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Multisymplectic structures and geometric integration

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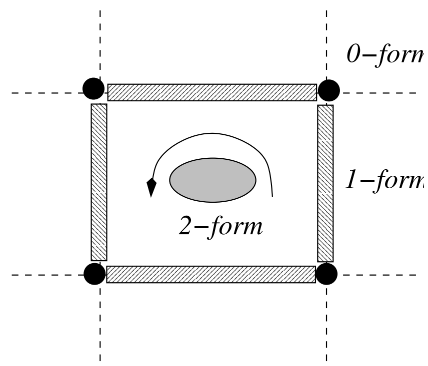


In these lectures, the concept of multisymplecticity and its role in the discretization of partial differential equations is discussed. The topics to be discussed include: overview of multisymplecticty, variational integrators and the Cartan form, continuous and discrete conservation of symplecticity, discrete multisymplectic structures, and implications for waves. A new approach to multisymplectic structures will be also introduced and its implications for numerics discussed. The latter idea is based on the observation that *any* Riemannian manifold has a natural coordinate-free multisymplectic structure on the total exterior algebra bundle, and this "canonical multisymplectic structure" turns out to be useful for analysis and numerics of Hamiltonian PDEs.

From Lagrangian to Hamiltonian for ODEs

Recall the relationships between symplecticity, Lagrangians and Hamiltonians for ordinary differential equations.

Historically, the construction of a "Hamiltonian system" started with a *Lagrangian* function

$$\mathscr{L} = \int L\,\mathrm{d}t\,, \quad \text{with} \quad L = T - V \quad \text{on} \quad TQ\,,$$

since a Lagrangian is derivable from physical (energy) considerations.

The *Legendre transform* then takes one from TQ to T^*Q. The Legendre transform delivers a canonical one-form on T^*Q and a Hamiltonian function. For example, if

$$Q = \mathbb{R}^1 \quad \text{and} \quad L = \tfrac{1}{2}\dot{q}^2 - V(q)\,,$$

then

$$p = \frac{\partial L}{\partial \dot{q}} = \dot{q}\,, \quad H = p\dot{q} - L \quad \text{and} \quad \theta = p\mathrm{d}q\,,$$

and the "Hamiltonian system" is

$$\begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{pmatrix} q \\ p \end{pmatrix}_t = \begin{pmatrix} H_q \\ H_p \end{pmatrix} .$$

One gets for free that $M = T^*Q$ is a *symplectic manifold* with *symplectic form* (in local coordinates),

$$\omega = \mathrm{d}\theta = \mathrm{d}p \wedge \mathrm{d}q\,.$$

Symplectic geometry

On the other hand, symplectic structures exist independent of differential equations, and independent of a Lagrangian. While determining if a given smooth even dimensional manifold supports a symplectic structure is a difficult problem in general, there is a class of smooth manifolds which always has a natural symplectic structure.

Starting with a smooth $n-$dimensional manifold Q, the manifold (M, ω) is a *symplectic manifold* when $M = T^*Q$. The two-form ω is the natural form on T^*Q, $\omega = \mathrm{d}p \wedge \mathrm{d}q$ (in local coordinates).

Given a symplectic manifold, the idea of a Hamiltonian system arises naturally from Cartan's formula,

$$\mathcal{L}_X \omega = X \;\lrcorner\; \mathrm{d}\omega + \mathrm{d}(X \;\lrcorner\; \omega)\,.$$

Vectorfields which preserve the symplectic form are generated by a Hamiltonian function,

$$\mathcal{L}_X \omega = 0 \quad \Rightarrow \quad X \;\lrcorner\; \omega = \mathrm{d}H\,.$$

or alternatively, Hamiltonian vectorfields are symplectic:

$$X \;\lrcorner\; \omega = \mathrm{d}H \quad \Rightarrow \quad \mathcal{L}_X \omega = 0\,.$$

Dynamical systems on the cotangent bundle

Consider an arbitrary smooth vectorfield on $Q = \mathbb{R}^n$,

$$\mathbf{q}_t = \mathbf{f}(\mathbf{q})\,, \quad \mathbf{q} \in Q\,.$$

The associated flows on the tangent bundle and cotangent bundle are

$$\begin{aligned} \mathbf{u}_t &= \mathbf{A}(t)\mathbf{u}\,, \quad \mathbf{u} \in TQ\,, \quad \mathbf{A}(t) = D\mathbf{f}(\mathbf{q}(t)) \\ \mathbf{p}_t &= -\mathbf{A}(t)^T\mathbf{p}\,, \quad \mathbf{p} \in T^*Q \end{aligned}$$

In stability computations and Lyapunov exponent computations it is usual to integrate the coupled system for $(\mathbf{q}, \mathbf{u})$. However, the coupled system $(\mathbf{q}, \mathbf{p})$ has a natural symplectic structure with symplectic form

$$\omega = \mathbf{dp} \wedge \mathbf{dq}\,.$$

What is the Hamiltonian system? Use the formula: $\mathbf{X}_h \;\lrcorner\, \omega = \mathrm{d}H$,

$$\begin{aligned} \mathbf{X}_h \;\lrcorner\, \omega &= \langle \mathbf{dq}, \mathbf{X}_h \rangle \mathbf{dp} - \langle \mathbf{dp}, \mathbf{X}_h \rangle \mathbf{dq} \\ &= \mathbf{q}_t\, \mathbf{dp} - \mathbf{p}_t\, \mathbf{dq} \\ &= \mathbf{f}(\mathbf{q})\, \mathbf{dp} + \mathbf{A}(t)^T\mathbf{p}\mathbf{dq} \\ &= \mathrm{d}H\,, \quad \text{with} \quad H = \langle \mathbf{p}, \mathbf{f}(\mathbf{q}) \rangle\,. \end{aligned}$$

Hence the coupled system for $(\mathbf{q}, \mathbf{p})$ is a Hamiltonian system

$$\begin{aligned} \mathbf{q}_t &= \tfrac{\partial H}{\partial \mathbf{p}} = \mathbf{f}(\mathbf{q}) \\ \mathbf{p}_t &= -\tfrac{\partial H}{\partial \mathbf{q}} = -\mathbf{A}(t)\mathbf{p}\,. \end{aligned}$$

From Lagrangian to Hamiltonian for PDEs

One way to view *multisymplecticity* is through a total Legendre transform. Consider a Lagrangian function for a scalar field

$$\mathscr{L}(\phi) = \int_{x_1}^{x_2} \int_{t_1}^{t_2} L(t, x, \phi, \phi_t, \phi_x)\, \mathrm{d}t \wedge \mathrm{d}x\,.$$

Introduce new coordinates – "polymomenta" – by

$$u = \frac{\partial L}{\partial \phi_t} \quad \text{and} \quad v = \frac{\partial L}{\partial \phi_x}\,.$$

Assuming that these equations can be uniquely solved for ϕ_t and ϕ_x as functions of u and v, a "Hamiltonian function" is then defined by the Legendre transform

$$S(t, x, \phi, u, v) = u\phi_t + v\phi_x - L\,.$$

The governing equations are then

$$\begin{aligned} -u_t - v_x &= S_\phi \\ \phi_t &= S_u \\ \phi_x &= S_v \end{aligned}$$

In addition to a new Hamiltonian function, *two* one forms have been generated

$$\theta_1 = u\,\mathrm{d}\phi \quad \text{and} \quad \theta_2 = v\,\mathrm{d}\phi\,.$$

with two forms $\omega_1 = \mathrm{d}u \wedge \mathrm{d}\phi$ and $\omega_2 = \mathrm{d}v \wedge \mathrm{d}\phi$. We have replaced the characterization of the PDE by a Lagrangian with three objects: a Hamiltonian function and a pair of two forms.

Multisymplectic Hamiltonian PDEs

Motivated by the form of the equations obtained by Legendre transform, it is natural to propose the following "canonical form" for a multisymplectic Hamiltonian PDE

$$\mathbf{J}Z_t + \mathbf{K}Z_x = \nabla S(Z)\,, \quad Z \in \mathbb{H} \tag{1}$$

where $\mathbb{H}$ is the "phase space" and will be taken to be a finite-dimensional vector space ($\mathbb{R}^n$ for simplicity), S is any smooth function and $\mathbf{J}$ and $\mathbf{K}$ are skew-symmetric operators. The operators $\mathbf{J}$ and $\mathbf{K}$ can depend on Z as long as they satisfy the Jacobi condition (i.e. associated with *closed* two forms).

