Multisymplectic Integration

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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 lead 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.

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