Multisymplectic Mechanics and Variational Integrators

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Variational Multisymplectic Integrators

Multisymplectic mechanics

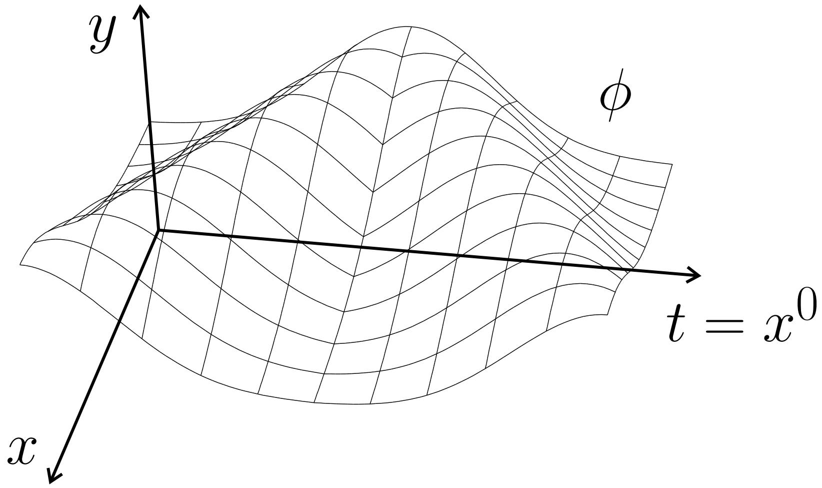
- Covariant classical field theory formalism.
- Takes a local spacetime point of view.
- Has a fully variational Lagrangian structure.
- Relationship of symmetries and conservation/constraint functions clearly presented.

Variational integrators

- Discretize and approximate the action function.
- Derive discrete equations of motion (the integrator) variationally.
- Automatically gives discrete multisymplectic structures and discrete Noether theorems (symplectic-momentum integrators).

Configuration Bundle

- ***Base space*** X is an oriented manifold (think $X =$ ***spacetime***). Coordinates x^μ, $\mu = 0, 1, \ldots, n$. May take $x^0 = t$.
- ***Configuration bundle*** $\pi_{XY} : Y \to X$ is a fiber bundle over X (think fiber $Y_x =$ ***field variables***). Coodinates (x^μ, y^a), $a = 1, \ldots, m$.
- ***Configuration*** of the system is a section ϕ of the bundle π_{XY} (a map $\phi : X \to Y$ with $\pi_{XY} \circ \phi = \mathrm{Id}$). Coordinates $\phi : (x^\mu) \mapsto (x^\mu, y^a = \phi^a(x))$.



Jet Bundles

- ***First jet bundle*** J^1Y of Y is the affine bundle with fibers $(J^1Y)_{y_x}$ consisting of linear maps $\gamma : T_xX \to T_yY$ with $T\pi_{XY} \circ \gamma = \mathrm{Id}$. Coordinates $(x^\mu, y^a, v^a{}_\mu)$. Think ***space of first derivatives***.

