Lattice based Multispace and Applications

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Joint work with :

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- Motivation 1 - Can Conservation laws be built *a priori* into numerical schemes via a discrete Noether's Theorem?
- Motivation 2 - simultaneous smooth and discrete invariants and their syzygies? e.g. for discrete integrable systems

- Definition of a multispace
- Group actions and moving frames on a multispace

- Application to variational shallow water systems
- A Lagrange interpolation variational calculus?

Current obsession: shallow water variational systems

I. Roulstone and J. Norbury, *Computing Superstorm Sandy*, Scientific American, **309** 2013

Consider $(u^\alpha) \mapsto \int_\Omega L(x, u^\alpha, u^\alpha_K)\, \mathrm{d}\mathbf{x}\mathrm{d}t$.

Noether's Theorem yields $\sum_\alpha Q^\alpha E^\alpha(L) + \frac{\mathrm{D}}{\mathrm{D}t} A_0 + \sum_i \frac{\mathrm{D}}{\mathrm{D}x_i} A_i = 0$

Symmetry	**Conserved Quantity**, A_0
Translation in time	Energy
Translation in space	Linear momentum
Rotation in space	Angular momentum
Particle relabelling	Potential vorticity*

Physically important symmetries involve smooth actions in the base space – which is discretised!

* Actually a differential consequence of momenta conservation laws for this class of symmetry.

Philosophy

1. Discretise the Lagrangian functional, $\mathcal{L}[u^\alpha] = \int_\Omega L(x, u^\alpha, u^\alpha_K)\,\mathrm{d}\mathbf{x}$ according to some scheme.

2. Insist the discretised Lagrangian has both the correct continuum limit and the Lie group invariance.*

3. Obtain discrete conservation laws via a discrete version of Noether's Theorem.

4. Prove the discrete Euler-Lagrange equations and the discrete laws converge to the smooth laws in some useful sense.

*Achieving this is the central part of this talk for a particular scheme.

Can we achieve all four of these?

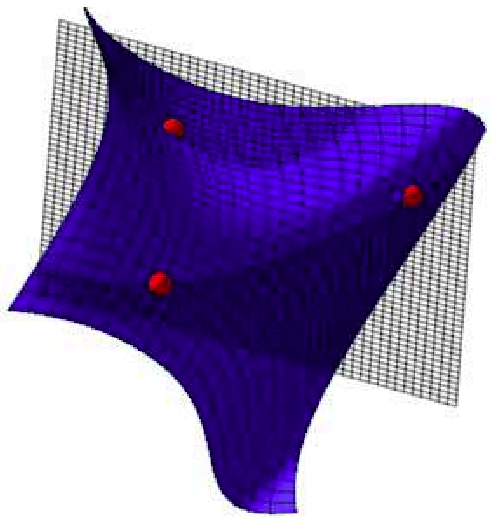
Yes! For FEM, see ELM and Pryer, 2015, FoCM. I also have a theoretical demonstration of weak $\rightarrow$ smooth PV conservation.

2. Insist the discretised Lagrangian has both the correct continuum limit and the Lie group invariance.

2.1. Construction of a manifold, multispace consisting of discrete curves and surfaces with the usual jet bundle embedded as a smooth sub manifold.

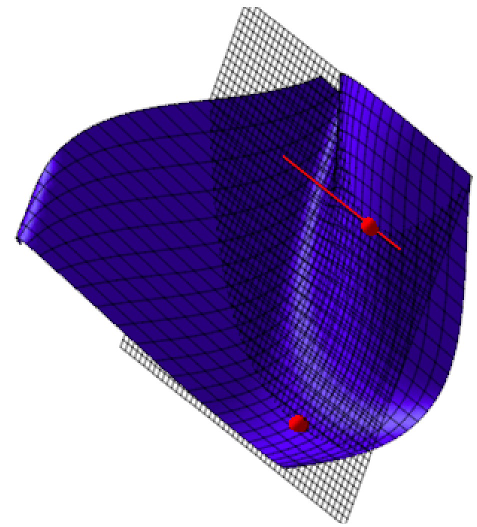
2.2. Algorithmic construction of discrete and differential invariants, together with their syzygies (recurrence relations), using the Lie group based moving frame.

We turn now to Step 2.1.

