

Copyright is owned by the Author of the thesis. Permission is given for a copy to be downloaded by an individual for the purpose of research and private study only. The thesis may not be reproduced elsewhere without the permission of the Author.

MULTISYMPLECTIC INTEGRATION

A thesis presented in partial fulfilment
of the requirements for the degree of

Doctor of Philosophy
in
Mathematical Physics

at Massey University, Palmerston North,
New Zealand.

Brett Nicholas Ryland

2007

Copyright © 2007 by Brett Nicholas Ryland

Abstract

Multisymplectic integration is a relatively new addition to the field of geometric integration, which is a modern approach to the numerical integration of systems of differential equations. Multisymplectic integration is carried out by numerical integrators known as multisymplectic integrators, which preserve a discrete analogue of a multisymplectic conservation law.

In recent years, it has been shown that various discretisations of a multi-Hamiltonian PDE satisfy a discrete analogue of a multisymplectic conservation law. In particular, discretisation in time and space by the popular symplectic Runge–Kutta methods has been shown to be multisymplectic. However, a multisymplectic integrator not only needs to satisfy a discrete multisymplectic conservation law, but it must also form a well-defined numerical method. One of the main questions considered in this thesis is that of when a multi-Hamiltonian PDE discretised by Runge–Kutta or partitioned Runge–Kutta methods gives rise to a well-defined multisymplectic integrator. In particular, multisymplectic integrators that are explicit are sought, since an integrator that is explicit will, in general, be well defined.

The first class of discretisation methods that I consider are the popular symplectic Runge–Kutta methods. These have previously been shown to satisfy a discrete analogue of the multisymplectic conservation law. However, these previous studies typically fail to consider whether or not the system of equations resulting from such a discretisation is well defined. By considering the semi-discretisation and the full discretisation of a multi-Hamiltonian PDE by such methods, I show the following:

- For Runge–Kutta (and for partitioned Runge–Kutta methods), the active variables in the spatial discretisation are the stage variables of the method, not the node variables (as is typical in the time integration of ODEs).
- The equations resulting from a semi-discretisation with periodic boundary conditions are only well defined when both the number of stages in the Runge–Kutta method and the number of cells in the spatial discretisation are odd. For other types of boundary conditions, these equations are not well defined in general.
- For a full discretisation, the numerical method appears to be well defined at first, but for some boundary conditions, the numerical method fails to accurately represent the PDE, while for other boundary conditions, the numerical method is highly implicit, ill-conditioned and impractical for all but the simplest of applications. An exception to this is the Preissman box scheme, whose simplicity avoids the difficulties of higher order methods.
- For a multisymplectic integrator, boundary conditions are treated differently in time and in space. This breaks the symmetry between time and space that is inherent in multisymplectic geometry.

The second class of discretisation methods that I consider are partitioned Runge–Kutta methods. Discretisation of a multi-Hamiltonian PDE by such methods has led to the following two major results:

1. There is a simple set of conditions on the coefficients of a general partitioned Runge–Kutta method (which includes Runge–Kutta methods) such that a general multi-Hamiltonian PDE, discretised (either fully or partially) by such methods, satisfies a natural discrete analogue of the multisymplectic conservation law associated with that multi-Hamiltonian PDE.
2. I have defined a class of multi-Hamiltonian PDEs that, when discretised in space by a member of the Lobatto IIIA–IIIB class of partitioned Runge–Kutta methods, give rise to a system of explicit ODEs in time by means of a construction algorithm. These ODEs are well defined (since they are explicit), local, high order, multisymplectic and handle boundary conditions in a simple manner without the need for any extra requirements. Furthermore, by analysing the dispersion relation for these explicit ODEs, it is found that such spatial discretisations are stable.

From these explicit ODEs in time, well-defined multisymplectic integrators can be constructed by applying an explicit discretisation in time that satisfies a fully discrete analogue of the semi-discrete multisymplectic conservation law satisfied by the ODEs. Three examples of explicit multisymplectic integrators are given for the nonlinear Schrödinger equation, whereby the explicit ODEs in time are discretised by the 2-stage Lobatto IIIA–IIIB, linear–nonlinear splitting and real–imaginary–nonlinear splitting methods. These are all shown to satisfy discrete analogues of the multisymplectic conservation law, however, only the discrete multisymplectic conservation laws satisfied by the first and third multisymplectic integrators are local.