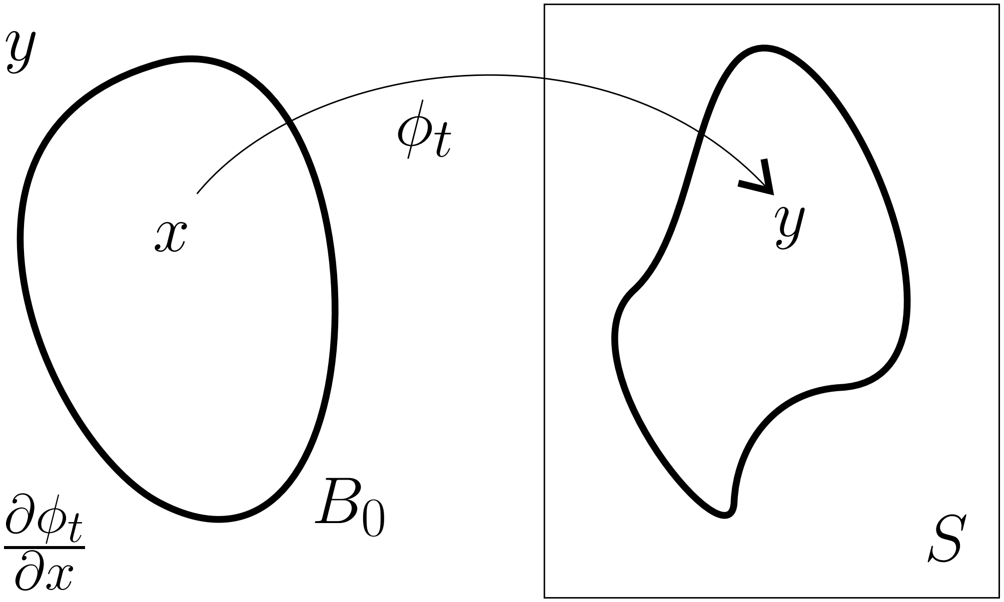
- Given a section ϕ of $Y \to X$, the ***first jet*** of ϕ is a section $j^1\phi$ of $J^1Y \to X$ with $j^1\phi : (x^\mu) \mapsto (x^\mu, \phi^a(x), \phi^a{}_{,\mu}(x))$. Think ***first derivatives of*** ϕ.

- ***Dual first jet bundle*** $J^1Y^\star$ of Y is the vector bundle with fibers $(J^1Y^\star)_{y_x}$ consisting of affine maps $(J^1Y)_{y_x}$ to $\Lambda^{n+1}X_x$ (volume forms on X at x). Coordinates $(p, p_a{}^\mu)$ represent the map $v^a{}_\mu \mapsto (p + p_a{}^\mu v^a{}_\mu)\ d^{n+1}x$. Think $p_a{}^\mu =$ ***spacetime momenta*** and $p =$ ***Hamiltonian***.

Classical Continuum Mechanics

Geometry

- Reference configuration B_0, coordinates x
- Ambient space S, coordinates y
- Configuration $y = \phi_t(x)$



Material

- Material density $\rho(x)$
- Stored energy $W(F)$
- Deformation gradient $F(x) = \frac{\partial \phi_t}{\partial x}$

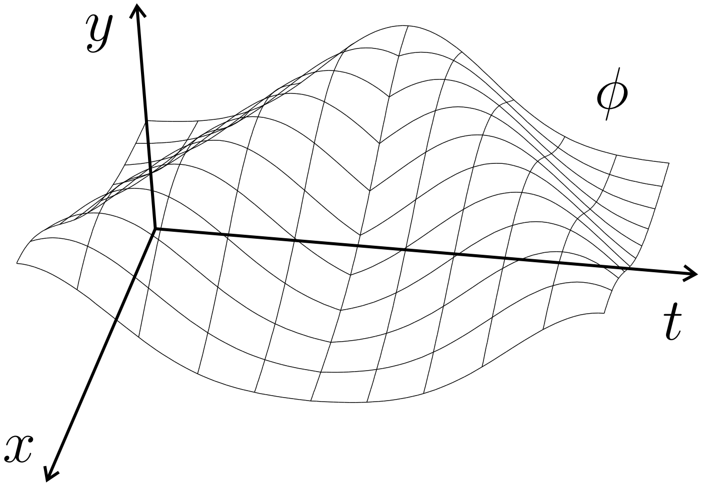
Dynamics

- First Piola-Kirchhoff stress tensor $P = \rho(x)\frac{\partial W}{\partial F}(F(x))$
- Equations of motion $\rho\ddot{\phi} = \mathrm{div}P + \mathrm{B.F.}$

Multisymplectic Continuum Mechanics

Geometry

- Base space $X = \mathbb{R} \times B_0$, coordinates (t, x)
- Fiber bundle $Y = X \times S$ with fiber coordinates y
- Configuration ϕ is a section of the fiber bundle



Material

- Lagrangian density $L(x, t, y, v, F) = \frac{1}{2}\rho(x)\|v\|^2 - \rho(x)W(F)$

