Introduction to multisymplectic integrators

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Abstract

The symplectic structure of Hamiltonian systems are well known, but for partial differential equations this is a global property. Many PDEs can be written as multisymplectic systems, in which each independent variable has a distinct symplectic structure. We give an introduction to multisymplecticity using differential forms, discuss some implications and show some examples of integrators for the nonlinear Schrödinger equation.
Overview

1. Motivation
2. Multisymplectic formulation of PDEs
3. Introduction to forms
4. Multisymplectic structure
5. Multisymplectic integrator
6. Numerical examples
Symplectic integration is proven to be a robust and stable way to integrate Hamiltonian system, both ODEs and PDEs.

- Preservation of symplectic structures gives excellent long integration-time behaviour.
- Geometric properties of the solution are often to preserved to a remarkable degree of accuracy.
- Multisymplecticity is a new approach going further in locating structures inherent in PDEs.
- Multisymplecticity often includes symplecticity as a special case.
- One wants to design *multisymplectic integrators* with additional appealing properties.
Symplectic schemes, examples

(Hairer, Lubich and Wanner 2002: Geometric Numerical Integration, page 12)
We start out with a partial differential equation we want to solve

$$\mathcal{L}_t u = \mathcal{L}_x u + \mathcal{V}(u), \quad u(0) = u_0$$

where $\mathcal{L}_t$ is differential operator in time, $\mathcal{L}_x$ is a differential operator in space and $\mathcal{V}$ is just some function of $u$.

This equation must be reformulated in order to be able to locate the possible multisymplectic structure:

- Introduce more phase space variables, typically $u_x$ and/or $u_t$.
- Alternatively, one may be able to start from first-order field theory defined by a Lagrangian. This will not be pursued here, but is the approach by Marsden et.al.

Håvard Berland  Multisymplectic integrators
A PDE is said to be multisymplectic if it can be written as

**Multisymplectic equation**

\[ Mz_t + Kz_x = \nabla_z S(z) \]

where \( z(x, t) \in \mathbb{R}^d \), and \( M, K \in \mathbb{R}^{d \times d} \) are skew-symmetric matrices and \( S: \mathbb{R}^d \to \mathbb{R} \) is a smooth function of the phase space variable \( z \).

\( (d \text{ will be } 3 \text{ or } 4 \text{ in our examples}) \)
An example, the nonlinear wave equation

We exemplify with the nonlinear wave equation

$$u_{tt} - u_{xx} + V'(u) = 0$$

where $V(u)$ is some smooth (potential) function. Define $z = (u, w, v)^T$ and write up

$$-v_t + w_x = V'(u)$$
$$-u_x = -w$$
$$u_t = v$$

which is $Mz_t + Kz_x = \nabla_z S(z)$ if $S(z) = V(u) + \frac{1}{2}v^2 - \frac{1}{2}w^2$, 

$$M = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad \text{and} \quad K = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$
The nonlinear wave equation and multisymplecticity

- The nonlinear wave equation is a Hamiltonian PDE. By only introducing $u_t = v$ it can be written as a Hamiltonian system, and thus has symplectic structure in time.

- The multisymplectic structure is obtained by also looking for a symplectic structure in space, introducing the additional phase space variable $w = u_x$.

- Given appropriate boundary conditions, multisymplecticity will include symplecticity in this case.
Recall symplectic structure and Hamiltonian systems

**Symplectic map**

A linear map $A$ in $\mathbb{R}^2$ is symplectic if $A^TJA = J$ where $J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$. Nonlinear maps are symplectic if their linearization is symplectic.

**Hamiltonian system**

\[ Jy_t = \nabla H(y) \]

where $y$ plays the role of $z$. $H(y)$ is the Hamiltonian.

- Flows of Hamiltonian systems are symplectic mappings (Poincaré 1899).
- Symplectic integrators are numerical schemes in which each step is a symplectic map. The simplest schemes are known as “Symplectic Euler” and “Störmer–Verlet”.

Multisymplectic integrators
Preservation of symplectic structure

(Hairer, Lubich Wanner 2002: Geometric Numerical Integration, page 176)
Through backward error analysis, it has been proved that

**Theorem**

*If a symplectic integrator is applied to a Hamiltonian system, the resulting modified equation is again Hamiltonian.*

Symplectic integrators are known to conserve some physical properties of the equation very well over long integration periods, mainly due to

**Theorem**

*The trajectory of a symplectic integrator is exponentially close to the exact trajectory of the modified Hamiltonian system.*
The description of symplectic and multisymplectic structure is written in terms of differential forms.