Since it is the stage variables that are active in a Runge–Kutta or partitioned Runge–Kutta discretisation in space of a multi-Hamiltonian PDE, the order of such a spatial discretisation is limited by the order of the stage variables. Moreover, the spatial discretisation contains an approximation of the spatial derivatives, and thus, the order of the spatial discretisation may be further limited by the order of this approximation. For the explicit ODEs resulting from an r -stage Lobatto IIIA–IIIB discretisation in space of an appropriate multi-Hamiltonian PDE, the order of this spatial discretisation is $r - 1$ for $r \leq 10$; this is conjectured to hold for higher values of r . For $r = 3$, I show that a modification to the initial conditions improves the order of this spatial discretisation. It is expected that a similar modification to the initial conditions will improve the order of such spatial discretisations for higher values of r .

Acknowledgements

First and foremost, I would like to say a big thank you to my main supervisor, Prof. Robert McLachlan, who has spent countless hours over the last decade (firstly as an undergraduate lecturer, then as my Master's supervisor and lastly as my Doctoral supervisor) enthusiastically instructing me in the theory and practice of geometric integration, numerical analysis, and various other fields of mathematics, all-the-while patiently explaining and re-explaining ideas that he had thought of since our previous meeting or getting overly excited whenever I brought a new result or interesting looking graph to his attention; hopefully I've taught you a few things along the way too.

Thanks also go to Robert's wife and two daughters for allowing Robert and me to have the occasional meeting while he was on parental leave, since, within a few weeks of becoming my supervisor (both for my Master's and my PhD), Robert announced that his wife was with child!

I would like to thank my parents for providing me with an education that has allowed me to reach this far, for their support and encouragement throughout my studies and for repeatedly moving and storing my stuff. A thank you also goes to my three brothers who have provided stiff competition for almost every challenge I have undertaken, encouraging me to strive even further than I might have otherwise.

My thanks go to my fellow PhD (or ex-PhD) friends, Priscilla, Dion, Philip, Patrick (Paddy) and Paul (PP) for numerous discussions over coffee and their entertaining observations of graduate life. A thank you also goes to my friends in the Phoenix medieval re-enactment company, Friday night role-playing group, canoe polo leagues and white water kayaking clubs, who have provided much in the way of entertainment and physical exercise when I have felt the need for procrastination.

Finally, I would also like to thank those who have been my friends since my early years at university. In particular, a special thank you goes to my dear friends, Miriam (who kindly provided some last minute grammar and spell checking), Nathan, Anita and Jane, who provide a relatively sane perspective on the world outside of university life and whose antics continue to keep me entertained.

Brett N. Ryland

November 5, 2007.

Contents

| | |
|--|----------|
| Acknowledgements | v |
| 1 Introduction | 1 |
| 1.1 General overview of this thesis | 3 |
| 1.2 Hamiltonian ODEs and PDEs | 5 |
| 1.2.1 Conservation laws | 7 |
| ODE conservation laws | 7 |
| PDE conservation laws | 8 |
| ODE differential conservation laws | 9 |
| PDE differential conservation laws | 10 |
| 1.3 Lagrangian mechanics | 11 |
| 1.3.1 Differential geometry for ODEs | 12 |
| 1.3.2 Differential geometry for PDEs | 15 |
| 1.3.3 \mathcal{E} - \mathcal{L} equations and the multisymplectic form formula | 19 |
| 1.3.4 Particle mechanics example | 20 |
| 1.4 Existing methods | 21 |
| 1.4.1 Finite differences | 21 |
| 1.4.2 Runge–Kutta | 22 |
| 1.4.3 Partitioned Runge–Kutta | 23 |
| 1.4.4 Splitting methods | 25 |
| 1.4.5 Discrete variational integrators | 26 |
| 1.5 Advantages and usage | 28 |

