**FoCM • Santander, Spain • July 2005**

# Some questions on symplectic and multisymplectic discretizations

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- Symplectic discretization from the viewpoint of the geometry of time
- Multisymplectic structures, multisymplectic Dirac operators and their discretization from the viewpoint of differential forms on $M$
- Geometric integration and simulation of breaking water waves

## Total exterior algebra bundle of time

Consider time as a one-dimensional orientable Riemannian manifold, $M$, and for simplicity take $M = \mathbb{R}^1$, with standard metric and volume form $\mathsf{vol} = \mathrm{d}t$.

(With nontrivial metric, $\langle u, v\rangle = g(t)uv$ and $\mathsf{vol} = \sqrt{g}\,\mathrm{d}t$.)

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

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

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

i.e. functions on $M$ and one-forms on $M$

Take elements $(q, P) \in \boldsymbol{\Omega}^0(M) \oplus \boldsymbol{\Omega}^1(M)$; i.e. in coordinates, $P = p(t)\mathrm{d}t$.

Consider the scalar form of Newton's equations for $q(t)$:

$$-q_{tt} = V'(q)\,,$$

for some potential $V(q)$. Claim: Hamilton's equations can be written in the form $\mathrm{d}q = P$ and $\boldsymbol{\delta} P = V'(q)$ or

$$\begin{pmatrix} 0 & \boldsymbol{\delta} \\ \mathrm{d} & 0 \end{pmatrix} \begin{pmatrix} q \\ P \end{pmatrix} = \begin{pmatrix} V'(q) \\ P \end{pmatrix}$$

This equation is the first variation of the functional

$$\int P \wedge \bigstar \mathrm{d}q - H(q, P)\mathrm{d}t$$

with $H\mathrm{d}t = \frac{1}{2} P \wedge \bigstar P + V(q)\mathrm{d}t$.

## Symplectic operator as a Dirac operator

The Newtonian equation $q_{tt} = -V'(q)$ is equivalent to

$$\boldsymbol{\delta}\mathrm{d}\, q = V'(q)\,,$$

which can be obtained as the first variation of the Lagrangian

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

where in coordinates, $\mathrm{d}q \wedge \bigstar\mathrm{d}q = g^{-1}q_t^2\sqrt{g}\mathrm{d}t$.

Legendre transform: let $v = \mathrm{d}q$,

$$\begin{aligned} L\mathrm{d}t &= \tfrac{1}{2}v \wedge \bigstar v - V(q)\mathrm{d}t + P \wedge \bigstar(dq - v) \\ &= P \wedge \bigstar\mathrm{d}q - H(q,P)\mathrm{d}t\,, \text{ with } H\mathrm{d}t = \tfrac{1}{2}P \wedge \bigstar P + V(q)\mathrm{d}t\,. \end{aligned}$$

Hamilton's equations: $\boldsymbol{\delta}P = V'(q)$ and $\mathrm{d}q = P$.

Now, $\boldsymbol{\delta}P = -\bigstar\mathrm{d}\bigstar p\mathrm{d}t = -\bigstar\mathrm{d}p = -p_t\bigstar\mathrm{d}t = -p_t$; the operator on the left is a coordinate-free formulation of $\mathbf{J}\frac{d}{dt}$.

Define $\mathbf{J}_\partial = \begin{pmatrix} 0 & \boldsymbol{\delta} \\ \mathrm{d} & 0 \end{pmatrix}$. It is a Dirac operator:

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

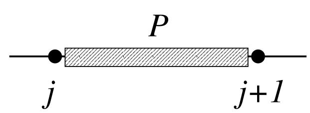
with the property: $\mathrm{Kernel}\begin{pmatrix} 0 & \boldsymbol{\delta} \\ \mathrm{d} & 0 \end{pmatrix}$ = the harmonic forms in $\boldsymbol{\Omega}^0 \oplus \boldsymbol{\Omega}^1$, on an appropriate space of functions.