Lagrangian and Action

- ***Lagrangian density*** $\mathcal{L} : J^1Y \longrightarrow \Lambda^{n+1}X$ bundle map over X. Coordinates $\mathcal{L} : (x^\mu, y^a, v^a{}_\mu) \mapsto L(x, y, v)\ d^{n+1}x$
- ***Legendre transform*** $\mathbb{F}\mathcal{L} : J^1Y \longrightarrow J^1Y^\star$ defined by

$$p_a{}^\mu = \frac{\partial L}{\partial v^a{}_\mu} \qquad p = L - p_a{}^\mu v^a{}_\mu$$

- ***Configuration space*** $\mathcal{C}(Y)$ is the space of sections ϕ of Y over X.
- ***Action integral*** $S : \mathcal{C}(Y) \longrightarrow \mathbb{R}$ defined by

$$S(\phi) = \int_X \mathcal{L}(j^1\phi)$$

Action Variations

- A ***variation*** $V : X \to TY$ of ϕ is a map

$$V : (x^\mu) \mapsto (x^\mu, \phi^a(x), V_X(x), V(x, \phi(x)))$$

- ***Hamilton's principle*** searches for configurations ϕ which are critical points of the action $S(\phi)$.
- More precisely, we require $dS(\phi) \cdot V = 0$ for all V zero on ∂X.
- Variation of S in the direction V gives

$$dS(\phi) \cdot V = \int_X D_{EL}\mathcal{L}(j^2\phi) \cdot V + \int_{\partial X} (j^1\phi)^* \left[i_{j^1 V} \Theta \right]$$

- First term is the ***Euler–Lagrange equations***:

$$\frac{\partial L}{\partial y^a}(j^1\phi) - \frac{\partial}{\partial x^\mu} \left(\frac{\partial L}{\partial {v^a}_\mu}(j^1\phi) \right) = 0$$

Multisymplectic Forms

- Boundary term in $dS(\phi)\cdot V$ gives the ***Lagrangian*** $(n+1)$–***form***:
$$\Theta_{\mathcal{L}} = p_a{}^{\mu}\, dy^a \wedge d^n x_\mu + p\, d^{n+1}x$$
where $d^n x_\mu = i_{\partial/\partial\mu} d^{n+1}x$ and $(p, p_a{}^{\mu}) = \mathbb{F}\mathcal{L}(x, y, v)$
- Exterior derivative of $\Theta_{\mathcal{L}}$ gives the ***Lagrangian*** $(n+2)$–***form***:
$$\Omega_{\mathcal{L}} = -d\Theta_{\mathcal{L}} = dy^a \wedge dp_a{}^{\mu} \wedge d^n x_\mu - dp \wedge d^{n+1}x$$
- Restricting to solutions ϕ of the EL equations, taking a second derivative of S, and recalling $d^2 = 0$ gives the ***multisymplectic form formula***:
$$\int_{\partial X} (j^1\phi)^* \left[i_{j^1 V} i_{j^1 W} \Omega_{\mathcal{L}} \right] = 0$$
for all first variations V, W of solutions ϕ.

Group Actions

- Consider a ***Lie group action*** $\Phi^Y : G \times Y \to Y$ by diffeomorphisms $g : Y \to Y$ covering the action $\Phi^X : G \times Y \to Y$ by diffeomorphisms $g_X : X \to X$.
- The ***prolonged action*** $\Phi^{J^1Y} : G \times J^1Y \to J^1Y$ is given by

$$g \cdot (x^\mu, y^a, v^a{}_\mu) = \left(g_X^\mu(x), g^a(x,y), \left[\frac{\partial g^a}{\partial x^\nu} + \frac{\partial g^a}{\partial y^b} v^b{}_\nu \right] \frac{\partial (g_X^{-1})^\nu}{\partial x^\mu} \right)$$

- The ***infinitesimal generator*** is $\xi_{J^1Y} : J^1Y \to T(J^1Y)$ given by

$$\xi_{J^1Y}(x,y,v) = \left.\frac{\partial}{\partial g}\right|_{g=e} \left(\Phi_g^{J^1Y}(x,y,v) \right) \cdot \xi$$

for each ξ in the Lie algebra $\mathfrak{g}$ of G.

