

between this and the other aspects of the subject that makes this book especially attractive.

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25[34C35, 58F05, 65L06, 65L07].—J. M. SANZ-SERNA & M. P. CALVO, *Numerical Hamiltonian Problems*, Applied Mathematics and Mathematical Computation, Vol. 7, Chapman & Hall, London, 1994, xii + 207 pp., 22 cm. Price \$48.50.

The story of numerical analysis is mostly about translating mathematical concepts and models into a quantitative medium, fleshing numbers on the formal mathematical skeleton. This, however, should not obscure the crucial role of *qualitative* aspects of computation. It is an illusion that, as soon as it comes to application, all questions are of a purely quantitative character. ‘Will the satellite stay in stable orbit?’, ‘Does a mixture undergo combustion?’, ‘Will the species survive in a given environment?’, are all qualitative questions. Presumably, they are modelled by differential equations. Presumably, these differential equations are solved numerically. Certainly, their numerical solution contains errors. Naively, the purpose of numerical analysis is to minimize the accretion of error, but this frequently misses the point of the whole calculation. Thus, let us consider the stability of a satellite and suppose that two alternative computational methods are available. The first produces a very small error which, however, consistently undershoots the elevation. The second is considerably more error-prone but gets the stability issue exactly right: the numerical orbit is stable if and only if so is the exact one. Little doubt that, for the specific purpose in hand, the second method is superior!

The emphasis on the recovery of qualitative attributes of a mathematical model, rather than just minimizing the error, is relatively a new one. It has led in the last decade to a profound new insight into computation and has changed the treatment of many important numerical problems. Arguably, the most significant advance has been associated with Hamiltonian problems.

A system of ordinary differential equations is said to be Hamiltonian if it can be represented in the form

$$\begin{aligned}\frac{d\mathbf{p}}{dt} &= -\frac{\partial H(\mathbf{p}, \mathbf{q})}{\partial \mathbf{q}}, \\ \frac{d\mathbf{q}}{dt} &= \frac{\partial H(\mathbf{p}, \mathbf{q})}{\partial \mathbf{p}},\end{aligned}$$

where H is a given C^1 function. A significant proportion of dynamical systems that occur in mechanics—classical and quantum alike—can be rendered in a Hamiltonian form. As Penrose comments, “Such unity of form in the structure of dynamical equations, despite all the revolutionary changes that have occurred in physical theories over the past century or so is truly remarkable!” [3].

The formulation of equations of motion by William Rowan Hamilton in the above form was highly significant for sound physical reasons. The letter \mathbf{p} stands for positions and \mathbf{q} for momenta of physical particles, whilst H is

the total energy. This dichotomy between position and momentum (and the consignment of velocity to an inferior role) was a crucial conceptual advance that augured the development of quantum mechanics. The practical significance of Hamiltonian systems, however, has less to do with their august historical role than with their intricate dynamics.

To put it in a nutshell, the problem with Hamiltonian equations is that they possess too much structure. For starters, total energy is conserved, $H(\mathbf{p}(t), \mathbf{q}(t)) \equiv \text{const}$. So is an infinity of other integral quantities. More importantly, the flow $\Phi_{H,t}(\mathbf{p}(0), \mathbf{q}(0)) = (\mathbf{p}(t), \mathbf{q}(t))$, which assigns the solution at fixed time t to an initial condition, has a *symplectic* property: if $\Phi_{H,t}(\Omega) = \tilde{\Omega}$, then the sum of the areas of the projections into all two-dimensional spaces (p_j, q_j) is the same for Ω and $\tilde{\Omega}$. Moreover, as long as we restrict our attention to simply-connected sets Ω , symplecticity characterizes Hamiltonian systems.

Symplecticity is at the root of a whole range of interesting phenomena. Thus, it implies that fixed points of the flow are surrounded in the phase space by stable centres—the phase plane of the humble linear equation $y'' + y = 0$ is a case in point.

Experienced applied mathematicians know that often there is a price to be paid for conservation. In the familiar case of nonlinear hyperbolic conservation laws, the price of conservation is discontinuity. For Hamiltonian systems it is the sheer complexity of the flow: chaotic trajectories are a rule rather than an exception. The situation becomes even more complicated in the case of numerical modelling—after all, centres are known as the most volatile dynamical objects. Every tiny perturbation (and what is a numerical error if not a perturbation?!) is likely to turn a centre into a (stable or unstable) spiral. Inasmuch as the numerical error per se might be small (at least, for solution intervals of moderate length), the qualitative picture becomes misleading.

Hamiltonian systems have been computed (often badly) for many decades, but only in the early Eighties had a serious effort been expanded to design algorithms that preserve symplecticity, thereby ensuring that the numerical solution is faithful to original differential equations. As often, both the impetus and early results originated in the work of mathematical physicists [1, 4]. They have employed algorithms based on generating functions which, their ingenuity notwithstanding, are labour-intensive and need be derived afresh—by a painful expansion into series—for virtually every new Hamiltonian.