Before we state the definitions, we should briefly discuss what differential forms are.

We do not need more than 2-forms.

Simply put, *forms* are linear maps from a vector space to the real line.

**Definition (1-form)**

A 1-form is map $\omega^1 : \mathbb{R}^n \to \mathbb{R}$.

The set of 1-forms trivially form a vector space, the dual space $(\mathbb{R}^n)^*$.

- If $\xi = (a, b, c)$ in $\mathbb{R}^3$, then $\omega^1(\xi) = c$ is an example 1-form.
Definition (2-form)

An exterior form of degree 2 is a map on pairs of vectors,

\[ \omega^2 : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R} \]

which is bilinear and skew-symmetric:

\[ \omega^2(\lambda_1 \xi_1 + \lambda_2 \xi_2, \xi_3) = \lambda_1 \omega^2(\xi_1, \xi_3) + \lambda_2 \omega^2(\xi_2, \xi_3) \]
\[ \omega^2(\xi_1, \xi_2) = -\omega^2(\xi_2, \xi_1) \]
Interpretation of 2-forms

- Let $n = 2$ and consider two vectors $\xi_1$ and $\xi_2 \in \mathbb{R}^2$.
- The *oriented area* $A(\xi_1, \xi_2)$ of the parallelogram spanned by $\xi_1$ and $\xi_2$ is an example of a 2-form:

  ![Parallelogram](image)

  Oriented area means that

  $$A(\xi_1, \xi_2) = -A(\xi_2, \xi_1)$$

  (skew-symmetry)
Exterior product of two 1-forms

The 2-forms will appear as the (exterior) product of two 1-forms, say $\omega_a$ and $\omega_b$:

**Definition**

Exterior product of two 1-forms

$$(\omega_a \wedge \omega_b)(\xi_1, \xi_2) = \begin{vmatrix} \omega_a(\xi_1) & \omega_b(\xi_1) \\ \omega_a(\xi_2) & \omega_b(\xi_2) \end{vmatrix}$$

- Let $\xi_1, \xi_2 \in \mathbb{R}^n$. Map this to the two vectors $(\omega_a(\xi_1), \omega_b(\xi_1))$ and $(\omega_a(\xi_2), \omega_b(\xi_2))$ in the plane $\mathbb{R} \times \mathbb{R}$.
- The value of the 2-form on the two vectors is then the oriented area of the spanned parallelogram in the $\omega_a, \omega_b$ plane:
Differential forms are forms which take vectors in a tangent space as inputs.

**Definition (Differential form)**

A differential 1-form on a manifold $\mathcal{M}$ is a smooth map

$$\omega: \bigcup_{x} T_x \mathcal{M} \rightarrow \mathbb{R},$$

linear on each tangent space $T_x \mathcal{M}$.

Take the differential $\omega = df = 2x \, dx$ of the function $f(x) = x^2$ as an easy example.
Differential 2-forms are maps

$$\omega^2 : \bigcup_{x} T_x M \times \bigcup_{x} T_x M \to \mathbb{R}$$

This is also written as $\omega^2 \in \wedge^2(TM)^*$

All 2-forms may be written as the wedge product of 1-forms. For example, in $\mathbb{R}^3$, there are $\binom{3}{2} = 3$ 2-forms, $dx \wedge dy$, $dy \wedge dz$ and $dz \wedge dx$. 
Given the multisymplectic formulation of the PDE,

$$Mz_t + Kz_x = \nabla_z S(z),$$

the multisymplectic structure is given by the two 2-forms:

$$\omega = dz \wedge Mdz \quad \text{and} \quad \kappa = dz \wedge Kdz$$
Conservation of multisymplecticity

**Lemma**

\[ \omega_t + \kappa_x = 0 \]

**Proof.**

\[
\begin{align*}
\omega_t + \kappa_x &= dz_t \wedge Mdz + dz \wedge Mdz_t + dz_x \wedge Kdz + dz \wedge Kdz_x \\
&= -(Mdz_t + Kdz_x) \wedge dz + dz \wedge (Mdz_t + Kdz_x) \\
&= -S_{zz}dz \wedge dz + dz \wedge S_{zz}dz \\
&= 0 
\end{align*}
\]

(using Leibniz’ rule, skew-symmetry, the differential equation and the fact that \( S_{zz} \) is symmetric)

This means that at each point \((x, t)\), the multisymplectic structure is conserved. This is a local property, opposed to conservation of symplectic structure.
A multisymplectic integrator is a map which preserves a *discrete* version of the multisymplectic structure.

