning GLMs for first order ODEs is due to J. C. Butcher to provide an unifying framework for the approach to the basic questions of consistency, convergence and stability of numerical methods for ODEs. It is important to observe that the discovery of a GLM theory "opened the possibility of obtaining essentially new methods which were neither Runge-Kutta nor linear multistep methods nor slight variations of these methods".

For second order ODEs (1) no systematic investigation on GLMs has begun till now: even if many linear and nonlinear methods appeared in the literature there is not yet a very wide and general class of methods for the numerical solution of the problem (1) together with a series of general theorems which provide an unifying framework to analyze the properties of such methods. In order to transfer to second order ODEs the same benefits obtained in the case of first order ODEs, the purpose of this work is the foundation of a theory of GLMs for the numerical solution of (1), starting from a suitable formulation of these methods.

Part 1 of this dissertation is devoted to laying the foundations of the theory of GLMs for second order ODEs. Part 2, instead, concerns with the construction and the theoretical analysis of special purpose methods, that represent an efficient approach to the problem (1) in presence of periodicity and high oscillations in the solution; in particular, we will concern with the so-called exponentially fitted methods. In fact, classical numerical methods for ODEs may not be well-suited to follow a prominent periodic or oscillatory behaviour of the solution, because, in order to catch the oscillations, a very small stepsize would be required with corresponding deterioration of the numerical performances, especially in terms of efficiency. For this reason, many classical numerical methods have been adapted in order to efficiently approach the oscillatory behaviour. One of the possible ways to proceed in this direction can be realized by imposing that a numerical method exactly integrate (whitin the round-off error) problems of type (1) whose solution can be expressed as linear combination of functions other than polynomials.