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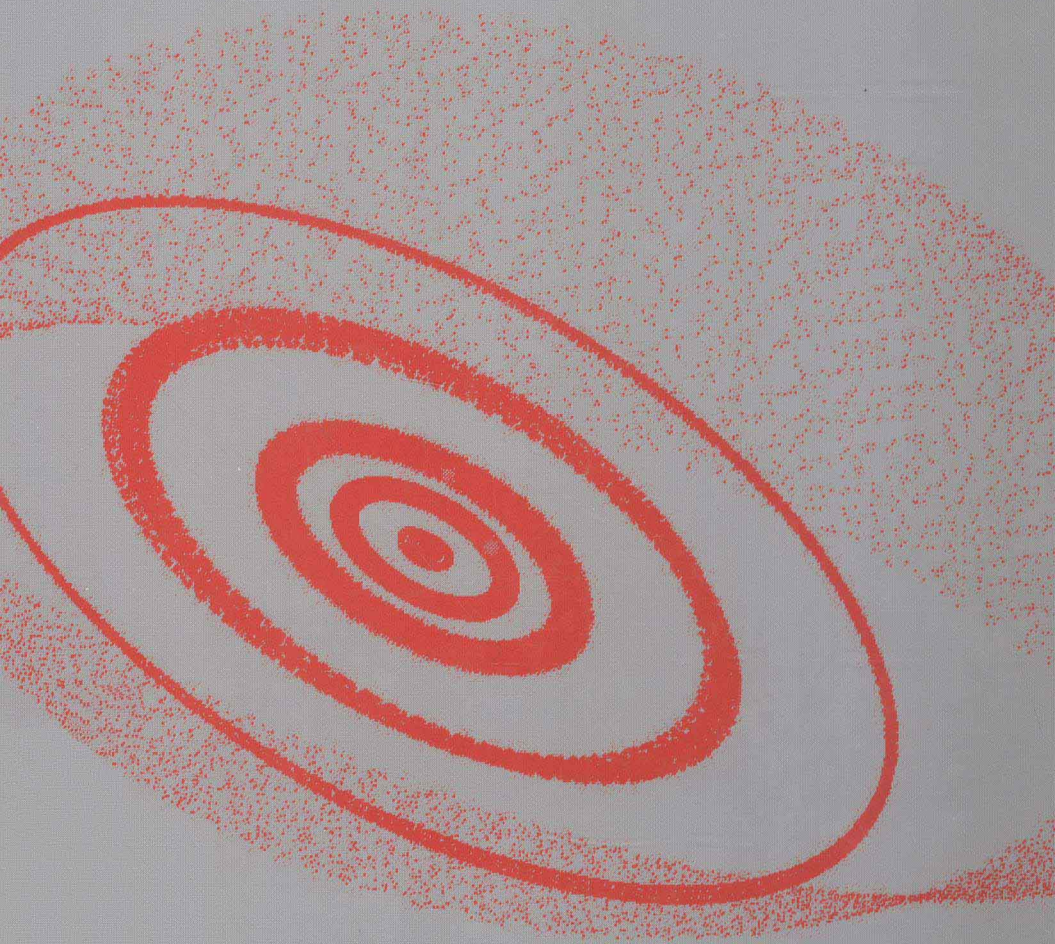
Simulating Hamiltonian Dynamics

Benedict Leimkuhler and Sebastian Reich



Simulating Hamiltonian Dynamics

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14 **Simulating Hamiltonian Dynamics**

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Preface

About geometric integration

This book is about simulating dynamical systems, especially conservative systems such as arise in celestial mechanics and molecular models. We think of the *integrator* as the beating heart of any dynamical simulation, the scheme which replaces a differential equation in continuous time by a difference equation defining approximate snapshots of the solution at discrete timesteps. As computers grow in power, approximate solutions are computed over ever-longer time intervals, and the integrator may be iterated many millions or even billions of times; in such cases, the qualitative properties of the integrator itself can become critical to the success of a simulation. *Geometric integrators* are methods that exactly (i.e. up to rounding errors) conserve qualitative properties associated to the solutions of the dynamical system under study.

