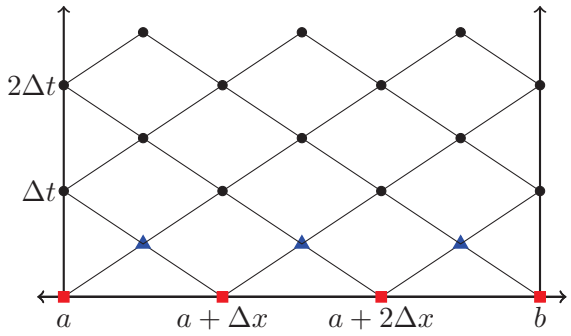
SYMPLECTIC INTEGRATORS FOR VAKONOMIC EQUATIONS AND FOR MULTI-HAMILTONIAN EQUATIONS



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Abstract

This thesis contains research contributions to two areas of geometric integration, one concerning ordinary differential equations (ODEs) and one concerning partial differential equations (PDEs).

The ODE contribution is a symplectic integrator for variational nonholonomic equations, also known as vakanomic equations. These systems include the Hamiltonian version of variational problems subject to position and velocity constraints that are nondegenerate in the velocities. Such constraints have the form $g_i(q) \cdot \dot{q} = 0$, and arise in sub-Riemannian geometry and control theory. An equivalence between variational equations with these constraints and generalized Hamiltonian systems of the form $J\dot{z} = \nabla H(z)$ (J not necessarily invertible) with such index 1 constraints is shown. This is extended to constraints of the form $g_i(q, \dot{q}) = 0$. It is shown that symplectic Runge–Kutta methods are also symplectic on generalized Hamiltonian systems and provide effective symplectic integrators for Hamiltonian systems with index 1 constraints. Two sample applications are given: finding the motion of a two-wheeled idealized vehicle, and finding the geodesics of the Heisenberg group.

The PDE contribution is a new multisymplectic integrator. A class of general purpose linear multisymplectic integrators for multi-Hamiltonian equations based on a diamond-shaped mesh is introduced. The class of integrators consists of a *simple diamond scheme*, and a *diamond scheme* parameterized by order r. On each diamond, the former discretizes the PDE on the corners of the diamond, and the latter discretizes the PDE with r-stage symplectic Runge–Kutta methods. Both schemes advance in time by filling in each diamond locally, leading to greater efficiency and parallelization, and easier treatment of boundary conditions compared to methods based on rectangular meshes. The simple diamond scheme is order two in both space and time, has solvable equations for the one-dimensional wave equation, satisfies a discrete conservation law, and can be extended to allow Dirichlet and Neumann boundary conditions for the wave equation. The diamond scheme is defined on all multi-Hamiltonian PDEs, has solvable nonlinear equations for the one-dimensional wave equation, satisfies a discrete symplectic conservation law, and scales exceedingly well with the number of processors

on which it is run. A method for handling Dirichlet and Neumann boundary conditions is presented. Discrete dispersion relations, and associated stability results, are found for the wave equation and the cubic nonlinear Schrödinger equation. Numerical experiments, for both the simple diamond and r diamond schemes, are presented to support an estimate of the order of the schemes. Difficulties and complications, including boundary treatment and the multi-step nature of the diamond scheme, are discussed.

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First, of course, I thank my family. My parents for their support and upbringing. My brother, Andy, who: was always interested in knowing the details, asked insightful questions that made me think from a different perspective, and helped me with isoparametric coordinate transformations between triangles and diamonds. My kids who suffered having an absentee dad, especially when I was close to submitting. My wife, Heather, who not only had to put up with me doing less about the house, but also: proofread the entire thesis; checked all my articles and documents; listened to all my practice talks; put up with me grumbling about proofs that didn't work or code that was buggy; and made suggestions when I was stumped.

I started my PhD on a part-time basis while working at ITS Massey University. I am thankful to ITS, in particular Clive Martis, the CTO at the time, for allowing me to do this. ITS partially paid my fees, and allowed me time to meet with my supervisors.

In the first year of study my supervisor had two visitors: Klas Modin and Olivier Verdier. Both are very clever Mathematicians, but equally important to me, was that they were kind, clear, and willing to explain things to a slow, inexperienced student such as myself. Around that time we had the 'pre-magic conference' at Waikanae; that, and these two gentlemen really brought some life to the beginning of my PhD.

New Zealand eScience Infrastructure (NeSI) provided the parallel computing resources for me to test my code. The process, from requesting access to actually using a cluster, was straightforward and very smooth. NeSI clusters have an enormous amount of software (I didn't have to request a single package be installed!) and are staffed by knowledgeable and helpful people.

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