Every system of the form (1) satisfies *conservation of symplecticity*

$$\mathscr{A}(Z)_t + \mathscr{B}(Z)_x = 0\,.$$

where

$$\mathscr{A}(Z) = \frac{1}{2\pi}\int_0^{2\pi} \tfrac{1}{2}\langle \mathbf{J}Z_\theta, Z\rangle \,\mathrm{d}\theta \quad \text{and} \quad \mathscr{B}(Z) = \frac{1}{2\pi}\int_0^{2\pi} \tfrac{1}{2}\langle \mathbf{K}Z_\theta, Z\rangle \,\mathrm{d}\theta\,,$$

and these functionals are averaged over an *ensemble* of solutions of (1)

$$Z(x,t,\theta) \quad \text{with} \quad Z(x,t,\theta+2\pi) = Z(x,t,\theta)\,.$$

This result is a generalization of the familiar result for Hamiltonian ODEs

$$\frac{d}{dt}\oint \mathbf{p}\cdot\mathbf{q}_\theta \,\mathrm{d}\theta = 0\,,$$

for an ensemble of solutions of Hamilton's equations.

Conservation of symplecticity – variations

The conservation of symplecticity that arises in numerics is the conservation law for variations.

Let $U(x,t)$ and $V(x,t)$ be any solutions of the first variation equation

$$\mathbf{J}\frac{\partial}{\partial t}\delta Z + \mathbf{K}\frac{\partial}{\partial x}\delta Z = D^2 S(Z)\delta Z$$

when $Z(x,t)$ is a solution of (1). Let

$$\omega(U,V) = \langle \mathbf{J}U, V\rangle \quad \text{and} \quad \kappa(U,V) = \langle \mathbf{K}U, V\rangle \,.$$

Then

$$\begin{aligned}
\omega_t + \kappa_x &= \omega(U_t,V) + \omega(U,V_t) + \kappa(U_x,V) + \kappa(U,V_x) \\
&= \langle (\mathbf{J}U_t + \mathbf{K}U_x), V\rangle - (\mathbf{J}V_t + \mathbf{K}V_x), U\rangle \\
&= \langle D^2 S(Z)U, V\rangle - \langle D^2 S(Z)V, U\rangle \\
&= 0\,,
\end{aligned}$$

since $D^2S(Z)$ is symmetric.

Conservation of energy and momentum

For a multisymplectic Hamiltonian PDE

$$\mathbf{J}Z_t + \mathbf{K}Z_x = \nabla S(Z)\,, \quad Z \in \mathbb{H} \tag{2}$$

If $\mathbf{J}$, $\mathbf{K}$ and S do not dependent explicitly on t, then *energy* is conserved

$$E(Z)_t + F(Z)_x = 0\,,$$

where

$$E(Z) = S(Z) - \tfrac{1}{2}\langle \mathbf{K}Z_x, Z\rangle \quad \text{and} \quad F(Z) = \tfrac{1}{2}\langle \mathbf{K}Z_t, Z\rangle\,.$$

If $\mathbf{J}$, $\mathbf{K}$ and S do not dependent explicitly on x, then *momentum* is conserved

$$I(Z)_t + \widetilde{S}(Z)_x = 0\,,$$

where

$$I(Z) = \tfrac{1}{2}\langle \mathbf{J}Z_x, Z\rangle \quad \text{and} \quad \widetilde{S}(Z) = S(Z) - \tfrac{1}{2}\langle \mathbf{J}Z_t, Z\rangle\,.$$

Remarks

- *energy flux* and *momentum density* are always quadratic functionals. But *energy density* and *momentum flux* are non-quadratic if the system is nonlinear, since then $S(Z)$ is not quadratic. This distinction is important when considering numerical integrators which preserve quadratic invariants.
- For steady solutions, the multisymplectic Hamiltonian function S equals the momentum flux $\widetilde{S}$. This is the origin of the use of S for the multisymplectic Hamiltonian functional.

Other variations on multisymplectic structures

- $k-$symplectic geometry of the frame bundle. It exploits the natural canonical soldering form of the linear frame bundle of an n-dimensional manifold to generate a vector-valued $k-$symplectic form. The Hamiltonian systems generated however have vector-valued Hamiltonian functions. (Norris, de Leon, Lawson, Awane, Salgado)
- Multisymplectic manifolds: a multisymplectic vector space of order $m + 1$ is a vector space of dimension $n + m$ with a closed $(m+1)-$form ω which is non-degenerate in the sense that $\mathbf{v} \,\lrcorner\, \omega = 0$ iff $\mathbf{v} = 0$ for all $\mathbf{v}$. It reduces to a classical symplectic manifold when $m = 1$. Some success with the case $m = 2$ with $n = 4$ (3 forms on 6-dimensional manifolds). Lacks a Darboux theory; non-uniqueness of canonical forms (Cantrijn, Ibort, De León)
- DeDonder-Weyl, Catheodory theory, Kijowski theory, Dedecker theory. Variations on the Lagrangian theory, Legendre transform, covariant Hamiltonian formulations (Śniatycki, GIMMSY, Crampin, Saunders, Marsden, Shkoller, Helein, Krupkova).
- Lepagean equivalents: looking at non-uniqueness of the Cartan form (Krupka, Gotay, Krupkova, Betounes).

Cartan form – *from ODEs to PDEs*

Ordinary differential equations: consider

$$\mathscr{L} = \int_{t_1}^{t_2} L(t, q, \dot{q})\,\Omega\,, \quad \Omega = \mathrm{d}t\,.$$

Reformulate as

$$\mathscr{L} = \int_{t_1}^{t_2} [L(t, q, v) + \alpha(\dot{q} - v)]\,\Omega\,.$$

But taking the variation with respect to v results in $L_v = \alpha$ and so

$$\mathscr{L} = \int_{t_1}^{t_2} [L(t, q, v) + L_v(\dot{q} - v)]\Omega\,.$$

But $\dot{q}\mathrm{d}t = \mathrm{d}q$,

$$\mathscr{L} = \int \theta_{\mathscr{L}}\,,$$

with $\theta_{\mathscr{L}}$ the *Cartan form*

$$\theta_{\mathscr{L}} = L\mathrm{dt} + L_v(dq - v\mathrm{d}t)\,.$$

Various interesting arguments about why the Cartan *form* is superior to the Lagrangian *function* (Dedecker, Crampin, Burke, Marsden).

Remark. By retaining α throughout (which is in the cotangent space), one can develop $\mathscr{L}$ on a submanifold of $T^*Q \oplus TQ$ leading to both Lagrangian and Hamiltonian dynamics (cf. SKINNER & RUSK).

- R. SKINNER & R. RUSK. *Generalized Hamiltonian Dynamics I: Formulation on $T^*Q \oplus TQ$*, J. Math. Phys **24** 2589–2601 (1983).

Cartan form – *PDEs*

For PDEs try to reproduce this strategy starting with a Lagrangian for a first order field theory

$$\mathscr{L} = \int_{x_1}^{x_2} \int_{t_1}^{t_2} L(t, x, q, q_t, q_x)\, \Omega\,, \qquad \Omega = \mathrm{dt} \wedge \mathrm{dx}\,.$$

Introduce new coordinates $u = q_t$ and $v = q_x$,

$$\mathscr{L} = \int_{x_1}^{x_2} \int_{t_1}^{t_2} [L(t, x, q, u, v) + \alpha(q_t - u) + \beta(q_x - v)]\, \Omega\,.$$

Taking u, v variations results in $\alpha = L_u$ and $\beta = L_v$, and so

$$\mathscr{L} = \int_{x_1}^{x_2} \int_{t_1}^{t_2} [L(t, x, q, u, v) + L_u(q_t - u) + L_v(q_x - v)]\, \Omega\,.$$

Now use

$$L_u q_t\, \Omega = L_u q_t\, \mathrm{dt} \wedge \mathrm{dx} = L_u(\mathrm{d}q - q_x \mathrm{d}x) \wedge \mathrm{dx} = L_u \mathrm{d}q \wedge \mathrm{d}x\,.$$

Similarly $L_v q_x \Omega = -\mathrm{dq} \wedge \mathrm{d}t$, leading to

$$\mathscr{L} = \int \Theta_{\mathscr{L}}$$

with $\Theta_{\mathscr{L}}$ the *Cartan form* in local coordinates

$$\Theta_{\mathscr{L}} = L_u \mathrm{d}q \wedge \mathrm{dx} - L_v \mathrm{d}q \wedge \mathrm{d}t + (L - uL_u - vL_v)\, \Omega$$

By retaining α and β, theory goes through for *singular* Lagrangians.