The increase in the use of simulation in applications has mirrored rising interest in the theory of dynamical systems. Many of the recent developments in mathematics have followed from the appreciation of the fundamentally chaotic nature of physical systems, a consequence of nonlinearities present in even the simplest useful models. In a chaotic system the individual trajectories are by definition inherently unpredictable in the exact sense: solutions *depend sensitively on the initial data*. In some ways, this observation has limited the scope and usefulness of results obtainable from mathematical theory. Most of the common techniques rely on local approximation and perturbation expansions, methods best suited for understanding problems which are "almost linear," while the new mathematics that would be needed to answer even the most basic questions regarding chaotic systems is still in its infancy. In the absence of a useful general theoretical method for analyzing complex nonlinear phenomena, simulation is increasingly pushed to the fore. It provides one of the few broadly applicable and practical means of shedding light on the behavior of complex nonlinear systems, and is now a standard tool in everything from materials modeling to bioengineering, from atomic theory to cosmology.

As models grow in complexity and dimension, and the demands placed on simulation have risen, the need for more sophisticated numerical methods and analytic techniques also grows. Longer time interval simulations require more stable methods. Larger problems call for more efficient schemes, tailored to a particular application or family of applications. And more intricate modeling of delicate behaviors or properties requires corresponding improvements in the resolution of those properties during simulation.

In writing this book for a broad audience of scientists, we have attempted to limit the introduction of technical detail, but in some places this cannot be avoided. The calculations are generally included for the benefit of students. We hope that appreciation of the general principles will not be lost in following the details of arguments. In the words of John Von Neumann, "One expects a mathematical theorem or a mathematical theory not only to describe and classify in a simple and elegant way numerous and a priori disparate special cases. One also expects elegance in its architectural, structural make-up. . . . If the deductions are lengthy or complicated there should be some simple general principle involved, which explains the complications and details, reduces the apparent arbitrariness to a few simple guiding motivations." If there is one such guiding principle underlying our work it is this: classical mechanics – on which all physical models are based – also provides the proper foundation for numerical simulation of those systems. We will attempt to show in this book that practical, efficient methods for simulating conservative systems can be realized by making judicious use of the methods of classical mechanics.

An emphasis on methods

In this book we address ourselves primarily to the following pair of questions:

Which properties should be fundamental to an integration method for a (conservative) model?

How can we design and implement schemes that respect physical principles regardless of timestep or traditional accuracy considerations?

Although our interest is always ultimately in the methods themselves and in quantifying the relative differences among them, we will find that in attempting to answer the above questions, we are drawn far afield from the usual domain of the numerical analyst. The first question will lead us into the field of mechanics so that we may appreciate something of the nature of those structures and symmetries that underlie physical models and contribute to their long-term evolution. The second question will take us outside even the areas that have traditionally been investigated by mathematicians, since the special forms of force

functions, presence of constraints, relationships among the variables, or efficiency considerations dictate to a large extent the features of appropriate (i.e. practical) methods used in applications.

It is important to emphasize that our treatment is not comprehensive; we have made a selection from the literature which comprises – in our view – the most important material from the standpoint of practical application.

Beginning with the idea of *splitting* we will show how many simple but effective integrators can be generated by using a few building blocks. The same techniques can be used to derive more sophisticated schemes. For example, explicit higher-order methods have a very natural derivation in the case of canonical mechanical systems developed in terms of the "kinetic+potential" form of the energy.

We survey recent work on methods for constrained systems and consider various approaches to the simulation of rigid body systems, methods which offer an efficient and – in many cases – demonstrably superior geometric alternative to more widespread schemes. Variable stepsize geometric integrators will be introduced based on a rescaling of the time variable. Methods for mixed systems possessing both rapidly and slowly varying degrees of freedom – or weak and strong forces – also call for the construction of specialized schemes. In all cases, our aim will be to present the ideas in as general a form as is prudent, highlighting instances where a given technique might be of use in other applications. Molecular dynamics applications are an important source of challenging problems for geometric integration, so we devote some time to their particular characteristics. Conservative partial differential equations introduce many new issues for the development of geometric integrators, a topic we touch on in the final chapter of the book.

