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

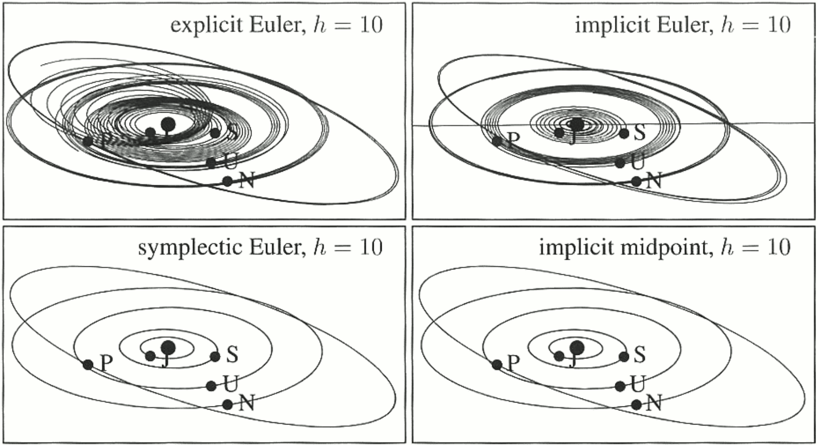
1. Motivation
2. Multisymplectic formulation of PDEs
3. Introduction to forms
4. Multisymplectic structure
5. Multisymplectic integrator
6. Numerical examples

Multisymplectic integration, motivation

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)

A PDE to be solved

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.

Multisymplectic PDE

A *PDE* is said to be multisymplectic if it can be written as

Multisymplectic equation

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

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

(d will be 3 or 4 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

$$\begin{aligned} -v_t + w_x &= V'(u) \\ -u_x &= -w \\ u_t &= v \end{aligned}$$

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 $\mathbf{R}^2$ is *symplectic* if $A^T J A = J$ where $J = \left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$. Nonlinear maps are symplectic if their linearization is symplectic.

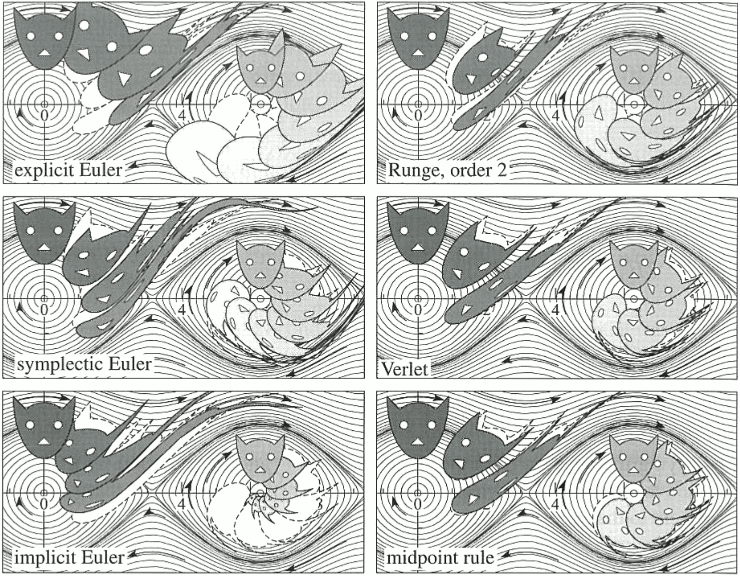
Hamiltonian system

$$J y_t = \nabla H(y)$$

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".

Preservation of symplectic structure



(Hairer, Lubich Wanner 2002: Geometric Numerical Integration, page 176)

Symplectic structure cont.

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.

Exterior algebraic forms

- 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 $\omega^1 \colon \mathbf{R}^n \to \mathbf{R}$.