A turning point in the history of symplectic integrators came in 1988, when three numerical analysts (F. M. Lasagni, J. M. Sanz-Serna and Y. B. Suris [2, 5, 7]) independently proved that, subject to a satisfaction of an algebraic condition, Runge-Kutta methods are symplectic. Specifically, if $A = (a_{k,l})$ is the RK matrix and $\mathbf{b} = (b_l)$ are the RK weights of an s -stage Runge-Kutta, the symplecticity condition is $b_k a_{k,l} + b_l a_{l,k} = b_k b_l$, $k, l = 1, 2, \dots, s$. Similar conditions can be derived for Runge-Kutta-Nyström and for partitioned Runge-Kutta methods (the latter apply different schemes to \mathbf{p} and \mathbf{q}). In particular, the familiar Gauß-Legendre methods are symplectic. Even more remarkably, in the important special case of the Hamiltonian being of the form $H(\mathbf{p}, \mathbf{q}) = \frac{1}{2}\mathbf{p}^T\mathbf{p} + V(\mathbf{q})$, the underlying equations can be solved by an *explicit* Runge-Kutta-Nyström method which is symplectic!

This pioneering work has been followed by a large number of publications

and generated a great deal of interest, not only among numerical analysts but also in the nonlinear dynamical systems community. The present monograph of Jesus Maria Sanz-Serna and Mari Paz Calvo, both leaders in the symplectic field, is very timely indeed. It started its life as an *Acta Numerica* survey [6] and has been subsequently expanded to a book form.

Writing a monograph for numerical analysts, symplectic geometers and users of Hamiltonian systems—astronomers, molecular biologists, mathematical physicists, quantum chemists, engineers, fluid dynamicists—presents a significant challenge, because of the great variability in numerical and mathematical proficiency of the target audience. Some will know good dynamics and no numerics, others good numerics and no dynamics. Yet others will know bad numerics and bad dynamics. A good monograph should dispel ignorance without putting to the test the attention span of the more knowledgeable readers. Sanz-Serna and Calvo managed this task in a most splendid manner!

The first part of the book is devoted to an exposition of analytic aspects of Hamiltonian equations. The dosage of mathematical sophistication is just right to present main qualitative properties of Hamiltonian systems and highlight the importance of symplecticity, but the authors admirably resist the temptation to wade into the deep waters of symplectic geometry or the KAM theory—a detour which, although replete with beautiful mathematics, is not necessary to understand the subject matter of this monograph.

Having explained dynamics to numericists, the authors devote the second part of the book toward the explanation of numerics (specifically, Runge-Kutta methods) to dynamicists. This is inclusive of both theory—in the main, application of rooted trees in the derivation of order conditions—and implementation.

The first two parts of the book set the stage for its extensive survey of symplectic Runge-Kutta methods. The algebraic condition for symplecticity is derived for standard, partitioned and Nyström methods. Moreover, there is a detailed consideration of the surprising, yet important, result of L. Abia and J. M. Sanz-Serna, namely that order conditions and the symplecticity condition interact! As soon as the algebraic condition for symplecticity is imposed on the RK matrix, most order conditions go away. This makes the derivation of symplectic Runge-Kutta methods substantially simpler.

Available symplectic methods of all kinds—explicit, implicit, singly-diagonally implicit, composite—are surveyed in great detail. This is accompanied by extensive numerical experiments that demonstrate vividly that symplectic methods easily outperform state-of-the-art (nonsymplectic) Runge-Kutta schemes.

An important consequence of symplecticity is that the solution can be subjected to backward error analysis. It is possible to prove that a symplectic numerical trajectory samples (within a uniformly small error) the exact solution of nearly Hamiltonian equations. Therefore, *global* behaviour of the solution is captured correctly, since the numerical trajectory reflects the properties of this nearby Hamiltonian. However, symplecticity and all its benefits are lost as soon as the step size is being amended in the course of the numerical solution and governed by (local) error control considerations. This flies in the face of received numerical wisdom: *always* control the error, *always* use a variable-step algorithm.

There is no such thing as a free numerical lunch. Symplecticity means that

the error cannot be controlled in the course of the solution: we must stick with an initial step length through thick and thin. Abandonment of symplecticity, on the other hand, spoils the qualitative picture, denies us the benefits of backward error analysis and in long-term integration brings about considerably faster accumulation of error. The authors debate this dilemma at some length and conclude that, provided the solution interval is relatively short, good (non-symplectic) Runge-Kutta methods, e.g., the Dormand-Prince algorithm, have the edge. However, there is little doubt that symplectic methods are superior when it comes to long-term integration.

The authors conclude with a long list of additional themes and extensions—generating functions, the Lie formalism, the Poisson bracket, generation of high-order symplectic Runge-Kutta. . . .

This is an important book on an important subject. As numerical analysis evolves, we are likely to witness growing interdependence of numerical and dynamical considerations. Numerical Hamiltonian equations are a showcase of this meeting of ideas and cultures, but its eventual influence is bound to spread significantly wider. No numerical analyst can afford to stay ignorant of this trend.

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26[65F10, 65–04].—RICHARD BARRETT, MICHAEL BERRY, TONY F. CHAN, JAMES DEMMEL, JUNE DONATO, JACK DONGARRA, VICTOR EIJKHOUT, ROLDAN POZO, CHARLES ROMINE & HENK VAN DER VORST, *Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods*, SIAM, Philadelphia, PA, 1994, xiv + 112 pp., 25½ cm. Price: Softcover \$18.00.

In 1971 James Wilkinson and Christian Reinsch edited a handbook of ALGOL programs for the solution of linear systems and eigenvalue problems [4]. The individual contributions had been previously published in *Numerische Mathematik* and were characterized by painstaking attention to detail, extensive testing, and complete documentation of both the algorithms and their implementations. Although the programming language ALGOL never caught on in the United States, the Handbook had an enormous influence on the later development of mathematical software. For my generation it was the place to turn to