

Book Reviews

Edited by Robert E. O'Malley, Jr.

Featured Review: Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations. By E. Hairer, C. Lubich, and G. Wanner. Springer-Verlag, New York, 2002. \$84.95. xiii+515 pp., hardcover. ISBN 3-540-43003-2.

Geometric integration is a field that was invented “too late,” and this book is an impressive record of a decade of catching up. It could have been invented at any time since Newton.¹ It could have been invented in 1957, with “a marvellous paper, short, clear, elegant, written in one week, submitted for publication—and never published” [4]. It could have been invented in 1967, when Loup Verlet introduced the leapfrog (Störmer/Verlet) method to molecular dynamics; its many desirable geometric properties were not appreciated for many years. In 1983 it was written that the symplecticity of leapfrog was well known, although perhaps it was only truly well known at SLAC and Los Alamos, and not known at all elsewhere. When I was a grad student in the late 1980s, photocopies of [3] were passed around and created a great stir, especially its Figure 2, which compared a new, symplectic integrator (showing a crisp, well-defined curve) to the hapless classical Runge–Kutta (a shapeless blur). Perhaps this mysterious word “symplectic” was also part of the appeal—some kind of secret weapon was in play. Of course, we students had no idea what was going on, and such comparisons were later criticized as unfair, but in any event, [3] unleashed the floodgates, and the 1990s saw a period of rapid development, first of symplectic integrators and then of more general geometric integrators.

It seems to me that in some areas there is a gulf between the theoreticians and the practitioners of numerical methods. Each group ignores the methods and experience of the other. Without wanting to make too much of it, geometric integration does seem to be such an area. For decades numerical analysts were either ignorant or skeptical of methods (such as leapfrog) developed and used to great effect in molecular dynamics, quantum mechanics, and elsewhere, perhaps because the methods didn't look good by the traditional criteria based on small and controllable local errors. This situation can only make it harder for numerical analysts to “sell” any new methods they may develop to their potential “customers,” which is, after all, the whole point of developing the methods.

Let us have a closer look at this leapfrog method. In [4], Hairer, Lubich, and Wanner offered a short preview of the book currently under review, exclusively from the point of view of this method. We start with a mechanical system with configuration space $\mathbb{R}^n$ (for example, a system of $n/3$ particles moving in three dimensions) and phase space $\mathbb{R}^{2n}$. Suppose the system has potential energy $V(q)$ and kinetic energy $T(p) = \frac{1}{2}\|p\|_2^2$, so that its total energy, or Hamiltonian, is $H(q, p) = T(p) + V(q)$. The

¹And perhaps it was: the leapfrog method, the prototype of all geometric integrators, has been traced back to the *Principia*—Book I, Theorem I [4].

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leapfrog method is

$$(1) \quad \frac{q_{n+1} - 2q_n + q_{n-1}}{(\Delta t)^2} = -\nabla V(q_n),$$

the form in which it was first introduced as a discretization of Hamilton's equations $\ddot{q} = -\nabla V(q)$. (In practice, the method is implemented as a map, $(q_n, p_n) \mapsto (q_{n+1}, p_{n+1})$, of phase space.) This method has many nice properties. It is explicit. It is second-order, yet requires only one evaluation of the force $-\nabla V(q)$ per time step. It conserves linear and angular momentum. Although it doesn't conserve energy exactly, in many computations one observes that the energy error is bounded. It is symmetric under $q_{n-1} \leftrightarrow q_{n+1}$, which is related to its time-reversibility. For all these reasons it was immediately adopted as the workhorse of computational molecular dynamics.

Now, for any Hamiltonian H , the flow of Hamilton's equations preserves a symplectic form on phase space. We now know that the main reason for the good long-time behavior of the leap-frog method is that it is symplectic; that is, it preserves the symplectic form exactly. Any features of the phase portrait of the flow of the system which are shared by all nearby symplectic maps (i.e., which are structurally stable under small perturbations of the system) will be inherited by the numerical integrator. To a physicist, perhaps, this means that all quantities of interest are preserved. Specifically, one expects that many qualitative features, such as quasi-periodic orbits and a lot of the fine structure of chaotic sets, will be preserved.

The symplectic property of leapfrog can be seen in several ways, each of which prompts a generalization to high-order methods and to larger classes of systems. The map can be derived from a generating function. It can be viewed as a partitioned Runge-Kutta method. It comes from the stationarity of a discrete Lagrangian. It is a splitting method: one splits the Hamiltonian $H = T + V$ and notes that the flows $\phi_{\Delta t, T}$ and $\phi_{\Delta t, V}$ of the kinetic and potential energies are simple to compute exactly, and hence are symplectic maps. The composition

$$(2) \quad \phi_{\frac{1}{2}\Delta t, T} \circ \phi_{\Delta t, V} \circ \phi_{\frac{1}{2}\Delta t, T}$$

then yields the leapfrog method (1). Symplecticity is preserved under composition because the symplectic maps form a group. In the form (2) the method preserves any symmetries, and any reversing symmetries, of the original system which are shared by the pieces T and V , for example, rotational symmetry, leading to preservation of angular momentum.