Symmetry Actions

- The Lagrangian $\mathcal{L} : J^1Y \longrightarrow \Lambda^{n+1}X$ is ***equivariant*** under the prolongation of the action $\Phi : G \times Y \longrightarrow Y$ if

$$\mathcal{L}(g(x, y, v)) = (g_X^{-1})^* \mathcal{L}(x, y, v)$$

- In such cases we say that G is a ***symmetry*** of $\mathcal{L}$. This implies that the action is ***invariant***:

$$S(g \cdot \phi) = \int_{g_X(X)} \mathcal{L}(g \cdot j^1\phi) = \int_{g_X(X)} (g_X^{-1})^* \mathcal{L}(j^1\phi)$$
$$= \int_X \mathcal{L}(j^1\phi) = S(\phi)$$

Momentum Maps

- ***Lagrangian momentum map*** $J_{\mathcal{L}} : J^1Y \to \mathfrak{g}^* \times \Lambda^n(J^1Y)$ is

$$J_{\mathcal{L}}(\xi) = i_{\xi_{J^1Y}} \Theta_{\mathcal{L}}$$

which has coordinate expression

$$J_{\mathcal{L}}(\xi) = ({p_a}^{\mu} \xi^a - p \xi^{\mu})\, d^n x_{\mu} - {p_a}^{\mu} \xi^{\nu}\, dx^a \wedge d^{n-1} x_{\mu\nu}$$

- Action variations in the group direction are

$$dS(\phi) \cdot \xi = \int_X D_E L(j^2\phi) \cdot \xi_Y + \int_{\partial X} (j^1\phi)^* \Big[i_{\xi_{J^1Y}} \Theta_{\mathcal{L}} \Big]$$

Noether's Theorem

- Symmetry action implies that action is invariant:

$$dS(\phi) \cdot \xi_{\mathcal{C}(Y)} = 0$$

- Also implies that the group action maps solutions of the Euler–Lagrange equations to other solutions.
- Using dS formula after integration by parts on solutions gives

$$dS(\phi) \cdot \xi_{\mathcal{C}(Y)} = \int_{\partial X} J_{\mathcal{L}}(\xi)$$

- Equating the above expressions gives ***Noether's theorem***:

$$\int_{\partial X} (j^1\phi)^* J_{\mathcal{L}}(\xi) = 0$$

- Taking this expression over subsets of X and using the divergence theorem gives the equivalent local form: $d\Big[(j^1\phi)^* J_{\mathcal{L}}(\xi)\Big] = 0$

Symmetries in Continuum Mechanics

- ***Translation*** group action $g^r(x,y)=(x,y+r)$ for $r\in\mathbb{R}^3$ has generator $\xi^r_Y(x,y)=(x,y,0,r)$ and momentum map $J_{\mathcal{L}}(\xi^r)={p_a}^\mu r^a\; d^n x_\mu$. Noether's theorem gives whole body linear momentum conservation and local linear momentum balance.
- ***Rotation*** group action $g^R(x,y)=(x,\exp(R)y)$ for skew R has generator $\xi^R_Y(x,y)=(x,y,0,Ry)$ and momentum map $J_{\mathcal{L}}(\xi^R)={p_a}^\mu {R^a}_b y^b\; d^n x_\mu$. Noether's theorem gives whole body angular momentum conservation and local symmetry of the Cauchy stress tensor σ.
- ***Time translation*** group action $g^\tau(t,x,y)=(t+\tau,x,y)$ for $\tau\in\mathbb{R}$ has generator $\xi^\tau_Y(t,x,y)=(t,x,y,\tau,0,0)$ and momentum map $J_{\mathcal{L}}(\xi^\tau)=(p\, d^n x_t-{p_a}^i\, dy^a\wedge d^{n-1}x_{it})\tau$. Noether's theorem gives whole body energy conservation and local energy balance.

