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Geometric Numerical Integration

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Abstract. The subject of this workshop was numerical methods that preserve geometric properties of the flow of an ordinary or partial differential equation. This was complemented by the question as to how structure preservation affects the long-time behaviour of numerical methods.

Mathematics Subject Classification (2010): 65xx.

Introduction by the Organisers

The subject of this workshop was numerical methods that preserve geometric properties of the flow of an ordinary or partial differential equation: symplectic and multisymplectic integrators for Hamiltonian systems, symmetric integrators for reversible systems, methods preserving first integrals and numerical methods on manifolds, including Lie group methods and integrators for constrained Hamiltonian mechanics, and methods for problems with highly oscillatory solutions. The unifying theme is structure preservation: not just the "how?" but also "why?", "where?" and "what for?".

The motivation for developing structure-preserving algorithms for special classes of problems arises independently in such diverse areas of research as astronomy, molecular dynamics, mechanics, theoretical physics, control theory, and numerical analysis with important contributions from other areas of both applied and pure mathematics. Moreover, it turns out that the preservation of geometric properties of the flow not only produces an improved qualitative behaviour, but also allows for a significantly more accurate long-time integration than with general-purpose methods.

Geometric numerical integration has developed into an active and interdisciplinary research area in the last two decades. While the core of the subject, for ordinary differential equations, is presented in the monographs

E. Hairer, Ch. Lubich, G. Wanner, Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations. Springer, Berlin, 2002,

and

B. Leimkuhler, S. Reich, Geometric Integrators in Hamiltonian Mechanics. Cambridge Univ. Press, 2004,

recent progress in the development and long-time theory of geometric integrators for classes of partial differential equations is documented in the book

E. Faou, Geometric numerical integration and Schrödinger equations. Zurich Lectures in Advanced Mathematics 15, European Math. Soc., Zürich, 2012.

In addition to the construction of geometric integrators, an important aspect of geometric integration is the explanation of the relationship between geometric properties of a numerical method and favourable error propagation in long-time integration. A very successful organising principle is backward error analysis, where the numerical one-step map is interpreted as (almost) the flow of a modified differential equation. In this way, geometric properties of the numerical integrator seamlessly translate into structure preservation on the level of the modified equation. Much insight and rigorous error estimates over long time intervals can then be obtained by combining backward error analysis with the KAM theory and related perturbation theories for Hamiltonian and reversible systems.

While backward error analysis has been very successful for ordinary differential equations, it does not extend directly to highly oscillatory systems and geometric integrators for partial differential equations. Only fairly recently, versions of backward error analysis based on Birkhoff normal form theory or on modulated Fourier expansions have allowed to explain favourable long-time energy behaviour for geometric integrators for some Hamiltonian partial differential equations. Highly oscillatory systems is another area with substantial recent progress where yet much remains to be understood and explored.

The workshop addressed the recent developments in theory and applications of geometric numerical integration and reflected the multidisciplinary nature of the topic.

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Workshop: Geometric Numerical Integration

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