PREFACE

Geometric Numerical Integration of Differential Equations

Geometric integration of *ordinary* differential equations

What is geometric integration?

'Geometric integration' is the term used to describe numerical methods for computing the solution of differential equations, while preserving one or more physical/mathematical properties of the system *exactly* (i.e. up to round–off error)[1].

What properties can be preserved in this way?

A first aspect of a dynamical system that is important to preserve is its phase space. If the phase space is $\mathbb{R}^n$, this is easily achieved by using any so-called one-step method. This means that, for example, all Runge–Kutta methods work, but no multi-step method does. If, on the other hand, phase space is a more complicated manifold, then more sophisticated methods are called for. If, for example, the phase space is a Lie group, traditional methods (Runge–Kutta methods and multi-step methods) generally do not work, and one must use a so-called Lie group integrator. That Lie groups are not necessarily esoteric phase spaces is demonstrated by the free rigid body, whose phase space is (the cotangent bundle of) SO(3).

Assuming one has got the phase space correct, the most important property for physicists to preserve is often the so-called symplectic structure of Hamiltonian systems. Symplectic integration methods, the discrete algorithms used to approximate the solution of Hamiltonian systems, themselves possess the desirable feature that they can be derived from a variational principle.

Other properties that can be important to preserve are phase-space volume (for divergence-free vector fields arising, for example, from incompressible fluid dynamics), continuous or discrete symmetries, time-reversal symmetry, first integrals such as energy, linear and angular momentum, Casimirs, the correct physical form of dissipation, Lyapunov functions, foliations, etc. Preservation of these various properties has many positive consequences for the faithful computation of dynamical orbits, and has led to myriad applications of geometric integration, ranging from celestial mechanics to particle accelerators, from molecular dynamics to quantum spin chains, and from classical mechanics to fluid dynamics.

Many, if not most, of the above properties are not preserved by traditional numerical methods. Therefore for each of these properties, novel geometric integration methods have been constructed preserving that property.

Many of the above properties (e.g. symplecticity, volume preservation, symmetries, first integrals and foliations) are examples of what one may call group properties. By this we mean that the vector fields having such a property (e.g. Hamiltonian vector fields) form a Lie algebra, and the associated discrete integrators (e.g. symplectic integrators) form a group

[1] Variations on this theme exist. Sometimes a 'nearby' property is preserved exactly; Sometimes a property is not preserved exactly, but more accurately than the solution in general.

(e.g. of symplectic maps)[2]. This important observation is the basis of the so-called splitting methods that are ubiquitous in geometric integration[3].

Splitting methods are familiar to physicists from the field of, for example, quantum spin chains. If a quantum system is described by a Hamiltonian $\mathcal{H}$, then its time evolution is given by $e^{t\mathcal{H}}$. If $\mathcal{H}$ can be split $\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2$, where $\mathcal{H}_1$ and $\mathcal{H}_2$ separately can each be 'solved' (diagonalized), then $e^{t\mathcal{H}}$ can be approximated by $e^{t\mathcal{H}_1}e^{t\mathcal{H}_2}$ (using the Campbell–Baker–Hausdorff formula).

It turns out that, analogously, the time evolution generated by a vector field f can (formally) be written e^{tf}. If f can be split as $f = f_1 + f_2$, where f_1 and f_2 separately can each be 'solved' (e.g. integrated exactly), then e^{tf} can be approximated similarly by $e^{tf_1}e^{tf_2}$. Here f_1 and f_2 are generally elements of a Lie algebra of vector fields (e.g. Hamiltonian, or divergence-free, or possessing some symmetry or first integral), and e^{tf_1} and e^{tf_2} are elements of the associated group of diffeomorphisms (e.g. symplectic, or volume-preserving, or possessing some symmetry or first integral). Since this group is closed under composition, $e^{tf_1}e^{tf_2}$ will also be an element in the same group.

This state of affairs became well understood following the pioneering works of Yoshida and Suzuki. Of course splitting methods are not the only methods used in the geometric integration of ordinary differential equations (ODEs). Other methods include the previously mentioned Runge–Kutta methods; the Lie group methods; and various projection methods (see the review by McLachlan and Quispel in this issue).