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

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

2-forms

Definition (2-form)

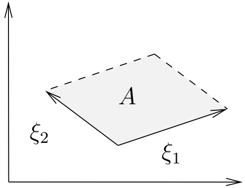
An exterior form of degree 2 is a map on pairs of vectors,

$$\omega^2 \colon \mathbf{R}^n \times \mathbf{R}^n \to \mathbf{R}$$

which is bilinear and skew-symmetric:

$$\omega^2(\lambda_1\xi_1 + \lambda_2\xi_2, \xi_3) = \lambda_1\omega^2(\xi_1, \xi_3) + \lambda_2\omega^2(\xi_2, \xi_3)$$
$$\omega^2(\xi_1, \xi_2) = -\omega^2(\xi_2, \xi_1)$$

- Let $n = 2$ and consider two vectors ξ_1 and $\xi_2 \in \mathbf{R}^2$.
- The *oriented area* $A(\xi_1, \xi_2)$ of the parallelogram spanned by ξ_1 and ξ_2 is an example of a 2-form:



- Oriented area means that

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

(skew-symmetry)

Exterior product of two 1-forms

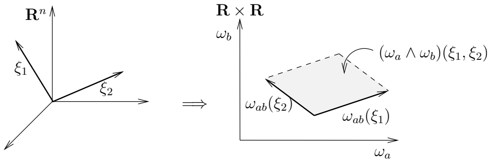
The 2-forms will appear as the (exterior) product of two 1-forms, say ω_a and ω_b:

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 $\xi_1, \xi_2 \in \mathbf{R}^n$. 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 $\mathbf{R} \times \mathbf{R}$.
- The value of the 2-form on the two vectors is then the oriented area of the spanned parallelogram in the ω_a, ω_b plane:



Differential forms

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

$$\omega\colon \bigcup_x T_x\mathcal{M} \to \mathbf{R},$$

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

Take the differential $\omega = \mathrm{d}f = 2x\,\mathrm{d}x$ of the function $f(x) = x^2$ as an easy example.

Differential forms

Differential 2-forms are maps

$$\omega^2\colon \bigcup_x T_x\mathcal{M} \times \bigcup_x T_x\mathcal{M} \to \mathbf{R}$$

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

All 2-forms may be written as the wedge product of 1-forms. For example, in $\mathbf{R}^3$, there are $\binom{3}{2} = 3$ 2-forms, $\mathrm{d}x \wedge \mathrm{d}y$, $\mathrm{d}y \wedge \mathrm{d}z$ and $\mathrm{d}z \wedge \mathrm{d}x$.

Multisymplectic structure

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:

$$\omega = \mathrm{d}z \wedge M\mathrm{d}z \qquad \text{and} \qquad \kappa = \mathrm{d}z \wedge K\mathrm{d}z$$

Conservation of multisymplecticity

Lemma

$$\omega_t + \kappa_x = 0$$

Proof.

$$\begin{aligned}\omega_t + \kappa_x &= \mathrm{d}z_t \wedge M\mathrm{d}z + \mathrm{d}z \wedge M\mathrm{d}z_t + \mathrm{d}z_x \wedge K\mathrm{d}z + \mathrm{d}z \wedge K\mathrm{d}z_x \\ &= -(M\mathrm{d}z_t + K\mathrm{d}z_x) \wedge \mathrm{d}z + \mathrm{d}z \wedge (M\mathrm{d}z_t + K\mathrm{d}z_x) \\ &= -S_{zz}\mathrm{d}z \wedge \mathrm{d}z + \mathrm{d}z \wedge S_{zz}\mathrm{d}z \\ &= 0\end{aligned}$$

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

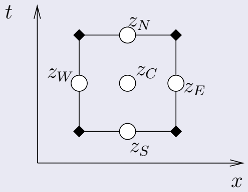
This means that at *each point* (x, t), the multisymplectic structure is conserved. This is a *local* property, opposed to conservation of symplectic structure.

Multisymplectic integrator

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

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

we have that for *time-independent* $S(z)$

$$\delta_t E(z) + \delta_x F(z) = 0$$

which is the locally conserved energy form.