- A. ECHEVERRÍA-ENRÍQUEZ, C. LÓPEZ, I. MARÍN-SOLANO, M.C. MUÑOZ-LECANDA, N. ROMÁN-ROY, *Lagrangian-Hamiltonian unified formalism for field theory*, J. Math. Phys. **45** 360–380 (2004).

Cartan form and integrability constraints

Replace $\int L$ by

$$\mathscr{L} = \int \Theta_{\mathscr{L}}$$

with

$$\Theta_{\mathscr{L}} = \frac{\partial L}{\partial q_t} \mathrm{d}q \wedge \mathrm{d}x - \frac{\partial L}{\partial q_x} \mathrm{d}q \wedge \mathrm{d}t + \left(L - q_t \frac{\partial L}{\partial q_t} - q_x \frac{\partial L}{\partial q_x} \right) \Omega$$

or

$$\Theta_{\mathscr{L}} = L_u \mathrm{d}q \wedge \mathrm{dx} - L_v \mathrm{d}q \wedge \mathrm{d}t + (L - uL_u - vL_v)\, \Omega$$

In the latter case, the relationship between u and v arises:

$$u = q_t \quad \text{and} \quad v = q_x \quad \Rightarrow \quad u_x = v_t$$

Is this condition automatically satisfied, or a constraint?

Consider the one form

$$\gamma = u\mathrm{d}t + v\mathrm{d}x$$

Then the above condition is equivalent to γ closed, since

$$\mathrm{d}\gamma = (v_t - u_x)\Omega\,.$$

On the Hamiltonian side, one encounters integrability conditions. How can one address these conditions?

Variational integrators

Suppose one has a scalar non-degenerate first-order field theory defined by a Lagrangian

$$\mathscr{L} = \int_{x_1}^{x_2} \int_{t_1}^{t_2} L(t, x, q, q_t, q_x)\,\Omega\,, \qquad \Omega = \mathrm{dt} \wedge \mathrm{dx}\,.$$

Instead of discretizing the Euler-Lagrange equation, MPS propose discretizing the Lagrangian density but without fixed boundary variations: *the variational route to the Cartan form*.

Space time is replaced by a lattice, and the Lagrangian is replaced by a discrete Lagrangian L_Δ. This discretization is called a *Veselov-type discretization*.

Variation of L_Δ leads to discrete E-L equations. However, the key is that nonzero variations at the boundary lead to a sum of terms which represent a discrete version of the Cartan form. If this sum vanishes the integrator is said to be *multisymplectic* (the exterior derivative of the Cartan form is called a multisymplectic form there).

Remarks:

- Elegant approach for discretizing Lagrangians.
- It is limited, however, to Lagrangians where the Cartan form can be uniquely defined; predominantly scalar first order field theories.
- Generalizations have been proposed however for fluids, second order fields, and constrained systems (Marsden, Kouranbaeva, Shkoller, Chen, Qin, Wang).
- Potential for backward error analysis (Oliver, West & Wulff).
- J.E. MARSDEN, G.W. PATRICK & S. SHKOLLER. *Multisymplectic geometry, variational integrators, and nonlinear PDEs*, Comm. Math. Phys. **199** 351–395 (1998).

Discrete conservation of symplecticity

One can start with the canonical form for a multisymplectic PDE

$$\mathbf{J}Z_t + \mathbf{K}Z_x = \nabla S(Z)\,. \tag{3}$$

and then use any scheme to discretize the equation

$$\mathbf{J}\Delta^t_{ij}Z^{ij} + \mathbf{K}\Delta^x_{ij}Z^{ij} = \nabla S(Z^{ij})\,.$$

If this discretization satisfies discrete conservation of symplecticity, we call it a multi-symplectic integrator

$$\Delta^t_{ij}\omega(U^{ij}, V^{ij}) + \Delta^x_{ij}\kappa(U^{ij}, V^{ij}) = 0 \quad \forall \quad i, j\,.$$

Remarks:

- Applies to any multisymplectic PDE in canonical form.
- Not clear, however, that "discrete form of multisymplectic conservation law" is unambiguous.
- Natural for concatenating 1D symplectic schemes in space time (i.e. GLRK).
- Agrees with variational integrators when (3) is obtained from a well-behaved Lagrangian.
- Backward error analysis results exist (Moore, Reich)
- S. REICH. *Multi-symplectic Runge-Kutta collocation methods for Hamiltonian wave equations*, J. Comput. Phys. **157** 473–499 (2000).
- B.E. MOORE & S. REICH. *Backward Error Analysis for Multi-Symplectic Integrators*, Numer. Math. **95** 625–652 (2003).

Discrete multisymplectic structures

Let $S : n \mapsto n+1$ be the forward shift operator and define

$$\Delta^+ = S - \mathrm{id} \quad \text{and} \quad \Delta^- = \mathrm{id} - S^{-1}\,.$$

HYDON shows that the semi-discrete analogue of $\mathbf{J}Z_t + \mathbf{K}Z_x = \nabla S(Z)$ is

$$J_{ij}Z^j_{,t} + K_{ij}\Delta^+ Z^j - K_{ji}\Delta^- Z^j = \frac{\partial S}{\partial Z^j}\,,$$

and this equation has a semi-discrete conservation of symplecticity,

$$D_t(\tfrac{1}{2}J_{ij}\mathrm{d}Z^i \wedge \mathrm{d}Z^j) + \Delta^+(K_{ij}\mathrm{d}(S^{-1}Z^i) \wedge \mathrm{d}Z^j) = 0\,.$$

As an example, consider the *Ablowitz-Ladik* equation,

$$\mathtt{i}u_t + (1+|u|^2)(\Delta^+\Delta^- u) + 2|u|^2 u = 0\,.$$

It is an integrable differential difference equation and is multisymplectic in the above sense.

In the same paper, HYDON introduces a new generalization of multisymplectic Noether theory for both continuous multisymplectic systems and semi-discrete systems. In application of this theory to the Ablowitz-Ladik equation, a new conservation law has been discovered.

- P.E. HYDON. *Multisymplectic conservation laws for differential and differential-difference equations*, Proc. Roy. Soc. London A (in press, 2005).

Towards intrinsic multisymplectic structures on any Riemannian manifold

So far, we have talked about multisymplectic structures that are dictated by PDEs. However, as noted earlier, one can obtain classical symplectic geometry from a manifold directly. The cotangent bundle of a smooth manifold has a natural symplectic structure.

Do manifolds, or bundles built on manifolds have a natural *multisymplectic* structure?

In going from ODEs to PDEs it is the base manifold that is changing; i.e. changing from the one-dimensional manifold time to the $m+1$ dimensional manifold space+time. The fibre structure does not change dramatically. This observation suggests that if multisymplectic structures appear naturally they will be induced by the geometry of the base manifold.

It turns out that there is a class of intrinsic multisymplectic structures on the *total exterior algebra bundle of the base manifold*. For the case of ODEs, the total exterior algebra reduces to the cotangent bundle (of time!). As soon as the dimension of the base exceeds one, interesting new geometry appears and it generates multisymplectic structures.

- TJB. *Canonical multisymplectic structure on the total exterior algebra of a Riemannian manifold*, Preprint (2004).

