Preface

"A basic idea behind the design of numerical schemes is that they can preserve the properties of the original problems as much as possible... Different representations for the same physical law can lead to different computational techniques in solving the same problem, which can produce different numerical results..." (Kang Feng, cited in [97]).

Differential equations play an important role in applied mathematics and are omnipresent in the sciences and in technical applications. They appear in many different fields such as chemical reaction kinetics, molecular dynamics, electronic circuits, population dynamics, control theory and astrodynamical problems, to name just a few. However, since the early days of the subject, it has become evident that very often finding closed solutions is either simply impossible or extremely difficult. Therefore, computing or approximating solutions of differential equations, partial as well as ordinary, linear or nonlinear, constitutes a crucial ingredient in all mathematical sciences.

Very often in applications, the differential equation modeling the physical phenomenon one aims to study possesses qualitative (geometric) properties which are absolutely essential to preserve under discretization. Hamiltonian systems constitute a clear example. These appear in many different contexts (classical, statistical and quantum mechanics, molecular dynamics, celestial mechanics, etc.) and have a number of features that are not shared by generic differential equations. These specific traits may be traced back to the fact that Hamiltonian flows define symplectic transformations in the underlying phase space.

The numerical integration of Hamiltonian systems by a conventional method results in discrete dynamics that are not symplectic, since there is *a priori* no reason whatsoever as to why numerical schemes should respect this property. If the time interval is short and the integration scheme provides a reasonable accuracy, the resulting violation of the symplectic character may be tolerable in practice. However, in many applications one needs to consider large time intervals so that the computed solution is useless due to its lack of symplecticity. One has then to construct special-purpose integrators that when applied to a Hamiltonian problem do preserve the symplectic structure at the discrete level. These are known as *symplectic integration algorithms*, and they not only outperform standard methods from a qualitative point of view, but also the numerical error accumulates more slowly. This of course becomes very important in long-time computations.

Starting from the case of symplectic integration, the search for numerical integration methods that preserve the geometric structure of the problem was generalized to other types of differential equations possessing a special structure worth being preserved under discretization. Examples include volume-preserving systems, differential equations defined in Lie groups and homogeneous manifolds, systems possessing symmetries or reversing symmetries, etc. Although diverse, all these differential equations have one important common feature, namely that they all preserve some underlying geometric structure which influences the qualitative nature of the phenomena they produce. The design and analysis of numerical integrators preserving this structure constitutes the realm of *Geometric Numerical Integration*. In short, in geometric integration one is not only concerned with the classical accuracy and stability of the numerical algorithm, but the method must also incorporate into its very formulation the geometric properties of the system. This gives the integrator not only an improved qualitative behavior, but also allows for a significantly more accurate long-time integration than with general-purpose methods. In the analysis of the methods a number of techniques from different areas of mathematics, pure and applied, come into play, including Lie groups and Lie algebras, formal series of operators, differential and symplectic geometry, etc.

In addition to the construction of new numerical algorithms, an important aspect of geometric integration is the explanation of the relationship between preservation of the geometric properties of a numerical method and the observed favorable error propagation in long-time integration.

Geometric Numerical Integration has been an active and interdisciplinary research area since the 1990s, and is nowadays the subject of intensive development. The monograph [227] played a substantial role in spreading the interest of symplectic integration within the international community working in the numerical analysis of ordinary differential equations. A more recent book on numerical Hamiltonian dynamics is [158], whereas the most authoritative monograph on Geometric Numerical Integration at present is [119], with two editions and more than 2800 citations in Google Scholar.

Although books [97, 119, 158, 227] constitute invaluable references in the field of Geometric Numerical Integration, it is the authors' belief that there is still a gap to be filled. On the one hand, books [97, 158, 227] are devoted almost exclusively to symplectic integration and numerical Hamiltonian dynamics. On the other hand, the monograph [119] is without any doubt the standard reference on the subject, but as such it might be too advanced for researchers or post-graduate students with different backgrounds wishing to initiate themselves in the field. The present book thus has a double goal. First, it is intended as a (concise) introduction to the main themes, techniques and applications of geometric integrators for researchers in mathematics, physics, astronomy or chemistry already familiar with numerical tools for solving differential equations. Second, it might constitute a bridge from the traditional training in the numerical analysis of differential equations to the most recent and advanced research literature in the field of numerical geometric integration.

It is assumed only that the reader has a basic undergraduate training in differential equations, linear algebra, and numerical methods for differential equations. More advanced mathematical material necessary in several parts of the book is collected in the Appendix. Also, for reader's convenience (and also for self-consistency) we have distributed along the book some of the basic features of Hamiltonian dynamical systems, in order to facilitate the discussion and understanding of their numerical treatment. Much emphasis is put on illustrating the main techniques and issues involved by using simple integrators on well known physical examples. These illustrations have been developed with the help of MATLAB®, and the corresponding codes and model files (including updates) can be dowloaded from the Web site accompanying the book

`http://www.gicas.uji.es/GNIBook.html`

Readers will find that they can reproduce the figures given in the text with the programs provided. In fact, it is not difficult to change parameters or even the numerical scheme to investigate how they behave on the systems provided. Although we have used MATLAB, there are of course other widely available free alternatives to this commercial package. We mention in particular OCTAVE, which is distributed under the Free Software Foundation's GNU Public License.

The book is based on a set of lectures delivered over the years by the authors to post-graduate students and also to an audience composed of mathematicians and physicists interested in numerical methods for differential equations. The actual project was suggested to one of the authors by Prof. Goong Chen (Texas A&M University at Qatar) during one of those lectures in Doha, Qatar, and has been made possible by NPRP Grant No. #5-674-1-114 from the Qatar National Research Fund (a member of Qatar Foundation) and by Project MTM2013-46553-C3 from the Ministerio de Economía y Competitividad (Spain).

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