**The (Preissman) Box scheme**

Use implicit midpoint in both $x$ and $t$ direction.

\[
M \frac{z_N - z_S}{\Delta t} + K \frac{z_E - z_W}{\Delta x} = \nabla_z S(z_C)
\]

where $z_N = \frac{z_{NW} + z_{NE}}{2}$ etc.

This scheme obeys

\[
\frac{\omega_N - \omega_S}{\Delta t} + \frac{\kappa_E - \kappa_W}{\Delta x} = 0
\]

i.e. *discrete conservation of the multisymplectic structure.*
Energy conservation

Defining

\[ E(z) = S(z) - \frac{1}{2} \langle Kz_x, z \rangle \quad \text{and} \quad F(z) = \frac{1}{2} \langle Kz_t, z \rangle \]

we have that for \textit{time-independent} \( S(z) \)

\[ \delta_t E(z) + \delta_x F(z) = 0 \]

which is the locally conserved energy form.

Proof.

\[ \delta_t E(z) = \delta_t S(z) - \frac{1}{2} \langle Kz_x, z_t \rangle - \frac{1}{2} \langle Kz_{xt}, z \rangle \]

\[ \delta_x F(z) = \frac{1}{2} \langle Kz_t, z_x \rangle + \frac{1}{2} \langle Kz_{xt}, z_t \rangle \]

and thus \( \delta_t E(z) + \delta_x F(z) = 0 \) for \textit{time-independent} \( S(z) \).
Energy conservation

Defining

\[ E(z) = S(z) - \frac{1}{2} \langle Kz_\times, z \rangle \quad \text{and} \quad F(z) = \frac{1}{2} \langle Kz_t, z \rangle \]

we have that for \textit{time-independent} \( S(z) \)

\[ \delta_t E(z) + \delta_x F(z) = 0 \]

which is the locally conserved energy form.

For suitable boundary conditions, this leads to global conservation of energy,

\[ \frac{d}{dt} \left( \int_0^L E(z) \, dx \right) = 0 \]
Momentum conservation

Defining
\[ I(z) = \frac{1}{2} \langle Mz_x, z \rangle \quad \text{and} \quad G(z) = S(z) - \frac{1}{2} \langle Mz_t, z \rangle \]

we can prove that for spatially invariant \( S(z) \)

\[ \delta_t I(z) + \delta_x G(z) = 0 \]

which is the locally conserved momentum form.

For suitable boundary conditions, this leads to global conservation of momentum,

\[ \frac{d}{dt} \left( \int_0^L I(z) \, dx \right) = 0 \]
When $S(z)$ is quadratic in $z$, the (multisymplectic) box scheme conserves local energy and momentum exactly.

This is similar to symplectic integrators which preserve quadratic Hamiltonians exactly, but note here that it is the local invariants that are preserved.

More generally, using a pair of Gauss–Legendre collocation schemes in space and time on selected PDEs, will result in a multisymplectic integrator.
In the end, we provide a simple numerical example, let the NLS be

\[
\psi_t = i\psi_{xx} - 2|\psi|^2\psi, \quad x \in (-L/2, L/2], \quad L = 4\sqrt{2}\pi
\]

\[
\psi(x, 0) = \frac{1}{2} \left(1 + 0.1 \cos \left(\frac{x}{2\sqrt{2}}\right)\right)
\]

with periodic boundary conditions.

The multisymplectic formulation is obtained by \(\psi = a + ib\), \(z = (a, b, v, w)\),

\[
M = \begin{pmatrix}
0 & 1 & 0 & 0 \\
-1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
\end{pmatrix}, \quad K = \begin{pmatrix}
0 & 0 & -1 & 0 \\
0 & 0 & 0 & -1 \\
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 \\
\end{pmatrix}
\]

and

\[
S(z) = \frac{1}{2}(v^2 + w^2 + (a^2 + b^2)^2)
\]
Solution plot, box scheme

Solution of NLS equation with the box scheme, N=64, dt=0.001
Local energy surface plot

Local energy NLS, box scheme, N=64, dt=0.001
Local momentum surface plot

Local momentum NLS, box scheme, N=64, dt=0.001
Global invariants
Multisymplectic integration is still to be considered as a new and not settled field of research.

Crucial theorems corresponding to theory on symplectic integrators are still missing, but numerical results are promising.

Multisymplectic integrators for PDEs are able to catch more physical features of the system than symplectic integrators.