Symplectic geometry on the *total exterior algebra bundle*

$$\left.\begin{array}{c} \frac{d^2q}{dt^2} = -V'(q) \\ \text{(base manifold)} \quad M = \mathbb{R}^1 \\ \bigwedge^0(T^*_m M) \oplus \bigwedge^1(T^*_m M) \end{array}\right\} \quad \to \quad \left\{\begin{array}{c} \frac{\partial^2 q}{\partial x_1^2} + \frac{\partial^2 q}{\partial x_2^2} = -V'(q) \\ \text{(base manifold)} \quad M = \mathbb{R}^2 \\ \bigwedge^0(T^*_m M) \oplus \bigwedge^1(T^*_m M) \oplus \bigwedge^2(T^*_m M) \end{array}\right.$$

$M = \mathbb{R}^1$, $\langle\cdot,\cdot\rangle$, vol $= \mathrm{d}t$

Hodge star operator: $\bigstar 1 = \mathrm{d}t$, $\bigstar \mathrm{d}t = 1$

co-differential: $\boldsymbol{\delta} u = -\bigstar \mathrm{d} \bigstar u$, $u \in \bigwedge^1(M)$

$\bigwedge(M) = \bigwedge^0(M) \oplus \bigwedge^1(M)$ (mappings from M into $\bigwedge(T^*_m M)$),

i.e. functions on M and oneforms on M

Take coordinates $(q, P) \in \bigwedge^0(M) \oplus \bigwedge^1(M)$; i.e. $P = p(t)\mathrm{d}t$. The natural form on $\bigwedge(M)$ is

$$\boxed{\boldsymbol{\Theta} = P \wedge \bigstar \mathrm{d}q}$$

$p\mathrm{d}q$ from the view of the *base manifold*

Consider the first variation of the functional $\int \boldsymbol{\Theta} - H(q, P)\mathrm{d}t$

$$\boldsymbol{\delta} P = H_q \quad \text{and} \quad \mathrm{d}q = H_P$$

$$\begin{pmatrix} 0 & \boldsymbol{\delta} \\ \mathrm{d} & 0 \end{pmatrix} \begin{pmatrix} q \\ P \end{pmatrix} = \begin{pmatrix} H_q \\ H_P \end{pmatrix}$$

In coordinates the operator on the left is $\mathbf{J}\frac{d}{dt}$.

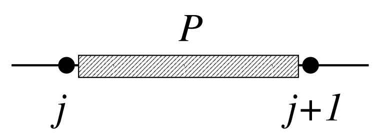
$$\text{Kernel} \begin{pmatrix} 0 & \boldsymbol{\delta} \\ \mathrm{d} & 0 \end{pmatrix} = \text{the harmonic forms in } \bigwedge^0 \oplus \bigwedge^1$$

Störmer-Verlet from the view of the base manifold

Consider Hamilton's equations for the classical mechanical system written in the "coordinate-free" way

$$\mathrm{d}q = P \quad \text{and} \quad \boldsymbol{\delta} P = V'(q)$$

Now introduce a discretization of time, with $q_j = q(j\Delta t)$,



On this lattice approximate the exterior derivative and one form P by

$$\mathrm{d}q \approx \Delta^+ q_j = q_{j+1} - q_j \quad \text{and} \quad P \approx \int_{t_j}^{t_{j+1}} p(t)\mathrm{d}t \approx p_{j+\frac{1}{2}} \Delta t\,.$$

How to approximate the co-differential $\boldsymbol{\delta}$? Recall that $\boldsymbol{\delta}$ is the adjoint of d with respect to the Riemannian metric on the base manifold, hence

$$\boldsymbol{\delta} P \approx \mathrm{d}^* P\Big|_{j,j+1} = (-p_{j+\frac{1}{2}} + p_{j-\frac{1}{2}})/\Delta t\,.$$

Using $(\Delta^+)^* = -\Delta^-$. Combining these equations

$$q_{j+1} = q_j + \Delta t\, p_{j+\frac{1}{2}} \quad \text{and} \quad p_{j+\frac{1}{2}} = p_{j-\frac{1}{2}} - \Delta t\, V'(q_j)\,.$$

i.e. obtain Störmer-Verlet (and its generalizations) by discretizing using *difference forms* or *discrete differential forms* (Bossavit, Hiptmair, Hydon, Leok, Mansfield).

Is Störmer-Verlet based on the cotangent bundle geometry of the base manifold (time) or the cotangent bundle geometry of the phase space?

Structure of the total exterior algebra of $M = \mathbb{R}^2$

Take $M = \mathbb{R}^2$ with coordinates (x_1, x_2).

M is taken to be a Riemannian manifold with

standard inner product $\langle \cdot, \cdot \rangle$ and volume form $\mathsf{vol} = \mathrm{d}x_1 \wedge \mathrm{d}x_2$

Mappings into the total exterior algebra built on $T_x^* M$:

$$\bigwedge(M) = \bigwedge^0(M) \oplus \bigwedge^1(M) \oplus \bigwedge^2(M)$$

i.e. functions on M, oneforms on M and twoforms on M

Hodge star operator: $\bigstar\mathsf{vol} = 1$,

$$\bigstar\mathrm{d}x_1 = \mathrm{d}x_2, \quad \bigstar\mathrm{d}x_2 = -\mathrm{d}x_1$$

co-differential: $\boldsymbol{\delta} u = -\bigstar\mathrm{d}\bigstar u, \quad u \in \bigwedge^k(M)$, $k = 1, 2$

Take a point $(q, P, R) \in \bigwedge^0(M) \oplus \bigwedge^1(M) \oplus \bigwedge^2(M)$;

i.e. $P = p_1(x)\mathrm{d}x_1 + p_2(x)\mathrm{d}x_2$ and $R = r(x)\,\mathrm{d}x_1 \wedge \mathrm{d}x_2$.

A natural form on $\bigwedge(M)$ is

$$\boxed{\boldsymbol{\Theta} = P \wedge \bigstar\mathrm{d}q + R \wedge \bigstar\mathrm{d}P}$$

Properties of Θ

$$\boldsymbol{\Theta}(Z) = P \wedge \bigstar \mathrm{d}q + R \wedge \bigstar \mathrm{d}P$$

Let $\langle\!\langle \cdot, \cdot \rangle\!\rangle$ be the induced inner product on $\bigwedge(T_x^* M)$.

Θ can be reformulated as

$$\Theta(Z) = \tfrac{1}{2} \langle\!\langle \mathbf{J}_\partial Z, Z \rangle\!\rangle \mathsf{Vol} + \mathrm{d}\Upsilon$$

where

$$\mathbf{J}_\partial = \begin{bmatrix} 0 & \delta & 0 \\ \mathrm{d} & 0 & \delta \\ 0 & \mathrm{d} & 0 \end{bmatrix}$$

and Υ is the one form

$$\Upsilon(Z) = \tfrac{1}{2}(q \bigstar P + \bigstar R\, P)$$

Now consider the integral of Θ: $\mathscr{T}(Z) = \int_{\mathscr{V}} \Theta(Z)$. Then

$$\frac{d}{d\epsilon} \mathscr{T}(Z + \epsilon\xi)\Big|_{\epsilon=0} = \int_{\mathscr{V}} \langle\!\langle \mathbf{J}_\partial Z, \xi \rangle\!\rangle \mathsf{vol}$$

with appropriate variations at the boundary.

Properties of the operator $\mathbf{J}_{\boldsymbol{\partial}}$ on $\bigwedge(M)$

Analyze $\mathbf{J}_{\boldsymbol{\partial}} Z$ in more detail.
In standard coordinates

$$\mathbf{J}_{\boldsymbol{\partial}} Z = \begin{bmatrix} 0 & \boldsymbol{\delta} & 0 \\ \mathrm{d} & 0 & \boldsymbol{\delta} \\ 0 & \mathrm{d} & 0 \end{bmatrix} \begin{pmatrix} q \\ P \\ R \end{pmatrix} = \begin{matrix} -(\frac{\partial p_1}{\partial x_1} + \frac{\partial p_2}{\partial x_2}) \\ (\frac{\partial q}{\partial x_1} + \frac{\partial r}{\partial x_2})\mathrm{d}x_1 + (\frac{\partial q}{\partial x_2} - \frac{\partial r}{\partial x_1})\mathrm{d}x_2 \\ (\frac{\partial p_2}{\partial x_1} - \frac{\partial p_1}{\partial x_2})\mathrm{d}x_1 \wedge \mathrm{d}x_2 \end{matrix}$$

It is a a *Cauchy-Riemann operator* with (q, r) and (p_1, p_2) conjugate pairs of harmonic functions.