Particle Relabeling Symmetry for Fluids

- $D_{\mathrm{vol}}(B)$ is the group of volume preserving diffeomorphisms of B with composition. The Lie algebra $\mathfrak{g}$ is the space of divergence free vector fields on B.
- $\eta \in D_{\mathrm{vol}}(B)$ acts on $Y = \mathbb{R} \times B \times S$ by $\eta \cdot (t, x, y) = (t, \eta(x), y)$. This is equivalent to composition on the right for sections so $\phi_t \mapsto \phi_t \circ \eta$.
- Lagrangian density is equivariant because volume preserving diffeomorphisms do not change $\|\phi_{,t}\|$ or the Jacobian $J(\phi_{,x})$ and $W = W(J)$.
- Noether's theorem gives circulation conservation (Kelvin's thm):

$$\frac{d}{dt} \oint_{\phi_t(\Gamma)} \dot{\phi}_t \cdot dl = 0$$

Variational Multisymplectic Discretizations

Geometry

- Discretize the base space (spacetime) into elements with fibers over them. Discrete configurations are sections of this fiber bundle.

Material

- Problem is specified by a discrete Lagrangian, which approximates the continuous action over one spacetime element.

Dynamics

- Discrete Euler-Lagrange equations (an integrator) are determined by stationarity of the discrete action.

Properties

- Methods have discrete multisymplectic form formulas and discrete Noether's theorems (symplectic-momentum integrators).

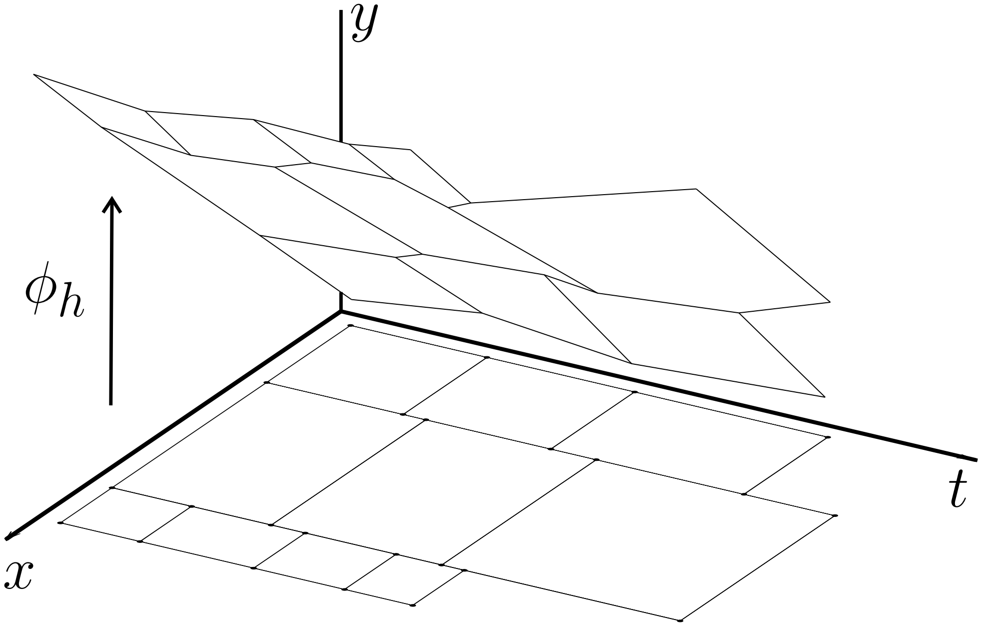
Variational Multisymplectic Discretizations

■ Examples

- Early examples include simple methods for nonlinear wave equations. (Marsden, Patrick, Shkoller)
- Hamiltonian multisymplectic methods such as product-PRK have variational derivations. (Bridges, Reich)
- Standard finite elements with Newmark is such a method. (Kane, Marsden, Ortiz, W.)
- Extensions to fluids via discrete symmetry reduction. (Pekarsky, Marsden, W.)
- Asynchronous methods for solid mechanics. (Lew, Marsden, Ortiz, W.)