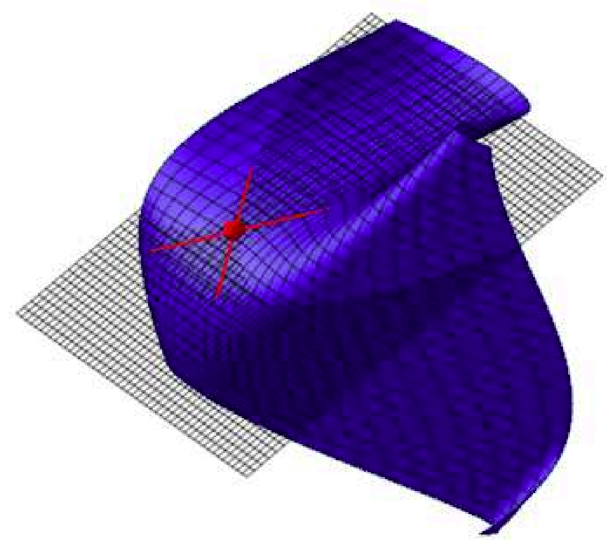


coalesce

$\rightarrow$



coalesce $\downarrow$



Lagrange, Hermite

and Taylor approximation

Basic idea

In Hirsch's defintion of a jet bundle, we have that

$$[x, f, U]_r = [x, T_r(f)|_x, U]_r$$

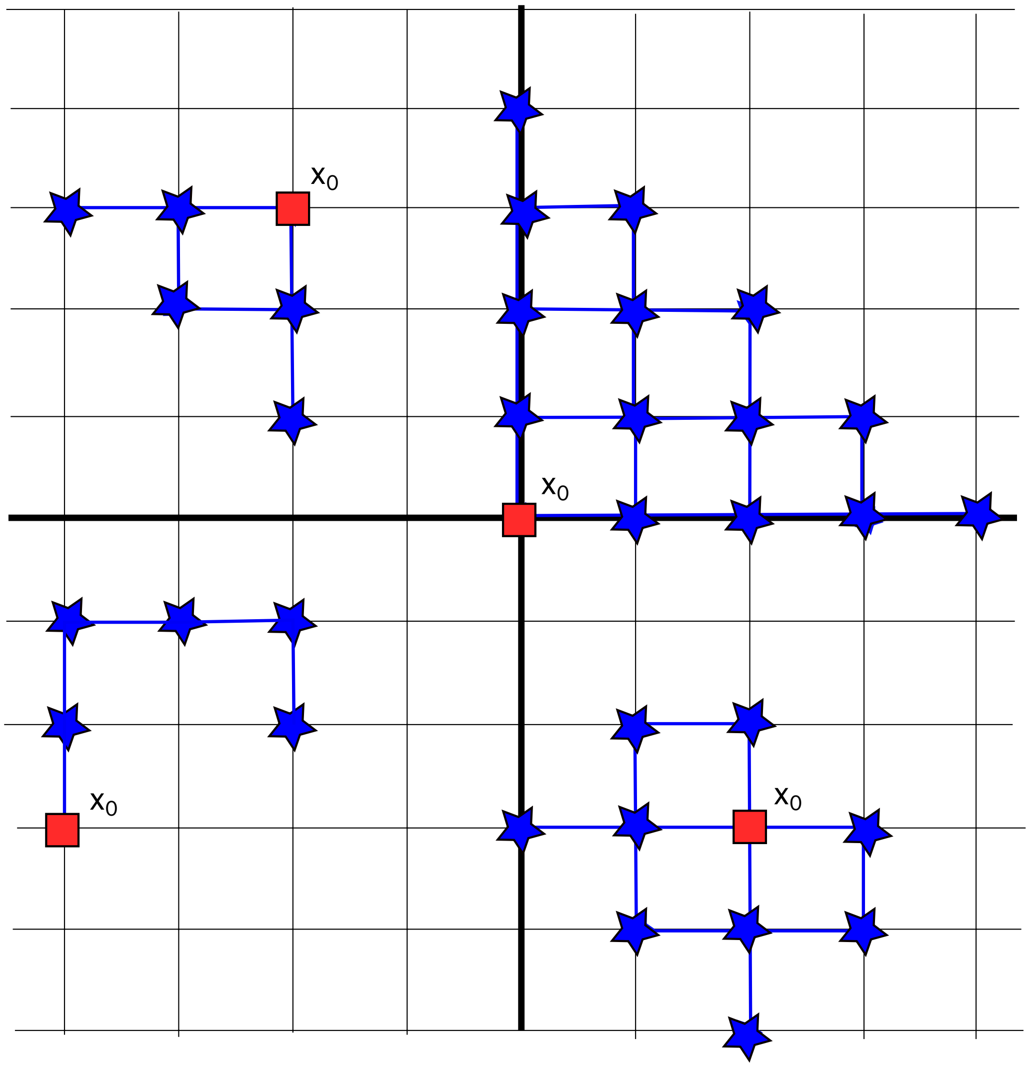
that is, a function on a domain U is equivalent to its r^{th} order Taylor polynomial calculated at the point x.

We view the Taylor polynomial as the coalesence limit of the Lagrange interpolation of the function on a lattice Γ:

$$\text{Lagrange}|_{\Gamma}(f) \to T(f)|_x, \qquad \Gamma \to x.$$

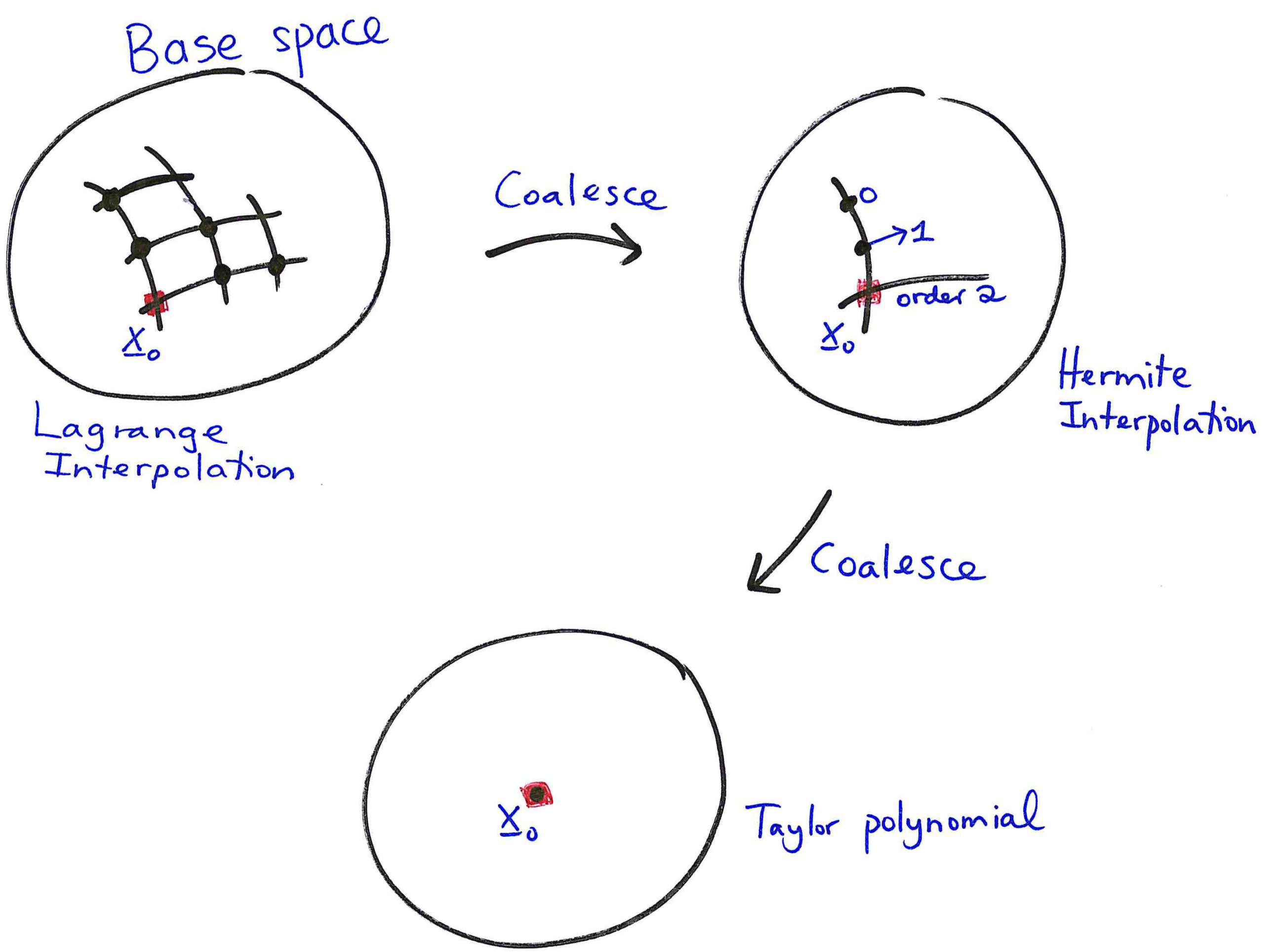
This process requires

- an appropriate lattice Γ
- a well controlled coalescence process.