In standard coordinates

$$\boxed{\mathbf{J}_{\boldsymbol{\partial}} = \mathbf{J}_1 \frac{\partial}{\partial x_1} + \mathbf{J}_2 \frac{\partial}{\partial x_2}}$$

with

$$\mathbf{J}_1 = \begin{bmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \quad \mathbf{J}_2 = \begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}.$$

In a coordinate representation, it is a *multisymplectic* operator.

Clifford algebra structure of $\mathbf{J}_{\boldsymbol{\partial}}$

In standard coordinates

$$\boxed{\mathbf{J}_{\boldsymbol{\partial}} = \mathbf{J}_1 \tfrac{\partial}{\partial x_1} + \mathbf{J}_2 \tfrac{\partial}{\partial x_2}}$$

with

$$\mathbf{J}_1 = \begin{bmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \quad \mathbf{J}_2 = \begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}.$$

The operators $\mathbf{J}_1$, $\mathbf{J}_2$ and $\mathbf{J}_{12} := \mathbf{J}_1\mathbf{J}_2$ satisfy

$\mathbf{J}_1^2 = -\mathbf{I}$, $\mathbf{J}_2^2 = -\mathbf{I}$ and $\mathbf{J}_1\mathbf{J}_2 + \mathbf{J}_2\mathbf{J}_1 = 0$,

$\{\mathbf{J}_1, \mathbf{J}_2, \mathbf{J}_{12}\}$ generate the quaternions; the Clifford algebra ($\mathscr{C}\ell_{0,2}$)

For any $\boldsymbol{\xi} \in \bigwedge(T_m^*M) \cong \mathbb{R}^4$ of unit length

$$\{\boldsymbol{\xi}, \mathbf{J}_1\boldsymbol{\xi}, \mathbf{J}_2\boldsymbol{\xi}, \mathbf{J}_{12}\boldsymbol{\xi}\}$$

provide an orthonormal basis for $\bigwedge(T_m^*M) \cong \mathbb{R}^4$.

Multi-symplectic Dirac operator

Square the operator $\mathbf{J}_\partial$

$$\mathbf{J}_\partial\,\mathbf{J}_\partial = \begin{bmatrix} 0 & \boldsymbol{\delta} & 0 \\ \mathrm{d} & 0 & \boldsymbol{\delta} \\ 0 & \mathrm{d} & 0 \end{bmatrix} \begin{bmatrix} 0 & \boldsymbol{\delta} & 0 \\ \mathrm{d} & 0 & \boldsymbol{\delta} \\ 0 & \mathrm{d} & 0 \end{bmatrix} = \begin{bmatrix} \delta\mathrm{d} & 0 & 0 \\ 0 & \mathrm{d}\delta + \delta\mathrm{d} & 0 \\ 0 & 0 & \mathrm{d}\delta \end{bmatrix}$$

But $\mathrm{d}\delta + \delta\mathrm{d} = -\Delta$. Hence

$$\mathbf{J}_\partial\,\mathbf{J}_\partial = -(\Delta_0 \oplus \Delta_1 \oplus \Delta_2)\,.$$

$\mathbf{J}_\partial$ can be interpreted as a multisymplectic Dirac operator.

In standard coordinates

$$\begin{aligned} \mathbf{J}_\partial\,\mathbf{J}_\partial &= (\mathbf{J}_1\tfrac{\partial}{\partial x_1} + \mathbf{J}_2\tfrac{\partial}{\partial x_2})(\mathbf{J}_1\tfrac{\partial}{\partial x_1} + \mathbf{J}_2\tfrac{\partial}{\partial x_2}) \\ &= \mathbf{J}_1^2\tfrac{\partial^2}{\partial x_1^2} + (\mathbf{J}_1\mathbf{J}_2 + \mathbf{J}_2\mathbf{J}_1)\tfrac{\partial^2}{\partial x_1 \partial x_2} + \mathbf{J}_2^2\tfrac{\partial^2}{\partial x_2^2} \\ &= -(\tfrac{\partial^2}{\partial x_1^2} + \tfrac{\partial^2}{\partial x_2^2})\mathbf{I}\,. \end{aligned}$$

since

$$\mathbf{J}_1^2 = -\mathbf{I}\,, \quad \mathbf{J}_2^2 = -\mathbf{I}\,, \quad \mathbf{J}_1\mathbf{J}_2 + \mathbf{J}_2\mathbf{J}_1 = 0\,.$$

$\mathrm{Kernel}(\mathbf{J}_{\boldsymbol{\partial}})$ = the harmonic forms in $\bigwedge^0 \oplus \bigwedge^1 \oplus \bigwedge^2$

PDEs on the total exterior algebra of $M = \mathbb{R}^2$

$$\boxed{\boldsymbol{\Theta} = P \wedge \bigstar \mathrm{d}q + R \wedge \bigstar \mathrm{d}P}$$

Consider the first variation of the functional

$$\mathscr{T}_S(Z) = \int_{\mathscr{V}} \boldsymbol{\Theta}(Z) - S(Z)\,\mathsf{vol}\,.$$

where $Z = (q, P, R) \in \bigwedge(M)$

$$\frac{d}{d\epsilon}\mathscr{T}_S(Z + \epsilon\xi)\Big|_{\epsilon=0} = \int_{\mathscr{V}} \langle\!\langle \mathbf{J}_\partial Z, \xi \rangle\!\rangle - \langle\!\langle \nabla S(Z), \xi \rangle\!\rangle\,\mathsf{vol}\,.$$

Setting the first variation to zero: $\mathbf{J}_{\boldsymbol{\partial}} Z = \nabla S(Z)$, or

$$\begin{bmatrix} 0 & \boldsymbol{\delta} & 0 \\ \mathrm{d} & 0 & \boldsymbol{\delta} \\ 0 & \mathrm{d} & 0 \end{bmatrix} \begin{pmatrix} q \\ P \\ R \end{pmatrix} = \begin{pmatrix} S_q \\ S_P \\ S_R \end{pmatrix}$$

or

$$\begin{aligned} \delta P &= S_q \\ \mathrm{d}q + \boldsymbol{\delta} R &= S_P \\ \mathrm{d}P &= S_R \end{aligned}$$

Elliptic PDEs generated by $\boldsymbol{\Theta}$

$$\mathbf{J}_{\boldsymbol{\partial}} Z = \nabla S(Z)\ : \qquad \begin{bmatrix} 0 & \boldsymbol{\delta} & 0 \\ \mathrm{d} & 0 & \boldsymbol{\delta} \\ 0 & \mathrm{d} & 0 \end{bmatrix} \begin{pmatrix} q \\ P \\ R \end{pmatrix} = \begin{pmatrix} S_q \\ S_P \\ S_R \end{pmatrix}$$

Consider two examples of $S(Z)$

$$S(Z) = \tfrac{1}{2}\langle P, P\rangle_1 + V(q) \quad \text{and} \quad S(Z) = \tfrac{1}{2}\langle P, P\rangle_1 + F(q,R)\,,$$

where $\langle \cdot, \cdot \rangle_k$ is the induced inner product on $\bigwedge^k(T_x^* M)$. Then

$$\begin{aligned} \boldsymbol{\delta} P &= V'(q) & \qquad \boldsymbol{\delta} P &= F_q(q,R) \\ \mathrm{d}q + \boldsymbol{\delta} R &= P & \qquad \mathrm{d}q + \boldsymbol{\delta} R &= P \\ \mathrm{d}P &= 0 & \qquad \mathrm{d}P &= F_R(q,R) \end{aligned}$$

Eliminating $P = \mathrm{d}q + \boldsymbol{\delta} R$ from both equations leads to

$$\begin{aligned} \Delta q &= -V'(q) & \qquad \Delta q &= -F_q(q,R) \\ \Delta R &= 0 & \qquad \Delta R &= -F_R(q,R) \end{aligned}$$

The first is obtainable by a (variant of the) Legendre transform, the latter is not.