Discrete Configuration Bundle

- Take a set of nodes X_d in the base space and let the ***discrete configuration bundle*** be the fiber bundle Y_d with fibers Y_x for $x \in X_d$.
- ***Discrete configurations*** are sections of this bundle.



Discrete Lagrangian and Action

- ***Discrete Lagrangian*** L_d approximates the continuous action over an element:

$$L_d(\{\phi_k \mid x_k \in E\}) \approx \int_E \mathcal{L}(j^1\phi)$$

where $\phi(x_k) \approx \phi_k$ is a solution of the system $\mathcal{L} : J^1Y \to \Lambda^{n+1}X$.

- ***Discrete action*** S_d approximates the total action:

$$\begin{aligned} S_d(\{\phi_k \mid \text{for all } x_k\}) &= \sum_E L_d(\{\phi_k \mid x_k \in E\}) \\ &\approx \int_X \mathcal{L}(j^1\phi) \end{aligned}$$

Discrete Euler–Lagrange Equations

- Taking action variations gives

$$
\begin{aligned}
dS_d(\phi_k)\cdot(\delta\phi_k,\delta x_k) &= \sum_E \left[\frac{\partial L_d(E)}{\partial \phi_k}\delta\phi_k + \frac{\partial L_d(E)}{\partial x_k}\delta x_k\right]\\
&= \sum_{k\in\mathrm{int}(X)}\left[\frac{\partial S_d^k}{\partial \phi_k}\delta\phi_k + \frac{\partial S_d^k}{\partial x_k}\delta x_k\right] + \sum_{k\in\partial X}\left[\frac{\partial S_d^k}{\partial \phi_k}\delta\phi_k + \frac{\partial S_d^k}{\partial x_k}\delta x_k\right]\\
&= \sum_{k\in\mathrm{int}(X)} D^k_{DEL}L_d(\phi)\cdot(\delta x_k,\delta\phi_k) + \sum_{k\in\partial X}\Theta^k_{L_d}(\phi)\cdot(\delta x_k,\delta\phi_k)
\end{aligned}
$$

  where $S_d^k(\phi) = \sum_{E|x_k\in E} L_d(E)$

- Interior terms are ***discrete Euler–Lagrange equations***.

- Boundary terms give ***discrete Lagrangian 1–forms*** and conservation laws.

Simple Example Variational Integrator

- Consider the system on $Y = \mathbb{R}^2 \times \mathbb{R}$ with Lagrangian density
$$\mathcal{L}(t, x, y, v_t, v_x) = \left[\frac{1}{2}v_t^2 - \frac{1}{2}v_x^2 + N(y)\right] dt \wedge dx$$
which gives the 1+1 nonlinear wave equation $\phi_{,tt} - \Delta\phi - N'(\phi) = 0$
- Take a regular fixed spacetime grid (t_i, x_k) with fibers $\phi_{i,k}$
- Take the discrete Lagrangian:

$$\begin{aligned} &L_d(\phi_{i,k}, \phi_{i+1,k}, \phi_{i,k+1}, \phi_{i+1,k+1}) \\ &= (\Delta t)(\Delta x)\left[\frac{1}{4}\left(\frac{\phi_{i+1,k} - \phi_{i,k}}{\Delta t}\right)^2 + \frac{1}{4}\left(\frac{\phi_{i+1,k+1} - \phi_{i,k+1}}{\Delta t}\right)^2\right. \\ &\quad \left. - \frac{1}{4}\left(\frac{\phi_{i,k+1} - \phi_{i,k}}{\Delta x}\right)^2 - \frac{1}{4}\left(\frac{\phi_{i+1,k+1} - \phi_{i+1,k}}{\Delta x}\right)^2 + N(\phi_{i,k})\right] \end{aligned}$$