Proof.

$$\begin{aligned} \delta_t E(z) &= \delta_t S(z) - \frac{1}{2}\langle Kz_x, z_t\rangle - \frac{1}{2}\langle Kz_{xt}, z\rangle \\ \delta_x F(z) &= \frac{1}{2}\langle Kz_t, z_x\rangle + \frac{1}{2}\langle Kz_{xt}, z_t\rangle \end{aligned}$$

and thus $\delta_t E(z) + \delta_x F(z) = 0$ for time-independent $S(z)$. □

Energy conservation

Defining

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

we have that for *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,

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\int_0^L E(z)\,\mathrm{d}x\right) = 0$$

Momentum conservation

Defining

$$I(z) = \frac{1}{2}\langle Mz_x, z\rangle \qquad \text{and} \qquad G(z) = S(z) - \frac{1}{2}\langle Mz_t, z\rangle$$

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,

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\int_0^L I(z)\,\mathrm{d}x\right) = 0$$

Numerical conservation of energy and momentum

Theorem

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.

Numerical example, nonlinear Schrödinger equation

In the end, we provide a simple numerical example, let the NLS be

$$\psi_t = \mathrm{i}\psi_{xx} - 2|\psi|^2\psi, \qquad x \in (-L/2, L/2], \quad L = 4\sqrt{2}\pi$$
$$\psi(x,0) = \frac{1}{2}\left(1 + 0.1\cos\left(x/(2\sqrt{2})\right)\right)$$

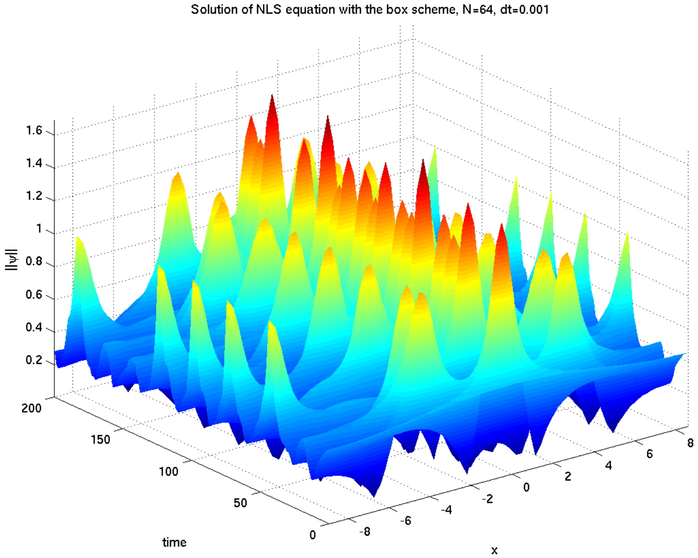
with periodic boundary conditions.
The multisymplectic formulation is obtained by $\psi = a + \mathrm{i}b$, $z = (a, b, v, w)$,