Generalities – $n-$dimensional manifolds

Starting point: an $n-$dimensional orientable Riemannian manifold M, orientable.

For illustration, take $M = \mathbb{R}^n$. The total exterior algebra at each point $m \in M$ has dimension 2^n and is of the form

$$\bigwedge(T_m^*M) = \bigwedge^0(T_m^*M) \oplus \cdots \oplus \bigwedge^n(T_m^*M).$$

with mappings

$$\bigwedge(M) = \bigwedge^0(M) \oplus \cdots \oplus \bigwedge^n(M).$$

On $\bigwedge(M)$ take a point

$$Z = (\boldsymbol{\alpha}^{(0)}, \ldots, \boldsymbol{\alpha}^{(n)}) \,, \quad \boldsymbol{\alpha}^{(j)} \in \bigwedge^j(M) \,,$$

and define

$$\boldsymbol{\Theta}(Z) = \sum_{j=1}^{n} \boldsymbol{\alpha}^{(j)} \wedge \bigstar \mathrm{d}\boldsymbol{\alpha}^{(j-1)}$$

Then

$$\boldsymbol{\Theta}(Z) = \tfrac{1}{2}\langle\!\langle \mathbf{J}_{\boldsymbol{\partial}} Z, Z \rangle\!\rangle \mathsf{vol} + \mathrm{d}\Upsilon$$

where Υ is an $n-1$ form and

$$\mathbf{J}_{\boldsymbol{\partial}} = \begin{bmatrix} 0 & \boldsymbol{\delta} & 0 & 0 & \cdots & 0 \\ \mathrm{d} & 0 & \boldsymbol{\delta} & 0 & \cdots & 0 \\ 0 & \ddots & 0 & \ddots & \cdots & 0 \\ 0 & \cdots & 0 & \mathrm{d} & 0 & \boldsymbol{\delta} \\ 0 & \cdots & 0 & 0 & \mathrm{d} & 0 \end{bmatrix}$$

Properties of $\mathbf{J}_\partial$ on $n-$dimensional manifolds

$\mathbf{J}_{\boldsymbol{\partial}}$ is a multisymplectic Dirac operator, satisfying

$$\begin{aligned}\mathbf{J}_{\boldsymbol{\partial}} \circ \mathbf{J}_{\boldsymbol{\partial}} &= \boldsymbol{\delta}\mathrm{d} \oplus \boldsymbol{\delta}\mathrm{d} + \mathrm{d}\boldsymbol{\delta} \oplus \cdots \oplus \boldsymbol{\delta}\mathrm{d} + \mathrm{d}\boldsymbol{\delta} \oplus \mathrm{d}\boldsymbol{\delta} \\ &= -\mathbf{I} \otimes \Delta\,.\end{aligned}$$

- A generalized Cauchy Riemann operator
- Kernel of $\mathbf{J}_{\boldsymbol{\partial}} = \cup_{k=1}^{n} \mathscr{H}^k(M)$ (the harmonic forms).

In standard coordinates

$$\mathbf{J}_{\boldsymbol{\partial}} = \sum_{j=1}^{n} \mathbf{J}_j \frac{\partial}{\partial x_j} \quad \text{with} \quad \mathbf{J}_i \mathbf{J}_j + \mathbf{J}_j \mathbf{J}_i = -2\delta_{ij} \mathbf{I}\,,$$

i.e. $\{\mathbf{J}_1, \ldots, \mathbf{J}_n\}$ are isomorphic as an associative algebra to the Clifford algebra $\mathscr{C}\ell_{0,n}$.

Adding a function $S : \bigwedge(M) \to \mathbb{R}$ generates a class of elliptic PDEs $\mathbf{J}_{\boldsymbol{\partial}} Z = \nabla S(Z)$ where ∇ is defined with respect to the induced inner product on $\bigwedge(T_m^* M) \cong \mathbb{R}^N$, $N = 2^n$.

Legendre Transformation

Consider the standard form for a Lagrangian which generates the PDE

$$\frac{\partial^2 q}{\partial x_1^2} + \frac{\partial^2 q}{\partial x_2^2} = -V'(q)\,,$$

that is, let $\mathscr{L} = \int\int L(q, q_{x_1}, q_{x_2})\,\mathrm{d}x_2 \wedge \mathrm{d}x_2$ with

$$L(q, q_{x_1}, q_{x_2}) = \tfrac{1}{2}\left((\frac{\partial q}{\partial x_1})^2 + (\frac{\partial q}{\partial x_2})^2 \right) - V(q)\,.$$

Introduce the classical Legendre transformation; i.e. let

$$p_1 = \tfrac{\partial L}{\partial q_{x_1}} \quad \text{and} \quad p_2 = \tfrac{\partial L}{\partial q_{x_2}} \text{ then}$$

$$S(q, p_1, p_2) = p_1 q_{x_1} + p_2 q_{x_2} - L = \tfrac{1}{2}(p_1^2 + p_2^2) + V(q).$$

The governing equations are

$$-\frac{\partial p_1}{\partial x_1} - \frac{\partial p_2}{\partial x_2} = V'(q)\,, \quad \frac{\partial q}{\partial x_1} = p_1\,, \quad \frac{\partial q}{\partial x_2} = p_2$$

or

$$\begin{bmatrix} 0 & -\frac{\partial}{\partial x} & -\frac{\partial}{\partial y} \\ \frac{\partial}{\partial x} & 0 & 0 \\ \frac{\partial}{\partial y} & 0 & 0 \end{bmatrix} \begin{pmatrix} q \\ p_1 \\ p_2 \end{pmatrix} = \begin{pmatrix} \partial S/\partial q \\ \partial S/\partial p_1 \\ \partial S/\partial p_2 \end{pmatrix}\,.$$

- The kernel of the operator on the left hand side is infinite dimensional!
- What about the constraint $\frac{\partial p_1}{\partial x_2} = \frac{\partial p_2}{\partial x_1}$?

Legendre transformation on forms

Look at the Legendre-transformation in a coordinate-free form.

$$\mathrm{d}q = \frac{\partial q}{\partial x_1}\mathrm{d}x_1 + \frac{\partial q}{\partial x_2}\mathrm{d}x_2\,,$$

and

$$\mathrm{d}q \wedge \bigstar\mathrm{d}q = \left((\frac{\partial q}{\partial x_1})^2 + (\frac{\partial q}{\partial x_2})^2 \right)\mathsf{vol}\,.$$

Hence $L = \frac{1}{2}\mathrm{d}q \wedge \bigstar\mathrm{d}q - V(q)\mathsf{vol}$.

In the Legendre transform one wants to replace "dq" with "P"

$$\mathrm{d}q = P$$

But, the Hodge decomposition says there is something missing.

Given $P \in \bigwedge^1(M)$,

$$P = \mathrm{d}q + \boldsymbol{\delta} R \qquad \text{(modulo harmonic forms)}$$

$$\text{for some } R \in \bigwedge^2(M)$$

Reconsider the Legendre transform on differential forms, using the above observations about the Hodge decompostion.

Towards a "Legendre-Hodge" Transformation

Consider $\Delta q = -V'(q)$ in coordinate-free form $\mathrm{d}\boldsymbol{\delta} q = V'(q)$,

with Lagrangian

$$\mathscr{L} = \int L \quad \text{and} \quad L = \tfrac{1}{2}\mathrm{d}q \wedge \bigstar \mathrm{d}q - V(q)\,\mathrm{vol}\,.$$

Transform as follows. Let $\mathrm{d}q = P$ for some $P \in \bigwedge^1(M)$,

$$L = \tfrac{1}{2} P \wedge \bigstar P - V(q)\,\mathrm{vol} + \boldsymbol{\alpha} \wedge \bigstar(\mathrm{d}q - P) + R \wedge \bigstar \mathrm{d}\boldsymbol{\alpha}\,.$$

Note the additional constrant $\mathrm{d}\boldsymbol{\alpha} = 0$.