## Discretization of differential forms on the time 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 $q_j = q(j\Delta t)$,




Approximate the differential forms using

- *discrete differential forms*: Bossavit, Hiptmair, Leok, Desbrun, Marsden, et al.
- *difference forms*: Mansfield & Hydon

resulting in a discretization

$$\Delta^+ q_j = P_j \quad \text{and} \quad \boldsymbol{\delta}^+ P_j = V'(q_j)$$

To be explicit, consider the use of difference forms following Mansfield & Hydon. Let $\Delta t = h_1 \Delta^1$, where $\Delta^1$ is a basis vector for discrete one forms and $h_1$ is a scale factor. Using forward differencing,

$$\Delta^+ q_j = (q_{j+1} - q_j) \wedge \Delta^1 = \frac{(q_{j+1} - q_j)}{h_1} \wedge h_1 \Delta^1 \,,$$

and the simplest approximation of the one form $P$ is

$$P_j \approx p_{j+\frac{1}{2}} \Delta t = p_{j+\frac{1}{2}} \, h_1 \Delta^1 \,.$$

How to approximate the co-differential $\boldsymbol{\delta}^+$?

## Discretizing the codifferential

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 – integrated over time. Use the discrete analog:

$$\begin{aligned}
\textstyle\sum_j P_j \wedge \bigstar \Delta^+ q_j &= \textstyle\sum_j \Delta^+ q_j \wedge \bigstar P_j \\
&= \textstyle\sum_j \Delta^+(q_j \wedge \bigstar P_{j-1}) - \sum_j q_j \wedge \Delta^- \bigstar P_j \\
&= -\textstyle\sum_j q_j \wedge \bigstar\bigstar \Delta^- \bigstar P_j \\
&= \textstyle\sum_j q_j \wedge \bigstar \boldsymbol{\delta}^+ P_j \,,
\end{aligned}$$

assuming suitable endpoint conditions, with

$$\boldsymbol{\delta}^+ = -\bigstar \Delta^- \bigstar \,,$$

where

$$\Delta^- q_j = (q_j - q_{j-1}) \wedge \Delta^1 = \frac{(q_j - q_{j-1})}{h_1} \wedge h_1 \Delta^1 \,.$$

Applying this formula to $P_j$ results in

$$\boldsymbol{\delta}^+ P_j = \frac{(-p_{j+\frac{1}{2}} + p_{j-\frac{1}{2}})}{h_1} \,.$$

Combining these equations

$$q_{j+1} = q_j + h_1\, p_{j+\frac{1}{2}} \quad \text{and} \quad p_{j+\frac{1}{2}} = p_{j-\frac{1}{2}} - h_1\, V'(q_j) \,.$$

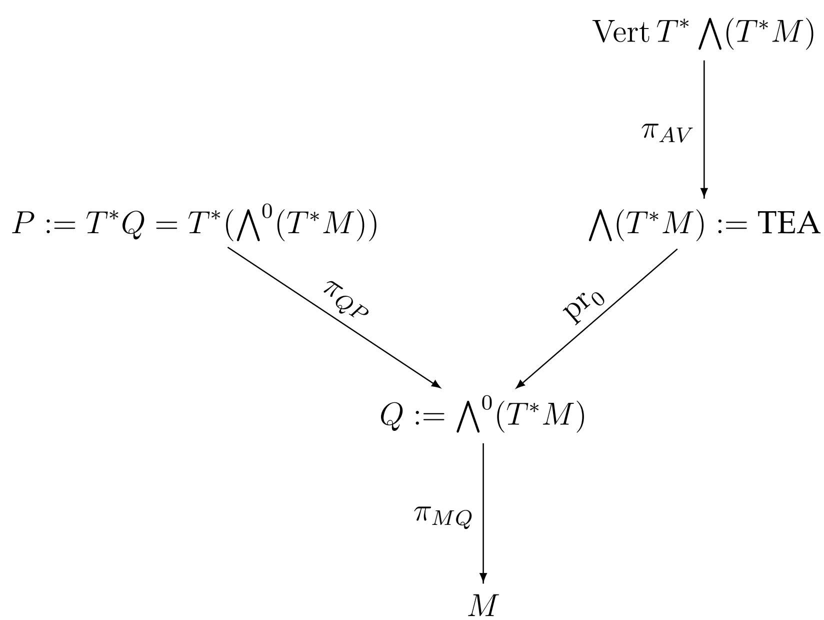
– yet another interpretation of the Störmer-Verlet method!

## Symplecticity, and Dirac operators on TEA

Summary: on the time manifold $M$, there is a canonical one-form on the TEA (total exterior algebra) bundle of $M$,

$$\Theta = P \wedge \bigstar \mathrm{d}q\,, \quad U := (q, P) \in \mathbf{\Omega}^0(M) \oplus \mathbf{\Omega}^1(M)\,,$$

and $\Theta = \frac{1}{2}\langle\!\langle \mathbf{J}_\partial U, U \rangle\!\rangle + \mathrm{d}(\cdot)$, with $\mathbf{J}_\partial$ a Dirac operator. Adding in a Hamiltonian function $H(t, q, P)\mathrm{d}t$ gives a form of Hamilton's equations. Where does the Hamiltonian function live?