| | | |
|----------|--|-----------|
| 2 | Runge–Kutta Discretisations | 31 |
| 2.1 | The multisymplectic conservation law | 33 |
| 2.2 | The spatial discretisation | 37 |
| 2.2.1 | Implicit ODEs | 38 |
| 2.2.2 | Odd behaviour | 40 |
| 2.3 | The full discretisation | 44 |
| 2.3.1 | Local integrators | 45 |
| 2.3.2 | Global integrators | 47 |
| 2.3.3 | The box scheme | 48 |
| 2.3.4 | The box scheme in higher dimensions | 49 |
| 3 | Partitioned Runge–Kutta Discretisations | 51 |
| 3.1 | Partitioned Runge–Kutta discretisation | 52 |
| 3.2 | Multisymplecticity of PRK | 53 |
| 3.2.1 | The importance of partitioning | 56 |
| 3.3 | Lobatto IIIA–IIIB | 58 |
| 3.4 | Explicit Discretisation | 61 |
| 3.4.1 | Examples | 66 |
| | Nonlinear wave equation | 66 |
| | NLS equation | 67 |
| | Boussinesq equation | 69 |
| | Korteweg-de Vries (KdV) equation | 69 |
| | Benjamin-Bona-Mahony (BBM) equation | 71 |
| | Padé–II equation | 72 |
| | A made-up example | 73 |
| 3.4.2 | A shortcut | 74 |
| 3.4.3 | Boundary conditions | 75 |
| 3.4.4 | Other PRK discretisations | 77 |

| | | |
|----------|--|------------|
| 4 | Time Integration | 79 |
| 4.1 | Hamiltonian systems and explicit integration | 79 |
| 4.2 | Semi-discrete Multisymplectic Conservation Law for NLS | 81 |
| 4.3 | Integration by 2-stage Lobatto IIIA–IIIB | 82 |
| 4.4 | Integration by symplectic splitting | 84 |
| 4.4.1 | 2-term (linear–nonlinear) splitting | 85 |
| 4.4.2 | 3-term (real–imaginary–nonlinear) splitting | 87 |
| 4.5 | Conservation laws | 89 |
| 5 | Dispersion and Order | 91 |
| 5.1 | Dispersion Relations | 91 |
| 5.1.1 | Stability | 93 |
| 5.2 | Order | 96 |
| 5.2.1 | Initial Conditions | 100 |
| 6 | Conclusion | 107 |
| 6.1 | Summary and closing remarks | 107 |
| 6.2 | Open questions | 109 |
| A | Proofs of various lemmas and theorems | 113 |
| A.1 | Proof of Lemma 2.0.1 | 113 |
| A.2 | Proof of Lemma 2.0.2 | 113 |
| A.3 | Proof of Lemma 3.4.2 | 115 |
| A.4 | Proof of Theorem 4.2.1 | 115 |
| A.5 | Proof of Theorem 4.3.1 | 117 |
| B | Theorems and lemmas of [33] | 121 |
| | Bibliography | 127 |

List of Figures

| | | |
|-----|--|-----|
| 1.1 | Differential conservation laws are evaluated on differentials, du , along a solution of the ODE. The differentials satisfy the first variation of the ODE. | 9 |
| 2.1 | A single cell demonstrating the labelling convention for a Runge–Kutta discretisation in space and time. | 34 |
| 2.2 | Collocation polynomials for periodic boundary conditions. (a) As the value on the left boundary decreases, the value on the right boundary increases. At some value they match. (b) As the value on the left boundary decreases, the value on the right boundary decreases at the same rate. | 43 |
| 5.1 | A comparison between the discrete dispersion relation (solid line) for $\rho(\Delta x)^2 = 1$ and the continuous dispersion relation (dashed line) for $\rho = 1$. | 94 |
| 5.2 | A waterfall plot of the norm $(p^2 + q^2)$ and the energy error for the NLS equation. | 96 |
| 5.3 | The values of p (solid line) and q (dashed line) after 10^7 steps of size 10^{-4} showing a lack of any high frequency wiggles in the solution. | 97 |
| 5.4 | The log of the fast Fourier transform of p after 10^7 steps of size 10^{-4} showing that the high frequency components are exponentially small. The log of the fast Fourier transform of q after 10^7 steps is almost identical. | 98 |
| 5.5 | The integrator for the sine–Gordon equation given by 3-stage Lobatto IIIA–IIIB discretisation in space and 2-stage Lobatto IIIA–IIIB discretisation in time, with unmodified initial conditions, has order 2. The dashed line gives the order at $i\Delta x$, the solid line gives the order at $(i + \frac{1}{2})\Delta x$. | 104 |
| 5.6 | The integrator for the sine–Gordon equation given by 3-stage Lobatto IIIA–IIIB discretisation in space and 2-stage Lobatto IIIA–IIIB discretisation in time, with modified initial conditions, has order 4. The dashed line gives the order at $i\Delta x$, the solid line gives the order at $(i + \frac{1}{2})\Delta x$. | 105 |