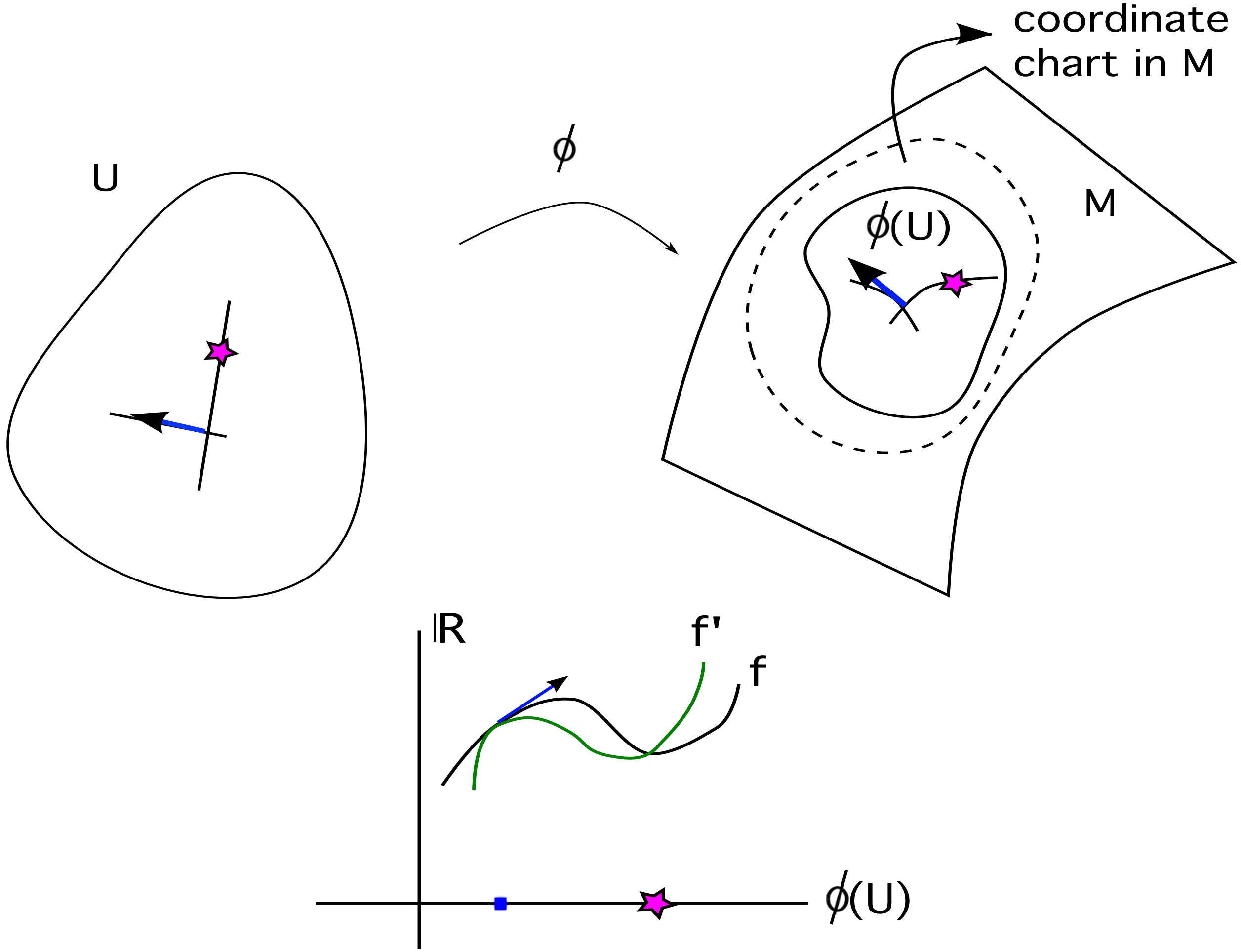


Some "corner lattices"

Hyperplane coalescence



Data for a multispace equivalence class $[\Gamma, f, \phi, U] \sim [\Gamma, f', \phi, U]$



Local coordinates on multispace

A function f defined on the plane $\mathbb{R}^2$, with values at the points $\mathbf{x}_0 = (x_0, x_1)$, $\mathbf{x}_1 = (x_1, y_1)$ and $\mathbf{x}_2 = (x_2, y_2)$, has the interpolation

$$p(f) = f(\mathbf{x}_0) + \frac{\begin{vmatrix} 1 & f(\mathbf{x}_0) & y_0 \\ 1 & f(\mathbf{x}_1) & y_1 \\ 1 & f(\mathbf{x}_2) & y_2 \end{vmatrix}}{\begin{vmatrix} 1 & x_0 & y_0 \\ 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \end{vmatrix}} (x - x_0) + \frac{\begin{vmatrix} 1 & x_0 & f(\mathbf{x}_0) \\ 1 & x_1 & f(\mathbf{x}_1) \\ 1 & x_2 & f(\mathbf{x}_2) \end{vmatrix}}{\begin{vmatrix} 1 & x_0 & y_0 \\ 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \end{vmatrix}} (y - y_0)$$

This multispace element has six coordinates.

A function f defined on the plane $\mathbb{R}^2$, with values at the points $\mathbf{x}_0 = (x_0, x_1)$, $\mathbf{x}_1 = (x_1, y_1)$ with multiplicity two and with $D(f)(v)\Big|_{\mathbf{x}_1} = v_1 f_x(x_1, y_1) + v_2 f_y(x_1, y_1)$, has the interpolation

$$p(f) = f(\mathbf{x}_0) + \frac{\begin{vmatrix} 1 & f(\mathbf{x}_0) & y_0 \\ 1 & f(\mathbf{x}_1) & y_1 \\ 0 & D(f)(v)\Big|_{\mathbf{x}_1} & v_2 \end{vmatrix}}{\begin{vmatrix} 1 & x_0 & y_0 \\ 1 & x_1 & y_1 \\ 0 & v_1 & v_2 \end{vmatrix}} (x - x_0) + \frac{\begin{vmatrix} 1 & x_0 & f(\mathbf{x}_0) \\ 1 & x_1 & f(\mathbf{x}_1) \\ 0 & v_1 & D(f)(v)\Big|_{\mathbf{x}_1} \end{vmatrix}}{\begin{vmatrix} 1 & x_0 & y_0 \\ 1 & x_1 & y_1 \\ 0 & v_1 & v_2 \end{vmatrix}} (y - y_0)$$

This multispace element has six coordinates.

Multispace approximations of curves and surfaces follows by applying the above multispace construction to each co-ordinate function separately.

Proofs rely on the multivariate interpolation results due to Carl de Boor and Amos Ron[†] which is in fact very much broader in scope than we have used here – a huge variety of functionals can be used in addition to point and derivative evaluation.