This example illustrates, then, what is meant by a "geometric" integrator. The flow of a dynamical system is a map (diffeomorphism) of phase space, and the set of diffeomorphisms forms a group. Since one can't preserve specific features, e.g., particular orbits, of this map exactly, one studies instead general features which control the dynamics. Crucially, each subgroup of the group of diffeomorphisms specifies a different class of dynamical systems with its own generic features. The infinite-dimensional subgroups—for example, of systems preserving a symplectic form, a volume form, an action of a symmetry group, or the level sets of some integrals—are small enough to constrain the dynamics in some way yet large enough to contain useful integrators.

This point of view is also useful in curing oneself of any inadvertently acquired "initial value problem...local error" brainwashing! It is true that if your goal is to compute the solution to a particular initial value problem on a fixed time interval, a classical method will usually do best. (Although because of more favorable error propagation, or because a difficult part of the problem can be treated specially, geometric integrators may still win even on this traditional test.) But a more typical

situation in dynamical systems is for orbits to separate, and hence errors to grow, exponentially in time. Individual orbits can then only be followed accurately for relatively short times, while many problems, in molecular and celestial dynamics, for example, demand extremely long simulations. For such problems classical methods give completely wrong results, and yet good results can be obtained by preserving the geometric structure of the system, which accords with the intuition that the phases of the planets and the exact positions of the gas molecules don't affect the systems' gross properties.

In *Geometric Numerical Integration* we have a rare collaboration among three mathematical generations. Hairer was a student of Wanner, the two now forming the productive "Geneva group" in numerical analysis. Lubich was a student of Hairer and is now a professor at Tübingen. Readers of the now-classic two-volume *Solving Ordinary Differential Equations* [5, 6] will know to look forward to the authors' trademarks: quotes from all the original works, photographs (or drawings) of all the actors, excellent graphics, and historically motivated examples.

This book is the first extensive treatment of its subject.² It covers the design, implementation, and especially the analysis of many types of novel integrators for many types of systems. The treatment is both broad and complete; all the theorems are proved entirely from scratch. The need to fit everything in has made the overall presentation fairly dense. It pays to read every sentence—for example, in the first paragraph, "The reader is encouraged to repeat the experiments." Absolutely! And the crucial fact that symplectic maps form a group under composition gets just one sentence on page 177. On the other hand, many proofs have been simplified from their first appearance in the literature, and the authors' experience means that the exposition of the (rather complicated) theory of order conditions via rooted trees is superb. There are so many topics that even dipping into the book is sure to reveal an interesting tidbit: on compensated summation, on QR as the flow of the Toda lattice, on an integrable discretization of the nonlinear Schrödinger equation, or the short proofs of the Baker–Campbell–Hausdorff and Kolmogorov–Arnold–Moser theorems. There are 148 exercises, many with hints, answers, or pointers to the literature. And the programs for all the algorithms and examples are on the authors' Web site.

The book's 14 chapters divide into two halves, on design and analysis of methods, respectively. The first half contains so many topics that even a summary would be too long. Considered are (partitioned) Runge–Kutta methods, splitting and composition methods, preservation of first integrals, ODEs on Lie groups, reversible and symplectic integration, Hamiltonian systems with constraints, Poisson and volume-preserving systems, and variable and multiple time-stepping. One theme is the analysis of order conditions via trees, an approach developed by John Butcher for Runge–Kutta methods but here extended in several ways, eventually to rooted trees labeled by positive integers; a whole sequence of simplifications reduces the number of conditions a certain composition method of order 6 must satisfy, for example, from 166 to just 4.

The treatment is analytical rather than geometrical and relies on a bare minimum of machinery—in theory only calculus is needed to build everything. This gives the book the widest possible potential audience. There were a few times, though, when I wished for a more geometrical approach, especially in the treatment of Lie groups and

²One earlier book, Sanz-Serna and Calvo [8], emphasized Hamiltonian systems, while McLachlan and Quispel [9] reviewed geometric integration. The current book is complemented by Budd and Piggott [2], which has a lot on PDEs, and the forthcoming Leimkuhler and Reich [7], which is more elementary and applications-oriented.

(e.g., symplectic) structures on manifolds. It is the geometry which motivates and unifies the subject, after all. The chosen examples are not typical (e.g., the pendulum is low-dimensional, and the Kepler problem is integrable, even super-integrable) and do not fully illustrate the power of a conservation law like symplecticity.