How to use this book

This book is intended, first, as a text for a course in computational mechanics or as a tool for self-instruction, and, second, as a basic reference for researchers and educators – regardless of discipline – interested in using and developing geometric integrators. The book should serve as a bridge from traditional training in the sciences to the recent research literature in the field of geometric integration. By emphasizing mathematical and computational issues and illustrating the various concepts and techniques with carefully developed model problems, it is hoped that the book can appeal to a wide audience, including mathematicians unfamiliar with modeling issues, and physicists, chemists, and engineers wishing to gain a better understanding of the mathematical underpinnings of existing methods or in developing effective methods for new applications.

The book assumes only that the reader has had undergraduate coursework in linear algebra and differential equations. At several points we introduce, but do

not thoroughly develop, topics from dynamical systems. A good introductory text in dynamical systems is the book of VERHULST [197]. We develop – in Chapters 2 and 3 – most of the necessary preliminaries of numerical analysis and classical mechanics from the ground up, however the reader should be aware that the treatment provided here of the required background material is necessarily brief; only those elements that are essential to our later study of geometric integrators are given. For an introduction to numerical analysis, the reader is referred to the classic books of ATKINSON [11], BURDEN AND FAIRES [37], and DAHLQUIST AND BJÖRK [48]. The book of GEAR [70] can provide a useful introduction to the numerical solution of differential equations. The books of HAIRER, NØRSETT AND WANNER [82] and HAIRER AND WANNER [84] can serve as references for obtaining a more complete picture of the mathematical issues associated with construction of methods and error analysis for ordinary differential equations. ISERLES [91] has written an integrated text that introduces numerical methods for both ordinary and partial differential equations.

First published at the end of the 19th century, ROUTH's *Dynamics of a System of Rigid Bodies (Elementary Part)*[1] remains a marvelous introduction to classical mechanics and provides a wealth of examples and exercises for the student (many of which could now be revisited with the aid of the modern computational techniques developed in this book). For a more systematic treatment to Hamiltonian classical mechanics the reader is referred to the following texts: LANDAU AND LIFSHITZ [105], MARION [121], GOLDSTEIN [73], and ARNOLD [7], all of which are well-worn occupants of our bookshelves. These books are quite varied in their use of notation and even in the way in which they motivate and explain identical material, but we have found all of them to be helpful on various occasions. If only one book is to be consulted, the elegant book of LANCZOS [104] is remarkable both in terms of its readability and its breadth, owing partly to the absence of detailed proofs. A modern rigorous treatment of classical mechanics may be found in MARSDEN AND RATIU [124], a book which also contains a number of useful examples and notes on history and applications.

The book by SANZ-SERNA AND CALVO [172] was the first to cover symplectic integration methods and applications to classical mechanics and is still an excellent introduction to the subject. The more recent book by HAIRER, LUBICH, AND WANNER [80] covers a wide range of topics from geometric integration and should be very useful as an additional reference.

In a graduate course in applied mathematics or computational physics, it is probable that much of the material of Chapters 1–3 could be skipped or skimmed, depending on the backgrounds of the students and the interests of the teacher. Some caution should be exercised here. In particular, it is essential

[1] Reprinted in 1960 as a Dover Edition.

that the student understand the concepts of convergence and order of convergence for a numerical method, the definition of the flow map, first integrals, and at least the condition for a symplectic map in terms of the Jacobian of the flow map.

Molecular dynamics provides a rich source of problems for geometric integration, and we often draw on examples from this field for motivation and for evaluation of concepts and methods. Here again, it is likely that the reader may, on occasion, wish for a more detailed description of the problems or of typical approaches used by chemists and physicists. One reference stands out in this area for clarity of presentation and breadth: ALLEN AND TILDESLEY [4]. More recent books of FRANKEL AND SMIT [66] and SCHLICK [174] help to fill in the picture.