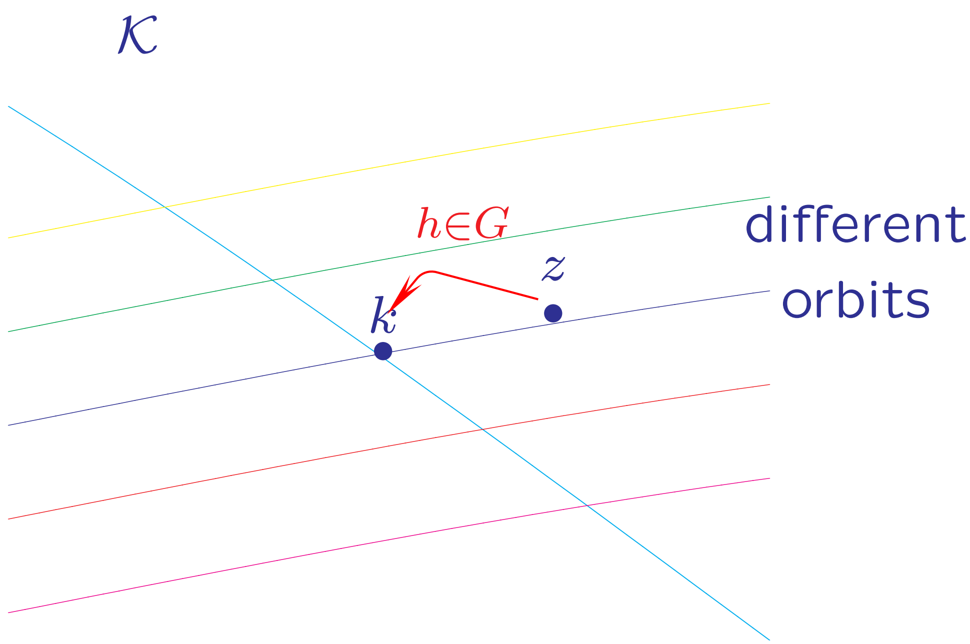
However, multivariate approximation is, on general sets of points, not well defined.

[†] *On Multivariate Polynomial Interpolation*, Constr. Approx. **6** (1990), 287-302.

We turn now briefly to Step 2.2. Moving frames can be used to describe complete, or generating, sets of invariants and their relations.
There are excellent algorithms to manipulate quantities derived from moving frames in symbolic computation environments.
Moving frames are flexible, to allow for ease of computation in specific applications, and they satisfy equations that allow them to be obtained numerically (if necessary).

Fels and Olver, Acta App. Math **51** (1998) and **55** (1999)

Moving Frame if $G \times M \to M$ is a regular, free action



$\rho : M \to G$ $\rho(z) = h$ is equivariant: $\rho(g \cdot z) = \rho(z) g^{-1}$

Calculation of a moving frame

Specify $\mathcal{K}$, the cross-section, as the locus of $\Phi(z) = 0$. Then solve $\Phi(g \cdot z) = 0$ for g. In practice, solve

$$\phi_j(g \cdot z) = 0, \qquad j = 1, \ldots, r = \dim(G)$$

for the r independent parameters describing g. Call the solution $\rho(z)$. Invoke IFT. Unique solution yields

$$\rho(g \cdot z) = \rho(z) \cdot g^{-1}.$$

- local solutions only this way: but see Hubert and Kogan, FoCM **7** (2007) and J. Symb. Comp., **42** (2007).

Equivariance is the key to success. In particular, we obtain:

Invariants: The components of $I(z) = \rho(z) \cdot z$ are invariant.

$$I(g \cdot z) = \rho(g \cdot z) \cdot (g \cdot z) = \rho(z) g^{-1} g \cdot z = \rho(z) \cdot z.$$

If $I(z_i)$ are the canonical invariants for $z = (z_1, z_2, \ldots, z_n)$, and $F(z_1, z_2, \ldots, z_n)$ is an invariant, then we have the Replacement rule,

$$\begin{aligned} F(z_1, z_2, \ldots, z_n) &= F(g \cdot z_1, g \cdot z_2, \ldots, g \cdot z_n) \\ &= F(g \cdot z_1, g \cdot z_2, \ldots, g \cdot z_n)|_{\text{frame}} \\ &= F(I(z_1), I(z_2), \ldots, I(z_n)) \end{aligned}$$

We designed multispace to solve the problem of co-ordinating moving frames on smooth curves and surfaces, and their discretisations. This is achieved by putting a moving frame on multispace.

First, a Lie group action. For example, $G = \mathbb{R} \ltimes \mathbb{R}$, with

$$(\epsilon, a) \cdot (x, y, u(x)) = (x, y, e^{\epsilon}u + a),$$

the group product being

$$(\epsilon, a) \cdot (\delta, b) = (\epsilon + \delta, a + e^{\epsilon}b).$$

The induced action on multispace is that the lattice points are fixed, while . . .