I found Chapter VII, which covers constrained, (Lie-)Poisson, and volume-preserving systems, the hardest to follow. Lie-Poisson systems are largely viewed as a reduction of a certain Hamiltonian system on (the cotangent bundle of) the square matrices, with holonomic constraints to a matrix Lie group. This is one way to do it, but then the main example, the free rigid body (p. 246) has some problems: $\dot{Q}Q^{-1}$ in equation (2.54) should be $Q^{-1}\dot{Q}$, the Hamiltonian should be left (not right) invariant, and the reduced equations (2.56) have the wrong sign. The treatment is much too brief to follow from scratch. The importance of preserving the symmetry of the full equations to allow reduction (p. 246) is not mentioned and it is hard to trace where it appears. Casimirs are defined locally through Darboux's theorem but are used globally. In equation (1.2), $M(q)\dot{v}$ should be $\frac{d}{dt}(M(q)v)$. On page 243, the terms "dual Lie algebra" and "Lie algebra $\mathfrak{g}^*$ " are not right. Apart from these minor errors I wonder how far a reader will be able to go here; perhaps there is just not enough space devoted to these topics, which, after all, have occupied workers in geometric mechanics for many years.

The second half of the book concerns the analysis of geometric integrators. Why do they work so well, especially for long times? The unifying theme here is backward error analysis. The integrator is matched to the flow of a *modified equation*, an ODE close to the original system. If the integrator is analytic, then the modified equation can be constructed recursively to any order in Δt , and by a careful truncation of its Taylor series, the error can be made exponentially small in Δt . Thus, a symplectic integrator, say, not only shares all the typical properties of symplectic *maps*, it also (very nearly) shares those of symplectic *flows*. The difference between the two is that the latter possess a conserved quantity, the Hamiltonian. Following up this idea allows the authors to prove that the energy error during a symplectic integration is bounded for exponentially long ($\mathcal{O}(e^{\text{const.}/\Delta t})$) times. Even in situations where flows and maps are not so different, backward error analysis provides a useful tool. It plays a role in reversible integration, in linear error growth for quasi-periodic orbits, in KAM theory, and in dissipatively perturbed systems. A different technique, of modulated Fourier expansions, is needed in Chapter XII on highly oscillatory ODEs. When the time step is large compared to the highest frequency of the system, the terms formerly exponentially small are now order 1, and, indeed, basic leapfrog doesn't perform well. A family of modifications is analyzed for performance on energy conservation, adiabatic invariance, and slow exchange of energy. Research on this topic is continuing as it has vital applications to solving the Schrödinger equation for the telecommunications industry.

The book will be most accessible to, and I suspect most read by, numerical analysts working (or wanting to work) in geometric integration. To drive the field forward, as indeed they have done so far, it's important that scientists with diverse backgrounds in dynamical systems, geometry, mechanics, and the numerous applications fields in physics and chemistry should read it as well.

I close by noting an interesting connection to another field. In 2002 Douglas Arnold [1] addressed the International Congress of Mathematicians in Beijing, saying, "The design of stable discretizations of systems of PDEs often hinges on capturing subtle aspects of the structure of the system in the discretization. . . . This new geometric viewpoint has provided a unifying understanding of a variety of innovative

numerical methods developed over recent decades.” Almost the same words could serve to introduce *Geometric Numerical Integration*! Now note the word *Numerical* in the title. As Hairer has remarked elsewhere, this word was included in order to distinguish the field from Hassler Whitney’s “geometric integration theory.” Arnold’s talk, however, shows that the two are not really that far apart: the function spaces introduced by Whitney in 1957 (“Whitney elements”) are exactly what is required for a *geometric* discretization of many PDEs.

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777 Mathematical Conversation Starters.
By John dePillis. Mathematical Association of America, Washington, D.C., 2002. \$37.95.
xvi+344 pp., softcover. ISBN 0-88385-540-2.

This book is a valuable and lively compilation of quotations about mathematics. It is organized by topic, with extensive cross-referencing between the various items. In addition, the book is decorated with a large number of cartoons by the author, who is an artist as well as a mathematician.

As there are 777 entries, I suspect that most readers will dip into the book in small doses, but it could be read in a more conventional way. Occasionally, for instance, the book deals at some length with particu-

lar themes, some related to the foundations of mathematics and the philosophical side of the subject.

But the main focus is on the quotations themselves, and even the most battle-hardened mathematician will find some new gems in this book. I was struck, for instance, by “There is no branch of mathematics, however abstract, which may not some day be applied to phenomena of the real world” (Lobachevsky), neatly cross-referenced with a famous quote by G. H. Hardy expressing an altogether different view. New to me, too, were, “An author most hurts his readers by concealing difficulties” (Galois), and, as an example of the light touch that runs through the book, “I