Exercises included at the end of each chapter are intended to be demanding but not overwhelming; some of the multi-part problems could be assigned as projects, especially those involving the use of computers.

Computer software

This book primarily emphasizes the mathematical properties of algorithms for solving differential equations. In later chapters, we will often see the methods introduced and analyzed as abstract maps of phase space. This approach, while essential to understanding and generalizing the methods, has the tendency to obscure both the intuitive basis for the theory and the ultimate importance of the subject. We would like emphasize that *the student must implement and test numerical methods in order to gain a full understanding of the subject.*

While any programming language and graphics package could, in principle, be employed, the need for flexibility in the coding and testing of methods and the need to be able to work easily with scientific functions of vectors and matrices makes a specialized, interpreted language system for mathematics the best environment for problem solving.

At the time of this writing, there are several widely distributed commercial software packages that support the simplified design and testing of algorithms, including the commercial packages MATLAB, MAPLE, and MATHEMATICA. Of these, the authors prefer the user interface and programming structure of MATLAB, but this is largely a matter of taste and any of the three mentioned systems would be suitable. These packages are all available to students at heavily discounted prices and run on a variety of computer platforms.

For a student on a severe budget, there are several widely available *free* alternatives to the commercial packages. These options include, notably, OCTAVE, which is distributed under the Free Software Foundation's GNU Public License. Our experience with this software is that it is adequate for most study purposes,

although the commercial alternatives are generally superior with regard to ease-of-use, documentation, and reliability.

We will occasionally describe algorithms in this text, but we will attempt to avoid system-specific details, so the student is expected to supplement the mathematical study with study of the the user's guide for the software system they are using, in particular the appropriate sections on programming.

Notation

Let us summarize some basic notation used throughout the book. Dependent variables, such as positions $\boldsymbol{q}$ and velocities $\boldsymbol{v}$ are elements of a Euclidean space $\mathbb{R}^d$, where $d \geq 1$ is the appropriate dimension. More specifically, we will always identify dependent variables with *column vectors*. When two column vectors $\boldsymbol{u} \in \mathbb{R}^k$, $\boldsymbol{v} \in \mathbb{R}^l$ are given we may write $(\boldsymbol{u}, \boldsymbol{v})^T$ for the column vector in $\mathbb{R}^{k+l}$ obtained by concatenating the two vectors. The transpose is there to remind us that the result is again a column vector. We will often need to refer to a set indexed by a parameter for which we write $\{a_t\}_{t \in P}$, where P is the index set. As a short-hand, we will write $\{a_t\}$ if the index set is clear from the context.

The set of $k \times k$ matrices with real coefficients is $\mathbb{R}^{k \times k}$ and capital bold-face letter are used to denote matrices, e.g., $\boldsymbol{A}, \boldsymbol{B} \in \mathbb{R}^{k \times k}$. The k-dimensional identity is $\boldsymbol{I}_k$ or $\boldsymbol{I}$ as a short-hand if the dimension is clear from the context.

A vector-valued function $\boldsymbol{F} : \mathbb{R}^n \to \mathbb{R}^m$ will be assumed to map column vectors of dimension n to column vectors of dimension m. The vector of partial derivatives of a scalar-valued function $f(\boldsymbol{q})$ is identified with a *row vector* in $\mathbb{R}^d$ and is denoted by $f_{\boldsymbol{q}}(\boldsymbol{q})$ or, equivalently, by $\partial f / \partial \boldsymbol{q}\,(\boldsymbol{q})$. Hence the *Jacobian matrix* of a vector-valued function $\boldsymbol{F}(\boldsymbol{q})$ is identified with the $m \times n$ matrix $\boldsymbol{F}_{\boldsymbol{q}}(\boldsymbol{q})$.