for example, the coefficient of $(x - x_0)$ in the first order interpolation of u moves as

$$(\epsilon, a) \cdot \frac{\begin{vmatrix} 1 & u_0 & y_0 \\ 1 & u_1 & y_1 \\ 1 & u_2 & y_2 \end{vmatrix}}{\begin{vmatrix} 1 & x_0 & y_0 \\ 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \end{vmatrix}} = \frac{\begin{vmatrix} 1 & e^{\epsilon}u_0 + a & y_0 \\ 1 & e^{\epsilon}u_1 + a & y_1 \\ 1 & e^{\epsilon}u_2 + a & y_2 \end{vmatrix}}{\begin{vmatrix} 1 & x_0 & y_0 \\ 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \end{vmatrix}} = e^{\epsilon} \frac{\begin{vmatrix} 1 & u_0 & y_0 \\ 1 & u_1 & y_1 \\ 1 & u_2 & y_2 \end{vmatrix}}{\begin{vmatrix} 1 & x_0 & y_0 \\ 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \end{vmatrix}}$$

where $u_i = u(\mathbf{x}_i)$. This is evidently consistent with the induced action on derivatives calculated via the chain rule, which is

$$g \cdot u_x = e^{\epsilon} u_x.$$

Continuing with $(\epsilon, a) \cdot (x, y, u) = (x, y, e^{\epsilon} u + a)$

If the interpolation of $u(x, y)$ on the lattice (x_i, y_i), $i = 0, 1, 2$ is

$$p(u) = u_0 + A(x - x_0) + B\,(y - y_0)$$

with $u_0 = u(x_0, y_0)$, then

$$(\epsilon, a) \cdot (u_0, A, B) = (e^{\epsilon} u_0 + a, e^{\epsilon} A, e^{\epsilon} B)$$

Definition: Given a Lie group action $G \times M \to M$, a moving frame is an equivariant map $\rho : M \to G$.

If we solve

$$(\epsilon, a) \cdot (u(x_0, y_0), A, B) = (0, 1, *)$$

for ϵ and a, we have the moving frame

$$\rho(u_0, A, B) = \left(-\log A, -\frac{u_0}{A}\right)$$

Working with the frame $\rho(u_0, A, B) = \left(-\log A, -\frac{u_0}{A}\right)$.

The equivariance of the frame is straightforward to show:

$$\rho(e^\delta u_0 + b, e^\delta A, e^\delta B) = \rho(u_0, A, B) \cdot \left(-\delta, -be^{-\delta}\right) = \rho(u_0, A, B) \cdot (\delta, b)^{-1}.$$

Depending on whether the coefficient A is determined by the grid being three distinct points, or a single point with multiplicity three, in which case A looks either like a quotient of determinants or is a derivative expression, the frame will either be in terms of the Lagrange 'discretisation', or in terms of the Taylor coefficients.

The point is that a frame on multispace is, under general conditions, simultaneously a smooth frame and a discretised frame, with equivariance maintained under coalescence.

Recall the frame was obtained by solving

$$(\epsilon, a) \cdot (u(x_0, y_0), A, B) = (0, 1, *).$$

Considering now the invariants of the action, we can evaluate $\rho \cdot B = (\epsilon, a) \cdot B\Big|_{(\epsilon,a)=\rho}$. This yields the invariant,

$$\rho \cdot B = \frac{B}{A} = \frac{\begin{vmatrix} 1 & u_0 & y_0 \\ 1 & u_1 & y_1 \\ 1 & u_2 & y_2 \end{vmatrix}}{\begin{vmatrix} 1 & x_0 & u_0 \\ 1 & x_1 & u_1 \\ 1 & x_2 & u_2 \end{vmatrix}} \quad \text{or} \quad \frac{u_x}{u_y}.$$

this last being if evaluated on the embedded jet bundle.

We have that ρ is a function of the multispace element, and so depends on Γ, and u evaluated on the lattice: $\rho = \rho(\Gamma, u)$.

We can also investigate invariants arising as the components of

$$\rho(\Gamma', u') \cdot \rho(\Gamma, u)^{-1}, \qquad u = u' \text{ or } u \neq u'$$

If $\Gamma' = \Gamma + h\mathbf{e}_1$ we expect, and indeed obtain,

$$\frac{\mathrm{d}}{\mathrm{d}h}\Big|_{h=0} \rho(\Gamma + h\mathbf{e}_1, u) \cdot \rho(\Gamma, u)^{-1} \rightarrow_{\Gamma \to x} \mathcal{D}_x \rho \, \rho^{-1}$$

where the RHS has the frame ρ evaluated on the embedded jet bundle.

That is, discrete Maurer-Cartan invariants limit to differential Maurer-Cartan invariants.

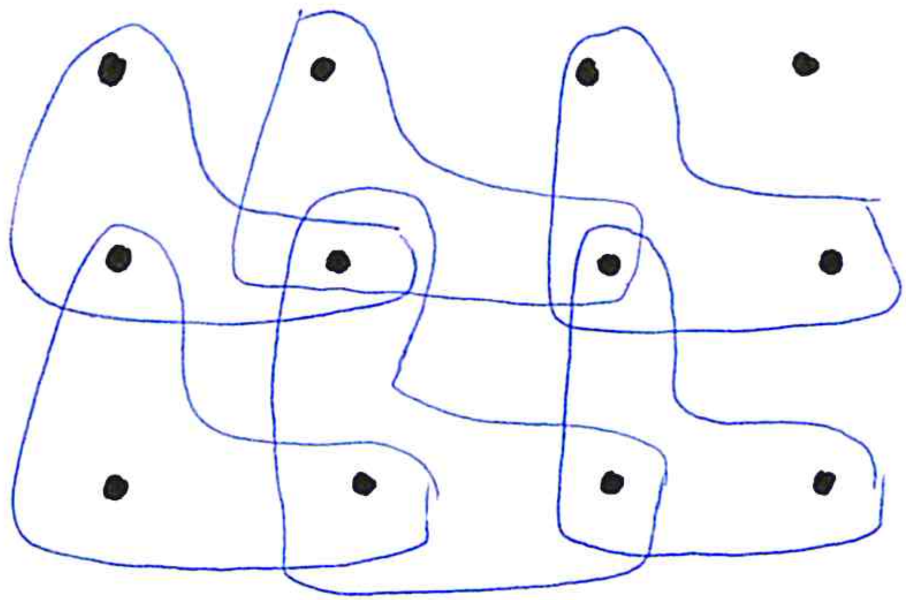
By virtue of having a moving frame on multispace, we can obtain discrete invariants matching the smooth ones. Hence we can build discrete Lagrangians matching the smooth, both in terms of continuum limit and invariance.