Now $\frac{\partial L}{\partial P} = 0 \quad \Rightarrow \quad \boldsymbol{\alpha} = P$, hence

$$L = P \wedge \bigstar \mathrm{d}q + R \wedge \bigstar \mathrm{d}P - \tfrac{1}{2} P \wedge \bigstar P - V(q)\,\mathrm{vol}$$

But this is $L = \boldsymbol{\Theta}(Z) - S(Z)$vol, and its first variation is

$$\begin{aligned} \boldsymbol{\delta} P &= V'(q) \\ \mathrm{d}q + \boldsymbol{\delta} R &= P \\ \mathrm{d}P &= 0\,. \end{aligned}$$

or

$$\mathbf{J}_{\boldsymbol{\partial}} Z = \nabla S(Z)\,, \quad Z \in \bigwedge(M)$$

The Hodge decomposition of P is a byproduct of the transformation.

Hyperbolic PDEs – *change the metric*

Take $M = \mathbb{R}^2$ with coordinates (x_1, x_2),
volume form vol $= \mathrm{d}x_1 \wedge \mathrm{d}x_2$, but inner product

$$\langle u, v \rangle = \varepsilon u_1 v_1 + u_2 v_2$$

The natural form on $\bigwedge(M)$ is still

$$\mathbf{\Theta} = P \wedge \bigstar \mathrm{d}q + R \wedge \bigstar \mathrm{d}P$$

The first variation of the functional $\int \mathbf{\Theta} - S(q, P, R)\mathsf{vol}$ leads to

$$\begin{bmatrix} 0 & \boldsymbol{\delta} & 0 \\ \mathrm{d} & 0 & \boldsymbol{\delta} \\ 0 & \mathrm{d} & 0 \end{bmatrix} \begin{pmatrix} q \\ P \\ R \end{pmatrix} = \begin{pmatrix} S_q \\ S_P \\ S_R \end{pmatrix}$$

The metric reappears when we take coordinate representations for $\bigstar$ and d. In coordinates, $\mathbf{J}_{\boldsymbol{\partial}} = \mathbf{J}_1 \frac{\partial}{\partial x_1} + \mathbf{J}_2 \frac{\partial}{\partial x_2}$ with

$$\mathbf{J}_1 = \begin{bmatrix} 0 & -\varepsilon & 0 & 0 \\ \varepsilon & 0 & 0 & 0 \\ 0 & 0 & 0 & -\varepsilon \\ 0 & 0 & \varepsilon & 0 \end{bmatrix}, \quad \mathbf{J}_2 = \begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & \varepsilon \\ 1 & 0 & 0 & 0 \\ 0 & -\varepsilon & 0 & 0 \end{bmatrix}.$$

$\mathbf{J}_1^2 = -\mathbf{I}$, $\mathbf{J}_2^2 = -\mathbf{I}$ – but now $\mathbf{J}_1\mathbf{J}_2 + \varepsilon \mathbf{J}_2 \mathbf{J}_1 = 0$.

Taking $S(Z) = \frac{1}{2}\langle P, P \rangle_1 + V(q)$ provides a multisymplectic formulation for

$$\varepsilon \frac{\partial^2 q}{\partial x_1^2} + \frac{\partial^2 q}{\partial x_2^2} + V'(q) = 0\,.$$

Discretizing multisymplectic structures on the TEA bundle

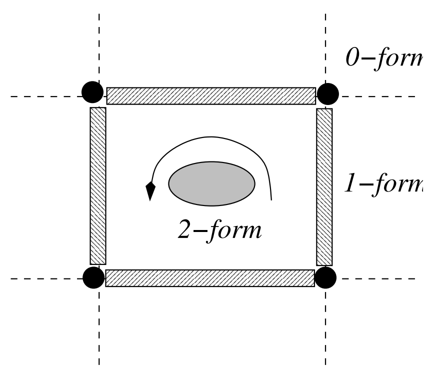
Discretizing multisymplectic structures on the total exterior algebra (TEA) bundle reduces to discretizing differential forms on a discretized Riemannian manifold.

Consider the case of $M = \mathbb{R}^2$ with S in standard form

$$\begin{aligned} \boldsymbol{\delta} P &= V_q(q) \\ \mathrm{d}q + \boldsymbol{\delta} R &= P \\ \mathrm{d}P &= 0\,. \end{aligned}$$

where $V : \bigwedge^0 \to \mathbb{R}$ is any smooth function.

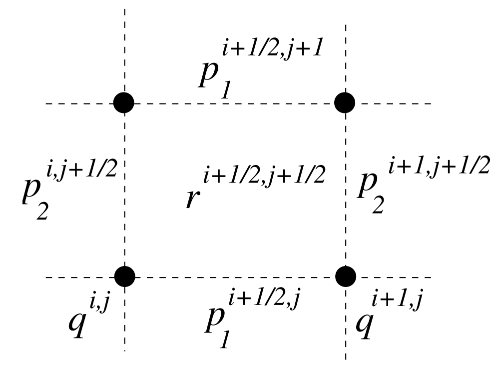
Introduce a lattice for $\mathbb{R}^2$, for example



and discretize q as a zero form, P as a one form and R as a two form, and introduced discretizations for d and $\boldsymbol{\delta}$.

Simplest multisymplectic TEA discretization

The simplest discretization leads to the staggered box scheme, which is a concatenation of Störmer-Verlet in space and time



$$
\begin{aligned}
-\left(\frac{p_1^{i+1/2,j}-p_1^{i-1/2,j}}{\Delta x_1}\right)-\left(\frac{p_2^{j,j+1/2}-p_2^{i,j-1/2}}{\Delta x_2}\right) &= V_q(q^{i,j}) \\
\left(\frac{q^{i+1,j}-q^{i,j}}{\Delta x_1}\right)+\left(\frac{r^{i+1/2,j+1/2}-r^{i+1/2,j-1/2}}{\Delta x_2}\right) &= p_1^{i+1/2,j} \\
-\left(\frac{r^{i+1/2,j+1/2}-r^{i-1/2,j+1/2}}{\Delta x_1}\right)+\left(\frac{q^{i,j+1}-q^{i,j}}{\Delta x_2}\right) &= p_2^{i,j+1/2} \\
\left(\frac{p_2^{i+1,j+1/2}-p_2^{i,j+1/2}}{\Delta x_1}\right)-\left(\frac{p_1^{i+1/2,j+1}-p_1^{i+1/2,j}}{\Delta x_2}\right) &= 0
\end{aligned}
$$

The full power of discrete differential forms or difference forms has yet to be applied in this context.

What is the appropriate geometric structure which is preserved or conserved?

Easy to show that the above scheme satisfies discrete conservation of symplecticity, but it is of interest to relate the structural properties of the discretization to the discrete properties of Θ.

Distortion of waves by dispersive truncation error

An interesting area is the effect of multisymplectic discretization on the *group velocity* of waves. There is recent interesting work on this by ASCHER & MCLACHLAN, MOORE & REICH and FRANKS & REICH.