Remark: metric on the configuration space versus that on $M$,

$$K = \tfrac{1}{2}\, g^{-1} h_{i,j} \frac{dq^i}{dt}\frac{dq^j}{dt}\,\sqrt{g}\,\mathrm{d}t\,.$$

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

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

$M$ is interpreted as an orientable 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 $T_x^* M$:

$$\mathbf{\Omega}(M) = \mathbf{\Omega}^0(M) \oplus \mathbf{\Omega}^1(M) \oplus \mathbf{\Omega}^2(M)$$

i.e. functions on $M$, one-forms on $M$ and two-forms 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: $\boldsymbol{\delta} u = -\bigstar \mathrm{d} \bigstar u, \quad u \in \mathbf{\Omega}^k(M)$, $k = 1, 2$

Take a point $(q, P, R) \in \mathbf{\Omega}^0(M) \oplus \mathbf{\Omega}^1(M) \oplus \mathbf{\Omega}^2(M)$;

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

Consider the natural generalization of $P \wedge \bigstar \mathrm{d}q$ on $\mathbf{\Omega}(M)$

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

## Properties of $\Theta$

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

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

$\Theta$ can be reformulated as

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

where

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

and $\Upsilon$ is the one form

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

Now consider the integral of $\Theta$: $\mathscr{T}(Z) = \int_{\mathscr{V}} \Theta(Z)$. 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 multi-symplectic Dirac operator $\mathbf{J}_{\partial}$

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

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

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

Another way to express this operator is

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

with

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

Each $\mathbf{J}_j$ is non-degenerate. In a coordinate representation, a set of symplectic operators is generated.

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

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

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

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 operators

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

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

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 $\bigwedge^0 \oplus \bigwedge^1 \oplus \bigwedge^2$,
with an appropriate choice of space of functions.

## Hamiltonian PDEs on the TEA bundle 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 $Z = (q, P, R) \in \boldsymbol{\Omega}(M)$

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

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 $\Theta$

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

Consider two examples of $S(Z)$

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

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 $M$.

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

$$\mathbf{\Omega}(M) = \mathbf{\Omega}^0(M) \oplus \cdots \oplus \mathbf{\Omega}^n(M).$$

Consider an element in $\mathbf{\Omega}(M)$,

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

and define

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

Then

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

where $\Upsilon$ 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 multi-symplectic Dirac operator, satisfying

$$\begin{aligned} \mathbf{J}_{\boldsymbol{\partial}} \circ \mathbf{J}_{\boldsymbol{\partial}} &= \boldsymbol{\delta}\mathrm{d} \oplus (\boldsymbol{\delta}\mathrm{d} + \mathrm{d}\boldsymbol{\delta}) \oplus \cdots \oplus (\boldsymbol{\delta}\mathrm{d} + \mathrm{d}\boldsymbol{\delta}) \oplus \mathrm{d}\boldsymbol{\delta} \\ &= -\mathbf{I}_N \otimes \Delta\,, \quad N = 2^n\,. \end{aligned}$$

- 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 $\mathscr{C}\ell_{0,n}$. Each $\mathbf{J}_j$ is symplectic.

Adding a function $S : \boldsymbol{\Omega}(M) \to \mathbb{R}$ generates a class of elliptic PDEs $\mathbf{J}_{\boldsymbol{\partial}} Z = \nabla S(Z)$ where $\nabla$ 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 $\mathscr{L} = \int\int L(q, q_{x_1}, q_{x_2})\,\mathrm{d}x_1\,\mathrm{d}x_2$ 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

Re-think the Legendre-transformation in a coordinate-free form, starting with

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

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 "$\mathrm{d}q$" with "$P$"

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

But, the Hodge decomposition says there is something missing.