Let's look at variational shallow water systems!!

The base space has particle labels (a, b), the dependent variables are the position of the particle at time t, given by $x = x(a, b, t)$, $y = y(a, b, t)$ with $x(a, b, 0) = a$ and $y(a, b, 0) = b$.

We want a Lagrangian which is invariant under translation in a, b and t, rotation in the (a, b) plane, and, if at all possible, a discrete analogue of the particle relabelling symmetry,

$$(a, b) \mapsto (A(a, b), B(a, b)), \qquad A_a B_b - A_b B_a = 1.$$



At each time step, we consider the mesh in (a, b) space to be the union of length one corner lattices, and we calculate the approximations to x and y via Lagrange interpolation.

Set the the lattice points to be,

$$(a_0, b_0, t_0), \quad (a_1, b_1, t_0), \quad (a_2, b_2, t_0), \quad (a_3, b_3, t_1)$$

where x takes the values x_0, x_1, x_2 and x_3 respectively, and similarly for y. Then the Lagrange interpolation coefficients for x are

$$\mathcal{M}(x_a) = \frac{\begin{vmatrix} 1 & x_0 & b_0 \\ 1 & x_1 & b_1 \\ 1 & x_2 & b_2 \end{vmatrix}}{\begin{vmatrix} 1 & a_0 & b_0 \\ 1 & a_1 & b_1 \\ 1 & a_2 & b_2 \end{vmatrix}}, \qquad \mathcal{M}(x_b) = \frac{\begin{vmatrix} 1 & a_0 & x_0 \\ 1 & a_1 & x_1 \\ 1 & a_2 & x_2 \end{vmatrix}}{\begin{vmatrix} 1 & a_0 & b_0 \\ 1 & a_1 & b_1 \\ 1 & a_2 & b_2 \end{vmatrix}}$$

where

$$p(x) = x_0 + \mathcal{M}(x_a)(a - a_0) + \mathcal{M}(x_b)(b - b_0) + \mathcal{M}(x_t)(t - t_0)$$

together with

$$\mathcal{M}(x_t) = \frac{\begin{vmatrix} 1 & x_0 & a_0 & b_0 \\ 1 & x_1 & a_1 & b_1 \\ 1 & x_2 & a_2 & b_2 \\ 1 & x_3 & a_3 & b_3 \end{vmatrix}}{(t_1 - t_0)\begin{vmatrix} 1 & a_0 & b_0 \\ 1 & a_1 & b_1 \\ 1 & a_2 & b_2 \end{vmatrix}} = \frac{x_3 - x_0}{t_1 - t_0}$$

if $(a_3, b_3) = (a_0, b_0)$, that is, if the mesh/initial parameter space is fixed.

We begin with the finite dimensional Lie group $SL(2) \ltimes \mathbb{R}^2$ acting linearly on (a, b)-space, in the neighbourhood of a lattice.

The group action is easily induced on these coordinates. If we take the normalisation equations to be

$$\widetilde{a_0} = 0, \quad \widetilde{b_0} = 0, \quad \widetilde{\mathcal{M}(x_a)} = 1, \quad \widetilde{\mathcal{M}(x_b)} = 0, \quad \widetilde{\mathcal{M}(y_a)} = 0$$

then the $SL(2)$ part of the frame is

$$\left.\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}\right|_{\text{frame}} = \begin{pmatrix} \mathcal{M}(x_a) & \mathcal{M}(x_b) \\ \frac{\mathcal{M}(y_a)}{\Delta} & \frac{\mathcal{M}(y_b)}{\Delta} \end{pmatrix}$$

where

$$\Delta = \frac{\begin{vmatrix} 1 & x_0 & y_0 \\ 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \end{vmatrix}}{\begin{vmatrix} 1 & a_0 & b_0 \\ 1 & a_1 & b_1 \\ 1 & a_2 & b_2 \end{vmatrix}} \quad \to_{\text{ctm limit}} x_a y_b - x_b y_a$$

The invariants are the remaining coordinates evaluated on the frame. We have

$$\widetilde{\mathcal{M}(y_b)}\Big|_{\text{frame}} = \Delta$$

and in fact $\mathcal{M}(x_t)$, $\mathcal{M}(y_t)$ are invariant, as is the denominator.