The *scalar product*, *inner product*, or *dot product* of two column vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ in $\mathbb{R}^d$ is denoted by $\langle \boldsymbol{a}, \boldsymbol{b} \rangle$ or $\boldsymbol{a} \cdot \boldsymbol{b}$, or, simply, $\boldsymbol{a}^T \boldsymbol{b}$, where $\boldsymbol{a}^T$ is the transpose of $\boldsymbol{a}$. The *cross product* of $\boldsymbol{a}$ and $\boldsymbol{b}$ is denoted $\boldsymbol{a} \times \boldsymbol{b}$. We will frequently use

$$\widehat{\boldsymbol{a}}\boldsymbol{b} = \boldsymbol{a} \times \boldsymbol{b},$$

where $\widehat{\boldsymbol{a}} \in \mathbb{R}^{3 \times 3}$ is a skew-symmetric matrix related to the vector $\boldsymbol{a} = (a_1, a_2, a_3)^T$ by

$$\widehat{\boldsymbol{a}} = \begin{bmatrix} 0 & -a_3 & a_2 \\ a_3 & 0 & -a_1 \\ -a_2 & a_1 & 0 \end{bmatrix}.$$

The *norm* of a vector $\boldsymbol{a}$ is defined by

$$\|\boldsymbol{a}\| = \langle \boldsymbol{a}, \boldsymbol{a} \rangle^{1/2}.$$

A real-valued function f defined on an interval I of the real line is said to be square-integrable if $\int_I f(x)^2 dx$ is bounded. In that case we say that f lies in the function space L_2 on the interval I. We say that the L_2-norm of f is

$$\|f\|_2 = \left(\int_I f(x)^2 dx \right)^{\frac{1}{2}},$$

and we define the L_2-inner product of two square integrable functions f and g by

$$(f, g) = \int_I f(x) g(x) dx$$

The *gradient* $\nabla_{\boldsymbol{q}} V(\boldsymbol{q})$ of a scalar-valued differentiable function $V(\boldsymbol{q})$ is defined by

$$\langle \nabla_{\boldsymbol{q}} V(\boldsymbol{q}), \boldsymbol{u} \rangle = \lim_{\varepsilon \to 0} \frac{V(\boldsymbol{q} + \varepsilon \boldsymbol{u}) - V(\boldsymbol{q})}{\varepsilon},$$

where the equality is to hold for all vectors $\boldsymbol{u}$ of the same dimension as $\boldsymbol{q}$. This definition leads to the relation

$$\nabla_{\boldsymbol{q}} V(\boldsymbol{q}) = V_{\boldsymbol{q}}(\boldsymbol{q})^T,$$

and, hence, the gradient $\nabla_{\boldsymbol{q}} V(\boldsymbol{q})$ is a column vector.

The time derivative of a function $\boldsymbol{q}(t)$ will normally be denoted by $d\boldsymbol{q}/dt(t)$, but whenever it is more convenient we may instead use the short-hand $\dot{\boldsymbol{q}}(t)$. If clear from the context, we will also frequently drop the argument in functions and write, for example, $\dot{\boldsymbol{q}}$ instead of $\dot{\boldsymbol{q}}(t)$, or $\boldsymbol{F}$ instead of $\boldsymbol{F}(\boldsymbol{q})$. The same conventions apply to higher-order derivatives.

If a variable u depends on several independent variables such as time t and space x, then the partial derivatives are often denoted by u_t and u_x, respectively.

Given two maps $\boldsymbol{\Psi}_1 : \mathbb{R}^n \to \mathbb{R}^n$ and $\boldsymbol{\Psi}_2 : \mathbb{R}^n \to \mathbb{R}^n$ with compatible range and domain, we define their composition $\boldsymbol{\Psi}_2 \circ \boldsymbol{\Psi}_1$ by

$$[\boldsymbol{\Psi}_2 \circ \boldsymbol{\Psi}_1](\boldsymbol{z}) = \boldsymbol{\Psi}_2(\boldsymbol{\Psi}_1(\boldsymbol{z})),$$

for all $\boldsymbol{z} \in \mathbb{R}^n$. The inverse of a one-to-one map $\boldsymbol{\Psi}$ is denoted by $\boldsymbol{\Psi}^{-1}$. Hence

$$\boldsymbol{\Psi}^{-1} \circ \boldsymbol{\Psi} = \mathbf{id},$$

where $\mathbf{id}(\boldsymbol{z}) = \boldsymbol{z}$ the identity map.