Simple Example Variational Integrator

- Computing the discrete Euler–Lagrange equations at (i, k) requires:

$$\frac{\partial}{\partial \phi_{i,k}} \Big[L_d(\phi_{i,k}, \ldots) + L_d(\phi_{i-1,k}, \ldots) + L_d(\phi_{i,k-1}, \ldots) + L_d(\phi_{i-1,k-1}, \ldots) \Big] = 0$$

- This gives the finite difference scheme:

$$\left(\frac{\phi_{i+1,k} - 2\phi_{i,k} + \phi_{i-1,k}}{2\Delta t} \right) - \left(\frac{\phi_{i,k+1} - 2\phi_{i,k} + \phi_{i,k-1}}{2\Delta x} \right) - N'(\phi_{i,k}) = 0$$

- This is a first order multisymplectic discretization.

Discrete Multisymplectic Forms

- Taking the exterior derivative of $\Theta^k_{L_d}$ gives ***discrete Lagrangian 2–forms***:

$$\Omega^k_{L_d} = -d\Theta^k_{L_d}$$

- Restricting to solutions $\{\phi_k\}$ of the discrete Euler–Lagrange equations, taking a second exterior derivative of S_d, and using $d^2 = 0$ gives the ***discrete multisymplectic form formula***:

$$\sum_{x_k \in \partial X} \Omega^k_{L_d}(\phi) \cdot \Big((\delta x^1, \delta\phi^1), (\delta x^2, \delta\phi^2) \Big)$$

for all first variations $(\delta x^1, \delta\phi^1)$,$(\delta x^2, \delta\phi^2)$ of solutions.

Group Actions

- Lie group actions $\Phi^Y : G \times Y \to Y$ of a continuous system can also act pointwise on the discrete system as $\Phi^{Y_d} : G \times Y_d \to Y_d$ by $\Phi_g^{Y_d}(x_k, y_k) = \Phi_g^Y(x_k, y_k)$.
- Infinitesimal generators of action on Y_d are pointwise versions of the continuous generators, so that

$$\xi_{Y_d}(x_k, y_k) = \xi_Y(x_k, y_k) = \left.\frac{\partial}{\partial g}\right|_{g=e} \left[\Phi_g^{Y_d}(x_k, y_k)\right] \cdot \xi$$

- A discrete Lagrangian is ***equivariant*** if it is invariant under the action, so that $L_d(g \cdot \{x_k, y_k\}) = L_d(\{x_k, y_k\})$
- Equivariance of the discrete Lagrangian implies invariance of the action, and so the action is a ***symmetry*** of the discrete system.

Discrete Noether's Theorem

- Symmetry actions preserve the discrete action:

$$dS_d(\phi_k) \cdot \xi_{\mathcal{C}(Y_d)} = 0$$

- Also implies that solutions map to solutions, so

$$dS_d(\phi_k) \cdot \xi_{\mathcal{C}(Y_d)} = \sum_{k \in \partial X} \Theta^k_{L_d}(\phi) \cdot \xi_{Y_d}(x_k, y_k)$$

- Identify the terms in the boundary sum as the ***discrete Lagrangian momentum maps***.
- Equating the above expressions gives the ***discrete Noether's theorem***:

$$\sum_{k \in \partial X} J^k_{L_d}(\xi) = 0$$

- Taking this over a single element gives a local discrete version.

Examples of Variational Integrators

Asychronous variational integrators

- Taking a spatial mesh and per-element timesteps, construct space-time elements $K \times [t_K^j, t_K^{j+1}]$
- Discrete Lagrangian uses finite element approximation in space and first order differences in time.
- Only use ϕ_k as degrees of freedom.
- Resulting integrator is an asynchronous method for hyperbolic problems (elastodynamics) with conservative energy and linear and angular momentum properties.

Examples of Variational Integrators

■ Circulation preserving fluid integrators

- Take spatial discretization with constant timesteps.
- Discrete Lagrangian uses isoparametric finite element approximation in space and low-order polynomial approximation in time.
- Consider both vertical and space–horizontal coordinates as degrees of freedom.
- Discrete Lagrangian is invariant under volume preserving actions on the reference configuration.
- Resulting integrator preserves discrete approximations to circulation integrals.

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