Given $P \in \mathbf{\Omega}^1(M)$,

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

for some $R \in \mathbf{\Omega}^2(M)$

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 $\mathrm{d}q = V$ for some $V \in \mathbf{\Omega}^1(M)$,

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

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

Now $\frac{\partial L}{\partial V} = 0 \quad \Rightarrow \quad V = P$ , 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 $L = \mathbf{\Theta}(Z) - S(Z)$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

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

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

$$\langle u, v\rangle = \varepsilon u_1 v_1 + u_2 v_2 \text{ with } \varepsilon = \pm 1.$$

The form $\Theta(Z)$ for $Z \in \mathbf{\Omega}(M)$ 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 $S(Z) = \frac{1}{2} P \wedge \bigstar P + V(q)$ 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 PDEs on the TEA bundle

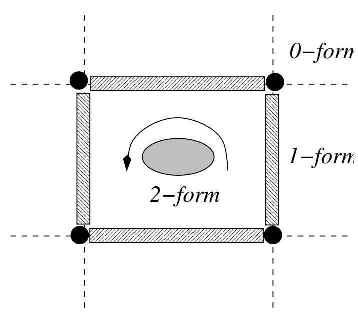
Consider the case of $M = \mathbb{R}^2$ with $S$ in standard form

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

where $V$ and $W$ are given smooth functions.

Discretizing multisymplectic PDEs on the TEA bundle reduces to discretizing differential forms on a discrete Riemannian manifold. Here the theory of "difference forms" of Mansfield & Hydon will be applied.

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




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

## Discretization using difference forms

Let $q^{i,j} = q(i\Delta x_1, j\Delta x_2)$ and define the shift operators

$$S_i q^{i,j} = q^{i+1,j} \quad \text{and} \quad S_j q^{i,j} = q^{i,j+1}$$

and the difference operator

$$\Delta^+ q^{i,j} = (S_i - I)q^{i,j} \wedge \Delta^1 + (S_j - I)q^{i,j} \wedge \Delta^2 \,,$$

where $\Delta^1$ and $\Delta^2$ are basis vectors for the the one-forms, and $\Delta x_k = h_k \Delta^k$, $k = 1, 2$ with scaling factors $h_1$ and $h_2$.

Hodge star is defined by

$$\begin{aligned} \bigstar 1 &= h_1 h_2 \Delta^1 \wedge \Delta^2 \,, \quad \bigstar h_1 h_2 \Delta^1 \wedge \Delta^2 = 1 \,, \\ \bigstar h_1 \Delta^1 &= h_2 \Delta^2 \,, \quad \bigstar h_2 \Delta^2 = -h_1 \Delta^1 \,. \end{aligned}$$

Take the simplest discrete representation for the one-forms and two-forms:

$$\begin{aligned} P^{i,j} &= p_1^{i+1/2,j} h_1 \Delta^1 + p_2^{i,j+1/2} h_2 \Delta^2 \\ R^{i,j} &= r^{i+1/2,j+1/2}\, h_1 h_2 \, \Delta^1 \wedge \Delta^2 \,. \end{aligned}$$

For the codifferential proceed as in the one-dimensional case, and define the discrete codifferential $\boldsymbol{\delta}^+$ to be the adjoint of $\Delta^+$ with respect to the induced inner product on $\mathbb{Z} \times \mathbb{Z}$. For example,

$$\sum_{i,j} \Delta^+ q^{i,j} \wedge \bigstar P^{i,j} = \sum_{i,j} q^{i,j} \wedge \bigstar \boldsymbol{\delta}^+ P^{i,j} \,,$$

with

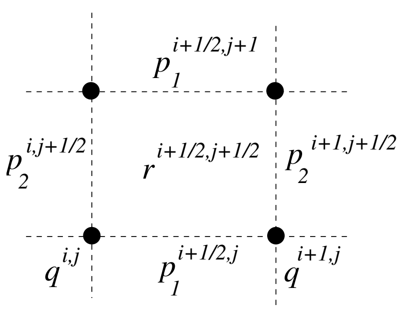
$$\boldsymbol{\delta}^+ P^{i,j} = -\bigstar \Delta^- \bigstar \, P^{i,j} \,.$$

## Simplest multisymplectic TEA discretization

Substituting the discretized forms into the governing equations results in

$$
\begin{aligned}
-\left(\frac{p_1^{i+1/2,j}-p_1^{i-1/2,j}}{h_1}\right)-\left(\frac{p_2^{j,j+1/2}-p_2^{i,j-1/2}}{h_2}\right) &= V'(q^{i,j}) \\
\left(\frac{q^{i+1,j}-q^{i,j}}{h_1}\right)+\left(\frac{r^{i+1/2,j+1/2}-r^{i+1/2,j-1/2}}{h_2}\right) &= p_1^{i+1/2,j} \\
-\left(\frac{r^{i+1/2,j+1/2}-r^{i-1/2,j+1/2}}{h_1}\right)+\left(\frac{q^{i,j+1}-q^{i,j}}{h_2}\right) &= p_2^{i,j+1/2} \\
\left(\frac{p_2^{i+1,j+1/2}-p_2^{i,j+1/2}}{h_1}\right)-\left(\frac{p_1^{i+1/2,j+1}-p_1^{i+1/2,j}}{h_2}\right) &= W'(r^{i+1/2,j+1/2})\,.
\end{aligned}
$$