Geometric integration of *partial* differential equations

The geometric integration of partial differential equations (PDEs) historically has not yet quite reached the same level of development as has that of ordinary differential equations. Partly this is because PDEs *per se* are not as easily systematized as ODEs. (Indeed it has been said that each PDE is different.) Partly it is also because PDEs are more difficult, if only because they can often be regarded as infinite-order ODEs, which means the correct phase space can never be preserved in numerical computation. But, precisely because they are so difficult, it has been found that preserving geometric structure is the key to constructing reliable methods; well-known examples are methods that preserve positivity (for systems of conservation laws) or ensure stability by preserving or decreasing some (e.g. energy) norm of the solution.

There is currently a lot of activity in the field of geometric integration of PDEs. Some of the geometric properties that are desirable to preserve are identical or similar to those of ODEs, such as Hamiltonian structure, symmetries, and first integrals, while some are unique to PDEs, such as the differential (div-grad-curl) complexes crucial to the Maxwell equations and the diffeomorphism group structure of fluid equations.

One of the approaches to numerical integration of evolution equations is to first apply a so-called semi-discretization, in which spatial derivatives are discretized, leading to (a large number of) coupled ODEs. Provided the semi-discretization preserves a spatially-discrete analogue of the desired geometric properties, the ensuing ODEs can then be integrated using a geometric method for ODEs. Other geometric methods for PDEs that have become very popular in recent years are multisymplectic integrators and variational integrators.

[2] This (infinite-dimensional) group is not to be confused with the (finite-dimensional) Lie group that can occur as phase space.

[3] Splitting methods can be used not only in the case of groups, but also for semigroups, which arise in dissipative systems, and for symmetric spaces, which arise for time-reversible systems.

Contents of this Special Issue

This Special Issue contains 4 review articles and 14 research papers on geometric integration.

McLachlan and Quispel review geometric integration for ODEs, and Bridges and Reich review Hamiltonian and multisymplectic PDEs.

Two further reviews concentrate on the application of geometric integration to one area of particular importance each. Forest presents a personal view of geometric integration for particle accelerators, and Jia and Leimkuhler review geometric integration for systems with multiple time scales, especially as they arise in molecular dynamics.

The research articles can roughly be divided into those that deal with ODEs and those that deal with PDEs. Among the papers on geometric integration for ODEs, Blanes and Casas investigate splitting methods for non-autonomous systems. Casas and Iserles study Lie group integrators for equations of the form $\dot{Y} = A(t, Y)Y$ where Y evolves in a given Lie group. Celledoni discusses the efficient time-symmetric simulation of torqued rigid bodies using Jacobi elliptic functions. Grimm and Hochbruck give a convergence analysis for exponential integrators applied to highly oscillating ODEs, that generalises results on the mollified impulse method due to Garcia-Archilla *et al* and on Gautschi-type exponential integrators. Jalnapurkar, Leok, Marsden and West discuss variational integration of mechanical systems with abelian symmetry. As examples they treat an Earth-orbiting satellite and a double spherical pendulum. Lall and West present a discrete Hamiltonian theory to parallel discrete Lagrangian mechanics. Moan considers the theory of modified equations of ODEs. Owren derives order conditions for commutator-free Lie group integrators. Shang proves that any n-dimensional volume-preserving map can be represented as a composition of $n - 1$ essentially 2-dimensional area-preserving maps, and studies the Lie algebra of skew-symmetric tensor potentials. Suzuki constructs exponential product formulas of higher order. Tuckerman *et al* derive a measure-preserving integrator for molecular dynamics simulations.

Finally, a number of research papers deal with geometric integration for PDEs. Budd and Williams study adaptive methods for PDEs with scaling symmetries. Frank shows that multisymplectic Runge–Kutta box schemes preserve a discrete conservation law of wave action. Last but not least, Munthe-Kaas investigates symmetry-preserving discretisations of PDEs and the computation of matrix exponentials.

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Guest Editors