An example. Suppose that a discretization of the wave equation

$$u_t + c\,u_x = 0\,, \quad c > 0 \quad (c \text{ constant})\,,$$

leads to a modified equation with dispersive truncation error

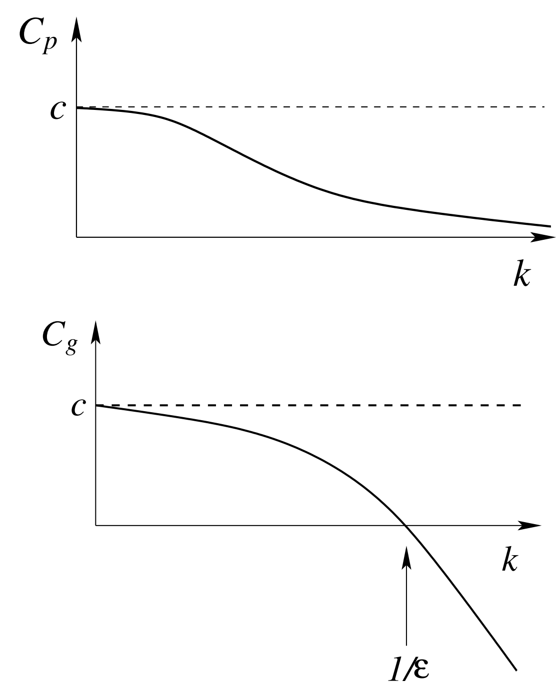
$$u_t + c\,u_x - \varepsilon^2 u_{txx} = 0\,, \quad 0 < \varepsilon << 1\,.$$

The *modified* dispersion relation is

$$\omega = \frac{ck}{1+\varepsilon^2 k^2}$$

which speeds

$$C_p = \frac{\omega}{k} = \frac{c}{1+\varepsilon^2 k^2} \quad \text{and} \quad C_g = \frac{d\omega}{dk} = \frac{c(1-\varepsilon^2 k^2)}{(1+\varepsilon^2 k^2)^2}\,.$$



Short waves have negative group velocity!

In two space dimensions new features arise. For example, consider the generalization of the above model problem to a modified equation with isotropic dispersion in two space dimensions,

$$u_t + c\,u_x - \varepsilon^2(u_{txx} + u_{tyy}) = 0\,,$$

The modified dispersion relation is now

$$\omega = \frac{ck}{1 + \varepsilon^2(k^2 + \ell^2)}\,.$$

In two space dimensions there may be directional error as well as magnitude error.

For the above example

$$\mathbf{C}_g = (\omega_k, \omega_\ell) = \frac{c}{1 + \varepsilon^2(k^2 + \ell^2)}\left(1 + \varepsilon^2(-k^2 + \ell^2), -2\varepsilon^2 k\ell\right)\,.$$

In the exact equation, the waves and the wave energy (dictated by the group velocity) travel in the same direction. But, when $\varepsilon > 0$, there is error in the *direction of propagation* of the wave, and error in the direction of propagation of the energy and the two forms of error are in different directions.

Action and symplectic periodic orbits

Consider a finite dimensional Hamiltonian system on $\mathbb{R}^{2n}$

$$\mathbf{J}U_t = \nabla H(U)\,, \quad U \in \mathbb{R}^{2n}$$

Periodic solutions can be characterized as *relative equilibria*: critical points of the Hamiltonian function restricted to level sets of the *action*

$$A(U) = \frac{1}{2\pi}\int_0^{2\pi} \tfrac{1}{2}\langle \mathbf{J}Z_\theta, Z\rangle \mathrm{d}\theta\,,$$

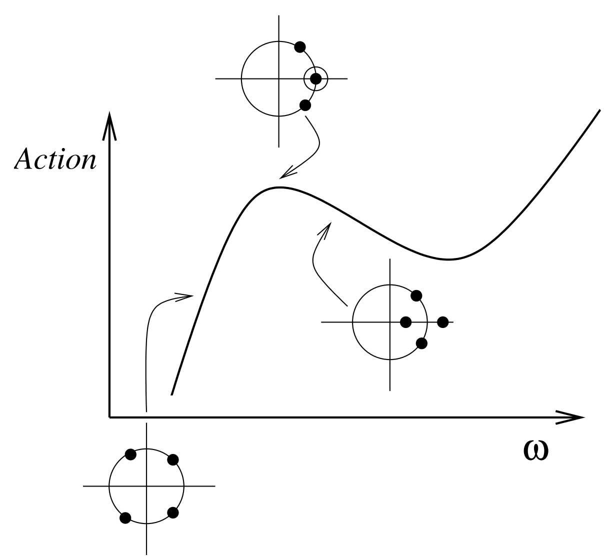
with Euler-Lagrange equation $\nabla H(U) = \omega \nabla A(U)$,

where ω, the frequency, is a Lagrange multiplier.

The constrained variational principle is said to be non-degenerate if

$$\frac{d\mathscr{A}}{d\omega} \neq 0,$$

where $\mathscr{A}$ is the value of the level set of $A(U)$.



Homoclinic bifurcation in nonlinear normal form near points $\mathscr{A}_\omega = 0$.

Action and multi-symplectic periodic patterns

Consider a elliptic operator of the form $\mathbf{J}_{\boldsymbol{\partial}}Z = \nabla S(Z)$ with $M = \mathbb{R}^2$ and standard coordinates and metric, i.e.

$$\mathbf{J}_1 \frac{\partial Z}{\partial x_1} + \mathbf{J}_2 \frac{\partial Z}{\partial x_2} = \nabla S(Z)\,.$$

Multi-periodic patterns can be characterized as critical points of $\int\int S \mathrm{d}\theta_1 \wedge \mathrm{d}\theta_2$ restricted to level sets of the actions

$$A_j(Z) = \frac{1}{(2\pi)^2}\int_0^{2\pi}\int_0^{2\pi} \tfrac{1}{2}\langle\!\langle \mathbf{J}_j Z_{\theta_j}, Z\rangle\!\rangle \mathrm{d}\theta_1 \wedge \mathrm{d}\theta_2\,,$$

with Euler-Lagrange equation $\nabla\overline{S(Z)} = \kappa_1 \nabla A_1(Z) + \kappa_2 \nabla A_2(Z)$,

where the wavenumbers (κ_1, κ_2) are Lagrange multipliers.

The constrained variational principle is said to be non-degenerate if

$$\det \begin{bmatrix} \frac{\partial \mathscr{A}_1}{\partial \kappa_1} & \frac{\partial \mathscr{A}_1}{\partial \kappa_2} \\ \frac{\partial \mathscr{A}_2}{\partial \kappa_1} & \frac{\partial \mathscr{A}_2}{\partial \kappa_2} \end{bmatrix} \neq 0\,,$$

where $\mathscr{A}_j$ is the value of the level set of $A_j(Z)$.

Points of degeneracy correspond to points of bifurcation of the Floquet-Bloch exponents.

“Spatial homoclinic bifurcation” near points where $\det = 0$?

Hyperbolic PDEs, periodic orbits and action

Consider a hyperbolic operator of the form $\mathbf{J}_{\boldsymbol{\partial}} Z = \nabla S(Z)$ with $M = \mathbb{R}^2$, coordinates (t,x) and minkowski metric i.e.

$$\mathbf{J}_1 Z_t + \mathbf{J}_2 Z_x = \nabla S(Z)\,, \quad \mathbf{J}_1\mathbf{J}_2 = \mathbf{J}_2\mathbf{J}_1\,.$$

Periodic travelling waves, i.e. solutions of the form $\widehat{Z}(\theta)$, $\theta = \kappa x + \omega t$ can be characterized as critical points of $\int S\,\mathrm{d}\theta$ restricted to level sets of the actions

$$A_j(Z) = \frac{1}{2\pi}\int_0^{2\pi} \tfrac{1}{2}\langle\!\langle \mathbf{J}_j Z_\theta, Z\rangle\!\rangle \mathrm{d}\theta\,,$$

with Euler-Lagrange equation $\nabla\overline{S(Z)} = \omega\nabla A_1(Z) + \kappa\nabla A_2(Z)$,

where (ω,κ) appear as Lagrange multipliers.

The constrained variational principle is said to be non-degenerate if

$$\det\begin{bmatrix} \frac{\partial\mathscr{A}_1}{\partial\omega} & \frac{\partial\mathscr{A}_1}{\partial\kappa} \\ \frac{\partial\mathscr{A}_2}{\partial\omega} & \frac{\partial\mathscr{A}_2}{\partial\kappa}\end{bmatrix} \neq 0\,,$$

where $\mathscr{A}_j$ is the value of the level set of $A_j(Z)$.

Theorem: *under suitable (reasonable) hypotheses, the travelling wave $\widehat{Z}(\theta;\omega,\kappa)$ is spectrally unstable (there exists a branch of unstable essential spectrum) if the above determinant is positive.*

Zero determinant is related to bifurcation of Floquet-Bloch exponents.

Interesting relation between the generation of homoclinic orbits in in the the nonlinear problem and the points of zero determinant of the action determinant.