Preservation of Phase Space Structure in Symplectic Integration

A thesis presented in partial
fulfilment of the requirements
for the degree of
Doctor of Philosophy
in Mathematics

at Massey University,
Palmerston North, New Zealand.

Dion Robert James O'Neale
2009

Abstract

This thesis concerns the study of geometric numerical integrators and how they preserve phase space structures of Hamiltonian ordinary differential equations.

We examine the invariant sets of differential equations and investigate which numerical integrators preserve these sets, and under what conditions. We prove that when periodic orbits of Hamiltonian differential equations are discretized by a symplectic integrator they are preserved in the numerical solution when the integrator step size is not resonant with the frequency of the periodic orbit.

The preservation of periodic orbits is the result of a more general theorem which proves preservation of lower dimensional invariant tori from dimension zero (fixed points) up to full dimension (the same as the number of degrees of freedom for the differential equation). The proof involves first embedding the numerical trajectory in a non-autonomous flow and then applying a KAM type theorem for flows to achieve the result. This avoids having to prove a KAM type theorem directly for the symplectic map which is generally difficult to do.

We also numerically investigate the break up of periodic orbits when the integrator's step size is resonant with the frequency of the orbit.

We study the performance of trigonometric integrators applied to highly oscillatory Hamiltonian differential equations with constant frequency. We show that such integrators may not be as practical as was first thought since they suffer from higher order resonances and can perform poorly at preserving various properties of the differential equation. We show that, despite not being intended for such systems, the midpoint rule performs no worse than many of the trigonometric integrators, and indeed, better than some.

Lastly, we present a numerical study of a Hamiltonian system consisting of two magnetic moments in an applied magnetic field. We investigate the effect of both the choice of integrator and the choice of coordinate system on the numerical solutions of the system. We show that by a good choice of integrator (in this case the generalised leapfrog method) one can preserve phase space structures of the system without having to resort to a change of coordinates that introduce a coordinate singularity.

Acknowledgements

Thanks first to my supervisor Robert McLachlan for guidance along the course of this thesis. Thanks also to other members of the mathematics department at I.F.S., including my co-supervisor Matt Perlmutter and fellow doctoral candidates Brett Ryland and Philip Zhang, for useful discussions, mathematical and otherwise.

During this thesis, financial support was received from the New Zealand Institute of Mathematics and its Applications, the New Zealand Mathematics Society, The Royal Society of New Zealand, Education New Zealand, and the IFS Postgraduate Research Fund. This was much appreciated and very helpful.

Much of this funding was used for travel to visit Zai-jiu Shang at the Chinese Academy of Sciences in Beijing, and to attend the program on highly oscillatory problems at the Isaac Newton Institute, in Cambridge, hosted by Arieh Iserles. The hospitality of both these people was greatly appreciated, as were the discussions.

Discussions with Ernst Hairer, Reinout Quispel and David Cohen during the INI program also contributed to work in this thesis.

Finally, thanks to family, friends and colleagues, for help and support over the duration of this thesis.

Contents

List of Figures

List of Tables