Shallow water variational systems arise from Lagrangians of the form

$$\int_{\Omega\times[t_0,t_1]} L(x, y, x_a y_b - x_b y_a, x_t, y_t)\, \mathrm{d}a\mathrm{d}b\, \mathrm{d}t.$$

The associated discrete Lagrangians are then

$$\sum_{\Gamma} L(x, y, \Delta, \mathcal{M}(x_t), \mathcal{M}(y_t)) \begin{vmatrix} 1 & a_0 & b_0 \\ 1 & a_1 & b_1 \\ 1 & a_2 & b_2 \end{vmatrix} (t_{n+1} - t_n)$$

Considering Lagrangians whose arguments are multispace co-ordinates, we can arrive readily at Euler Lagrange equations and a discrete Noether theorem.

To give an idea: The first order multispace approximation of $u(x)$ is $p(u)(x) = u_0 + \mathcal{M}(u_x)(x - x_0)$ and then

$$\mathcal{L}[u] = \int_\Omega L(x, u, u_x)\,\mathrm{d}x \rightsquigarrow \mathcal{L}[x, u] = \sum_{x_0} L\left(x_0, u_0, \mathcal{M}(u_x)\right)\,(x_1 - x_0).$$

Induce the infinitesimal Lie group action

$$\tilde{x} = x + \epsilon\xi(x, u) + \mathcal{O}(\epsilon^2), \qquad \tilde{u} = u + \epsilon\phi(x, u) + \mathcal{O}(\epsilon^2),$$

we have the induced action is, miraculously,

$$\widetilde{\mathcal{M}(u_x)} = \mathcal{M}(u_x) + \epsilon\left(\mathcal{M}(\phi_x) - \mathcal{M}(u_x)\mathcal{M}(\xi_x)\right) + \mathcal{O}(\epsilon^2)$$

which compares to the induced action on the derivative as obtained by the chain rule, $\widetilde{u_x} = u_x + \epsilon\left(\frac{\mathrm{d}\phi}{\mathrm{d}x} - u_x\frac{\mathrm{d}\xi}{\mathrm{d}x}\right) + \mathcal{O}(\epsilon^2)$.

The invariance condition of the (multispace) Lagrangian is

$$0 = \left.\frac{\mathsf{d}}{\mathsf{d}\epsilon}\right|_{\epsilon=0} \mathcal{L}[x + \epsilon\xi, u + \epsilon\phi]$$

which gives

$$0 = \text{“}E^x(L)\text{”}\,\xi_0 + E^u(L)\phi_0 + (S - \mathsf{id})(A)$$

where

	Smooth	Discrete
$\mathcal{L}[x,u]$	$\int L\left(x, u, \frac{u_t}{x_t}\right) x_t\,\mathsf{d}t$	$\sum_{x_0} L\left(x_0, u_0, \mathcal{M}(u_x)\right)\,(x_1 - x_0)$
$0 = E^x$	$0 = \frac{\partial L}{\partial x} - \frac{\mathsf{d}}{\mathsf{d}t}\left[L - \frac{u_t}{x_t} D_3(L)\right]$	$0 = (x_1 - x_0)\frac{\partial L}{\partial x_0} + \left(S^{-1} - \mathsf{id}\right)\left[L - \mathcal{M}(u_x)\frac{\partial L}{\partial \mathcal{M}(u_x)}\right]$
$0 = E^u$	$0 = x_t\frac{\partial L}{\partial u} - \frac{\mathsf{d}}{\mathsf{d}t}D_3(L)$	$0 = (x_1 - x_0)\frac{\partial L}{\partial u_0} + \left(S^{-1} - \mathsf{id}\right)\frac{\partial L}{\partial \mathcal{M}(u_x)}$
$c = A$	$c = \frac{\partial L}{\partial u_x}\phi + \left(L - u_x\frac{\partial L}{\partial u_x}\right)\xi$	$c = \frac{\partial L}{\partial \mathcal{M}(u_x)}\phi_1 + \left(L - \mathcal{M}(u_x)\frac{\partial L}{\partial \mathcal{M}(u_x)}\right)\xi_1$

Something interesting about this 1-d case.

The smooth Euler Lagrange equations satisfy

$$u_t E^u(L) + x_t E^x(L) = 0$$

by virtue of

$$\frac{\mathrm{d}L}{\mathrm{d}t} = x_t \frac{\partial L}{\partial x} + u_t \frac{\partial L}{\partial u} + u_{tt} \frac{\partial L}{\partial u_t} + \cdots$$

The compatibility condition of the discrete-Lagrange Euler Lagrange equations is

$$\begin{aligned} \left(\mathrm{id} - S^{-1}\right) L \; &= (x_1 - x_0)\left[\tfrac{\partial L}{\partial x_0} + \mathcal{M}(u_x)\tfrac{\partial L}{\partial u_0}\right] \\ &\qquad + S^{-1}\tfrac{\partial L}{\partial \mathcal{M}(u_x)}\left(\mathrm{id} - S^{-1}\right)(\mathcal{M}(u_x)) \end{aligned}$$

Still to be fully elucidated:

1. A discrete exterior calculus based on Lagrange interpolation as part of an exact variational complex.

2. The weak form of the potential vorticity that can be obtained for the discrete variational SWW systems.

3. Consequences of the conserved multi-symplectic forms – these are readily written down.

3. And last but not least: achieving stable numerical calculations. (!!)

Thank you!!