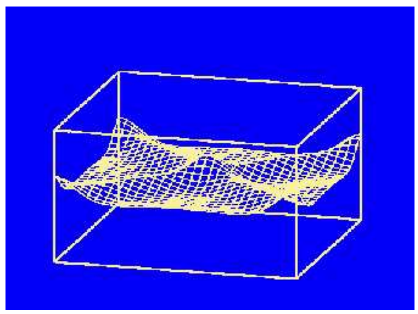
This discretization leads to the staggered box scheme, which is a concatenation of Störmer-Verlet in each space direcftion




The discretization methodology reduces to discretization of differential forms on $M$. To construct a multi-symplectic discretization, discretize $M$, the $k-$forms, the exterior derivative, Hodge star, and then deduce the discrete codifferential.

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 $\Theta$. Work in progress!

## Breaking water waves and geometric integration



The widely used governing equations for modelling water waves are Hamiltonian, and therefore one would expect that symplectic integrators would be appropriate for time integration.

For a simple free surface (a graph) the Hamiltonian formulation is canonical, but still the use of symplectic integrators is not straightforward. To simulate breaking waves one needs to represent the surface parametrically.

The Hamiltonian formulation for this case is not well known but was discovered by BENJAMIN & OLVER (1982). However, the Hamiltonian structure is no longer canonical: the symplectic form depends on the position of the surface.To determine the appropriate numerical scheme, new ideas from geometric integration are needed.

## Benjamin-Olver Hamiltonian formulation

The coordinates for the Hamiltonian formulation are $X(a,t)$, $Y(a,t)$ and $\Phi(a,t)$ where

$$\Phi(a,t) = \phi(x,y,t)\big|_{x=X(a,t),y=Y(a,t)} .$$

The equations are

$$\begin{bmatrix} 0 & -\Phi_a & Y_a \\ \Phi_a & 0 & -X_a \\ -Y_a & X_a & 0 \end{bmatrix} \begin{pmatrix} X \\ Y \\ \Phi \end{pmatrix}_t = \begin{pmatrix} \delta H/\delta X \\ \delta H/\delta Y \\ \delta H/\delta \Phi \end{pmatrix}$$

or

$$\mathbf{K}(\mathbf{U})\mathbf{U}_t = \nabla H(\mathbf{U}) ,$$

which can also be cast into the illuminating form

$$\mathbf{U}_a \times \mathbf{U}_t = \nabla H(\mathbf{U}) , \quad \mathbf{U} = (X, Y, \Phi) .$$

The Hamiltonian function is the total energy and the symplectic form is generated by

$$\Theta = \int_S \Phi \, \mathrm{d}\mathbf{X} \cdot \mathbf{n} \, \mathrm{d}S = \int_{a_1}^{a_2} \Phi(X_a \mathrm{d}Y - Y_a \mathrm{d}X) \, \mathrm{d}a ,$$

with $\omega = \mathrm{d}\Theta$.

Kernel of $\mathbf{K}$ is $\{\mathbf{U}_a\}$. The kernel is due to the reparameterization symmetry.

## Explicit equations for time integration

$$\mathbf{K}(\mathbf{U})\mathbf{U}_t = \nabla H(\mathbf{U})\,,$$

with

$$\mathbf{K} = \begin{bmatrix} 0 & -\Phi_a & Y_a \\ \Phi_a & 0 & -X_a \\ -Y_a & X_a & 0 \end{bmatrix} = \mathbf{U}_a \times$$

Now

$$\mathbf{K}^T\mathbf{K} = \|\mathbf{U}_a\|^2 \left[\mathbf{I} - \frac{\mathbf{U}_a\mathbf{U}_a^T}{\|\mathbf{U}_a\|^2}\right]\,,$$

and so

$$\mathbf{U}_t = \mathbf{J}(\mathbf{U})\nabla H(\mathbf{U}) + \mathrm{Ker}(\mathbf{K})\,, \quad \mathbf{J} = \frac{1}{\|\mathbf{U}_a\|^2}\mathbf{K}^T$$

or

$$\mathbf{U}_t = \mathbf{J}(\mathbf{U})\nabla H(\mathbf{U}) + \gamma(a,t)\mathbf{U}_a\,.$$

- $\gamma(a,t)$ is arbitrary.
- Nonzero $\gamma$ is equivalent to a time-dependent reparameterization. What are the implications?
- While $\mathbf{K}(\mathbf{U})$, the symplectic operator, is a linear function of $\mathbf{U}$, $\mathbf{J}(\mathbf{U})$ is a nonlinear function of $\mathbf{U}$.
- How to choose $\gamma$ to optimize the numerical scheme? Mesh relabelling?

