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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 (2000): 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 mechanical systems, 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, control theory, theoretical physics, electrical and electronic engineering 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 been an active and interdisciplinary research area in the last two decades. While the core of the subject is well documented in the monographs

> E. Hairer, Ch. Lubich, G. Wanner, Geometric Numerical Integration. Springer, Berlin, 2nd edition, 2006,

> K. Feng, M. Qin, Symplectic Geometric Algorithms for Hamiltonian systems. Springer, Berlin, 2010

and

> B. Leimkuhler, S. Reich, Simulating Hamiltonian Dynamics. Cambridge Univ. Press, 2004,

the area in its wider sense has in recent years undergone substantial and exciting developments:

1. Backward error analysis for infinite-dimensional systems, using modulated Fourier expansions and normal forms. This has, for the first time, brought partial differential equations to within the realm of backward error analysis, thereby helping to understand the long-term behaviour of numerical methods;
2. The understanding of numerical methods using tools from Hopf algebra and graph theory. This has clarified the sort of invariants that B-series-based numerical methods can respect. Thus, for example, such methods cannot conserve volume but they can be designed to respect Hamiltonian energy;
3. Understanding of symplectic structure of exponential integrators and the design of exponential integrators best capable of dealing with highly oscillatory solutions;
4. The design of asymptotic numerical approaches to numerical integration of highly oscillatory ODEs and DAEs, applications in electronic engineering and in control theory;
5. The analysis of multiscale algorithms, not least of the Heterogeneous Multiscale method, with modulated Fourier series;
6. The understanding how symmetries in differential equations and in discretized systems can be exploited by means of group theory and harmonic analysis, to reduce the cost of computations;
7. Geometric integrators for Maxwell and wave equations, applications in astrophysics, plasma physics and nano-optics;
8. Application of geometric integrators to the Schrödinger equation and reduced models in quantum mechanics;
9. Better understanding of geometric integrators in the context of molecular dynamics and macro-molecule modelling.

The intention of this second Oberwolfach workshop on geometric numerical integration (a first one was held in 2006) was to address these recent developments. Geometric numerical integration is by its very nature a multidisciplinary topic and this was well reflected in the workshop.