**Geometry, compatibility and structure preservation in computational differential equations**

**Isaac Newton Institute Cambridge**

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## Short Report

Differential equations have been used to formulate the laws of physics since the dawn of science and their computation is a fundamental activity in applied mathematics. However, it is important that the mathematics does not stop once computation starts.

In the past, much effort has been devoted to finding reliable methods for the most commonly used equations. Today, we seek to encode the laws of physics themselves directly into the numerical discretization, all the while maintaining good convergence and error bounds, having competitive efficiency and demonstrating excellent qualitative properties. The models considered originate from the full range of applications of interest in the modern era.

The effort to encode physics and geometry into discretizations, has proceeded along very different lines, depending on whether the differential equations were ordinary (ODEs) or partial (PDEs). To give an idea, symplecticity and the preservation of first integrals, such as energy, has been a holy grail for people studying ODEs. Meanwhile, for PDEs, compatibility with the approximation of the exterior derivative operator has been of prime importance when designing finite element methods.

One central aim of this six month programme, was to bring these two disparate communities together. Two strands of research of interest to both groups are the preservation of conservation laws and the structure of the manifold on which the solutions live, and these were among our main themes. The first workshop was devoted to tutorials and surveys originating in both groups, and there was a lively seminar series throughout, attended by all resident participants. All these talks are available on-line.

Specific geometric and topological structures needing to be preserved in numerical simulations are application-dependent. The second workshop focused on general relativity, in which the relevant differential equations expressly concern Riemannian geometry of space. An important theme of the workshop was the challenge of developing stable discretization methods preserving appropriate geometric structures, and the workshop was very successful in introducing participants from other areas of structure-preserving discretizations to these challenges.

Other focus periods included methods for plasma physics, quantum dynamics, virtual element methods and sampling algorithms on manifolds, addressing questions related to deep neural networks and statistical problems which involve smooth constraint structures. Our Kirk Lecturer, Donatella Marini, talked on advances in the application of virtual elements, while the Rothschild Lecture, given by Jesus Maria Sanz-Serna, concerned Hamiltonian Monte Carlo methods for ODEs. Further, the Open for Business day devoted to Advances in Numerical Modelling was a great success, attracting speakers on applications of geometric integration in meteorology and climate, medical imaging, and robotics.

Three immediate breakthroughs were noted. The first concerns photochemistry, or more precisely light harvesting, the study of how molecules transfer energy of light into motion. The new insight provides a mathematical justification of ring-polymer molecular dynamics (Caroline Lasser). The

second is in the preservation of multi-symplectic structures in finite element methods (Robert McLachlan and Ari Stern). Further, a group of participants (Fernando Casas, Sergio Blanes, and J.M. Sanz-Serna) obtained very promising results on splitting methods for Hamiltonian Monte Carlo simulations.

Fruitful discussions during one of the focus study periods covered space and time discretizations for Vlasov's equations and for gyrokinetic simulations, facilitating exchanges between experts of plasma physics and numerical analysis. Nuclear fusion for generating clean energy depends on plasma simulation and heavily employs structure preserving algorithms. Plasma physics simulation continues to be a source of open challenges for the field of structure preserving methods.

The final workshop, which took place at the ICMS in Edinburgh, concerned cutting edge and future research directions. A collection of open problems and of short communications of collaborative research initiated during the semester is being compiled.

The concurrent programme in Complex Analysis: Techniques Applications and Computation, had several participants and themes of great interest to our own programme, and monthly joint seminars were organised.

Awareness of the need for gender diversity in all our activities, was maintained throughout the time of the programme, as was attention to participation of people from ethnic minorities. Further, a good age balance was important to us. A luncheon discussion on gender and minorities was organized together with the Complex Analysis programme.

In addition, the friendly social programme, the excellent library facilities, the help with school and child care, and provisions for disabled participants, all created a good natured, welcoming environment and mental space for our outstanding participants.