## Curvature driven free surface flow

A model problem which is useful for studying the reparameterization question in isolation is the normal motion of a closed plane curve driven by its local curvature.

This "curve-shortening" problem is a model for a number of phase transition and front dynamics.

Let $\mathbf{X}(a,t) = (X(a,t), Y(a,t))$ where $a$ parameterizes the curve. Then the governing equation for the curve $X(a,t)$ is

$$\mathbf{n} \cdot \mathbf{X}_t = \kappa \,,$$

where $\mathbf{n}$ is the unit normal

$$\mathbf{n} = \frac{1}{\ell} \begin{pmatrix} -Y_a \\ X_a \end{pmatrix} \,, \quad \ell = \sqrt{X_a^2 + Y_a^2} \,,$$

and $\kappa$ is the surface curvature

$$\kappa(a,t) = \frac{X_a Y_{aa} - Y_a X_{aa}}{\ell^3} \,.$$

The dynamics of $\mathbf{X}(a,t)$ is not unique since only the normal velocity is prescribed. This becomes apparent when the governing equation is expressed in the form

$$\mathbf{X}_t = \kappa \mathbf{n} + \gamma(a,t)\mathbf{t} \,, \quad \mathbf{t} = \frac{1}{\ell} \begin{pmatrix} X_a \\ Y_a \end{pmatrix} \,,$$

with $\gamma(a,t)$ arbitrary.

## Curvature driven free surface flow

$$\mathbf{X}_t = \kappa \mathbf{n} + \gamma(a,t)\mathbf{t}\,,$$

Can choose $\gamma(a,t)$ to optimize the numerical scheme.

Choosing $\gamma$ is equivalent to a time-dependent reparameterization. To see this, first suppose $\gamma$ is zero,

$$\mathbf{X}_t = \kappa \mathbf{n}\,,$$

Introduce a time-dependent reparameterization

$$a = h(b,t) \quad \text{for some } h(b,t) \text{ satisfying } h_b \neq 0 \text{ for all } (b,t)$$

Then with

$$\widehat{\mathbf{X}}(b,t) = \mathbf{X}(h(b,t))$$

it follows that $\widehat{\mathbf{n}} = \mathbf{n}$, $\widehat{\mathbf{t}} = \mathbf{t}$ and $\widehat{\kappa} = \kappa$ and so

$$\begin{aligned} \tfrac{\partial}{\partial t}\widehat{\mathbf{X}}(b,t) &= \mathbf{X}_t + \mathbf{X}_a h_t \\ &= \kappa \mathbf{n} + h_t \ell \mathbf{t} \\ &= \widehat{\kappa}\widehat{\mathbf{n}} + \ell h_t \widehat{\mathbf{t}} \end{aligned}$$

that is,

$$\widehat{\mathbf{X}}_t = \widehat{\kappa}\widehat{\mathbf{n}} + \gamma\widehat{\mathbf{t}} \quad \text{with} \quad \gamma = \frac{h_t}{h_b}\,\widehat{\ell}\,.$$

The water-wave problem has the same structure but with the normal velocity determined by a third equation for $\Phi$.

## Summary and comments

- Appropriate geometric integrator for time evolution of water waves is still largely unsolved.
- When the surface is a graph, the symplectic structure associated with the Zakharov Hamiltonian formulation is canonical, but (a) infinite-dimensional, (b) non-local, and (c) the kinetic energy depends on the position of the free surface.
- The Hamiltonian structure changes when using the coordinate-free Hamiltonian formulation for a parametrically-defined surface, proposed by Benjamin & Olver.
- Symplectic form in the BO formulation is non-constant – a "Lie-Poisson type" structure on the "left". What is the appropriate geometric integrator in this case?
- There is a potential to take advantage of reparameterization symmetry in designing numerical schemes.
- Analogy with curvature-driven curve-shortening flow.
- The coordinate-free Hamiltonian formulation generalizes to the case of interfacial waves and problems like the nonlinear Kelvin-Helmholtz roll-up problem.

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