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

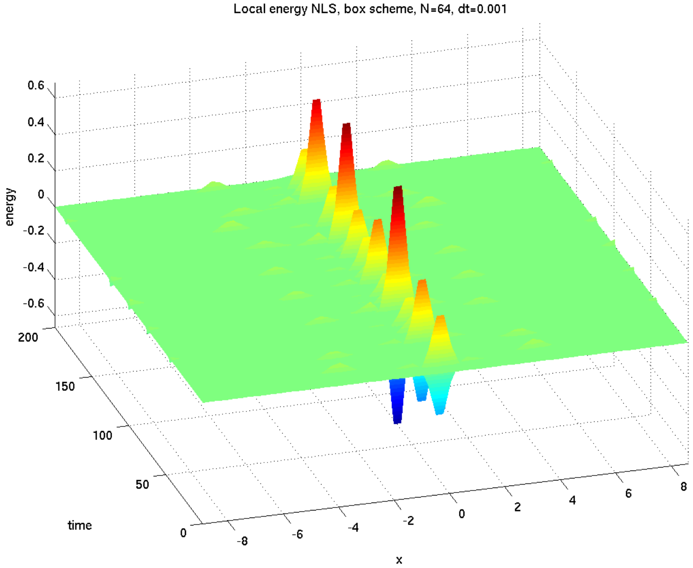
and

$$S(z) = \frac{1}{2}(v^2 + w^2 + (a^2 + b^2)^2)$$

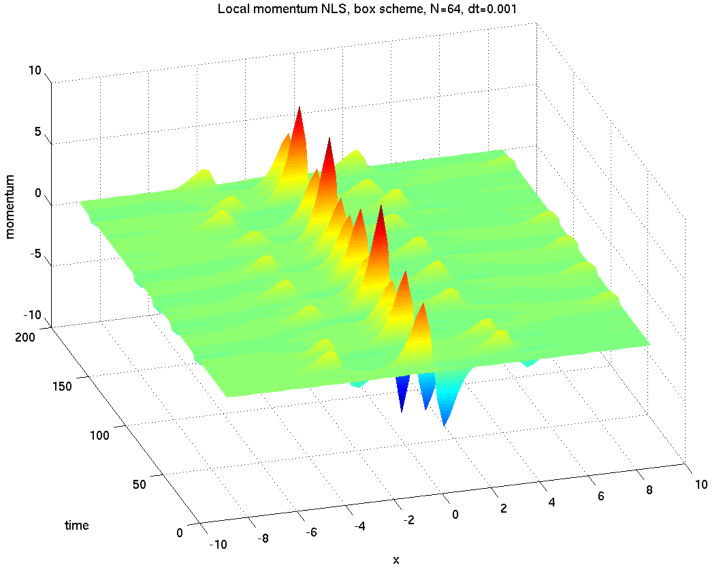
Solution plot, box scheme



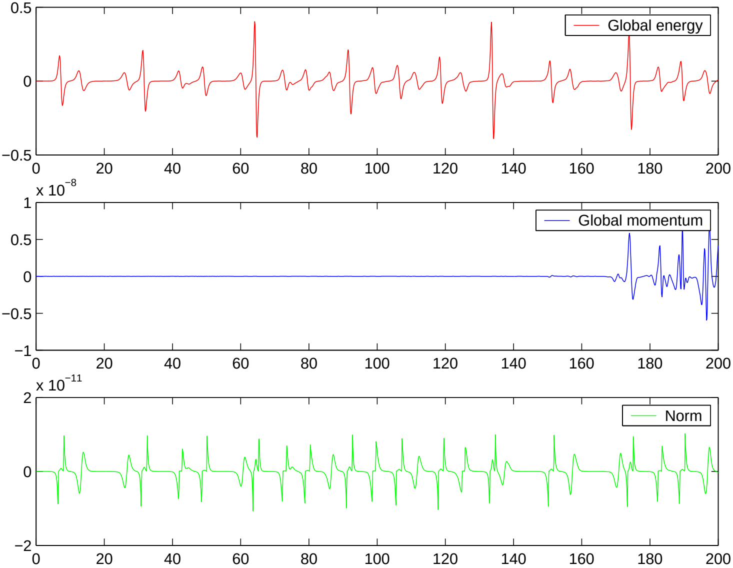
Local energy surface plot



Local momentum surface plot



Global invariants



Ending remarks

- 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.

Recommended literature

- Bridges and Reich 2001: *Multi-symplectic integrators: numerical schemes for Hamiltonian PDEs that conserve symplecticity*, Phys. Lett. A **284**, 184–193.
- Islas, Karpeev and Schober 2001: *Geometric integrators for the nonlinear Schrödinger equation*, J. of Comp. Phys. **173**, 116–148.
- Reich 1999: *Multi-Symplectic Runge–Kutta Collocation Methods for Hamiltonian Wave Equations*, J. of Comp. Phys. **157**, 473–499.