Finally the Landau-order notation $\mathcal{O}(\Delta t)$ is used to denote a quantity that goes to zero as rapidly as Δt goes to zero. More generally, we will write $g(\Delta t) = \mathcal{O}(\Delta t^p)$ if $g(\Delta t)/\Delta t^p$ is bounded as $\Delta t \to 0$ but $g(\Delta t)/\Delta t^q$ is unbounded if $q > p$.

Acknowledgements

We have to admit that when we began this project, we had no appreciation for its ultimate complexity. The only thing that has kept the project going at some critical points was the broad support and encouragement we received from our families, our colleagues, and our students.

A key aspect of the book is the emphasis on applications. Brian Laird proposed the Lennard–Jones model discussed in Chapter 4 and made several other helpful comments. Chris Sweet contributed most of the numerical experiments in Chapter 6, including the long-term simulations of the solar system, and Eric Barth provided the alanine dipeptide simulation in Chapter 11. Jason Frank helped with many of the experiments in Chapter 12. Jason's tireless proofreading of the entire manuscript must also be remarked!

We hope that the book will be useful for teaching upper-division undergraduate and graduate courses. In 2002, Ph.D. students from various fields and various parts of Europe – Martin Dahlberg (chemistry), Thomas Sauvaget (mathematics/physics), Marko Vranicar (physics), and Fredrick Hedman (mathematics) – attended an informal summer school in Leicester taught from an early draft of the book. Part of the book formed the basis for a series of survey lectures given by one of us in Bari, Italy in 2002. Mitch Luskin, Claudia Wulff, and Steve Bond have subjected their classes to a preliminary draft of the book for testing in this setting, and provided useful comments.

We would like also to thank Teijo Arponen, Jeff Cash, Colin Cotter, Ernst Hairer, Zhidong Jia, Per-Christian Moan, Brian Moore, and Antonella Zanna for reading various parts of the manuscript and providing feedback. We have also relied on the extraordinary patience of Cambridge University Press, particularly our editors David Tranah and Joseph Bottrill.

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1

Introduction

This book is about numerical methods for use in simulating dynamical phenomena governed by conservative processes. In this chapter, we review a few basic principles regarding conservative models. In general, we are concerned here with initial value problems for systems of ordinary differential equations (ODEs) of the form

$$\frac{d}{dt}z = \boldsymbol{f}(z), \qquad z(t_0) = z^0,$$

where $\boldsymbol{z} : \mathbb{R} \to \mathbb{R}^k$. The basic questions encountered early on in a first course on ODEs concern existence and uniqueness of solutions, a topic addressed, for example, by Picard's theorem. Discussion then turns to various techniques for analytically solving the differential equations when $\boldsymbol{f}$ has a prescribed form. In particular, the scalar case $k = 1$ is an instance of a *separable differential equation* and such models are in principle solvable in quadratures (i.e. by evaluating certain integrals and solving certain algebraic equations). Linear systems are exactly solvable after determination of the eigenvalues and eigenvectors (or generalized eigenvectors, in the degenerate case). Beyond these and a few other special cases, most models are not exactly integrable. In this book we are mostly interested in complex models that do not admit exact solutions.

The emphasis of this book is on the particular models which are formulated naturally as *conservative systems* of ODEs, most importantly *Hamiltonian systems*. As a general rule, mechanical systems resulting from physical principles are Hamiltonian until (usually for prudent modeling purposes) subjected to simplifying reductions or truncations. For example, in typical fluid dynamics applications, the incorporation of diffusive effects due to friction with a boundary plays an essential role in the modeling. However, in many situations, the conservative paradigm can be retained and remains the most appropriate foundation for the construction of models, since it is in no small measure due to properties such as conservation of energy and angular momentum that matter behaves as it does.

The existence of Kepler's laws which approximately describe the motion of the planets in the solar system are reflections of the conservative nature of