Variational Integrators in Plasma Physics

Part I: Discrete Action Principles and Conservation Laws

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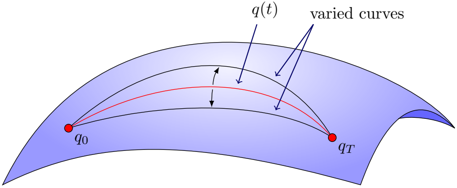
Outline

Continuous Variational Principle

- action: functional of a curve $q(t)$

$$\mathcal{A}[q(t)] = \int_0^T L\big(q(t), \dot{q}(t)\big)\, dt$$



- variation and integration by parts ($\delta q(0) = \delta q(T) = 0$)

$$\delta\mathcal{A} = \int_0^T \left[\frac{\partial L}{\partial q} \cdot \delta q + \frac{\partial L}{\partial \dot{q}} \cdot \delta \dot{q} \right] dt = \int_0^T \left[\frac{\partial L}{\partial q} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) \right] \cdot \delta q \, dt$$

- the variation of the action has to vanish for all δq, thus the term in square brackets has to vanish, and we get the Euler-Lagrange equations

$$\frac{\partial L}{\partial q}(q, \dot{q}) - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}}(q, \dot{q}) \right) = 0$$

Discrete Lagrangian and Discrete Action

- exact discrete Lagrangian: defined w.r.t. two points on a curve $q_d = \{q_k\}_{k=0}^{N}$

$$L_d^{\mathrm{e}}(q_k, q_{k+1}) = \int_{t_k}^{t_{k+1}} L(q, \dot{q})\, dt$$

- approximate velocities $\dot{q}$ with finite differences (timestep h_t)

$$\dot{q} \rightarrow \frac{q_{k+1} - q_k}{h_t}$$

- approximate discrete Lagrangian with discrete quadrature formula
  - trapezoidal

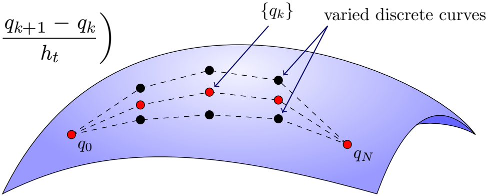
$$L_d^{\mathrm{tr}}(q^k, q^{k+1}) \approx \frac{h_t}{2} \left[L\left(q_k, \frac{q_{k+1} - q_k}{h_t} \right) + L\left(q_{k+1}, \frac{q_{k+1} - q_k}{h_t} \right) \right]$$

  - midpoint

$$L_d^{\mathrm{mp}}(q^k, q^{k+1}) \approx h_t\, L\left(\frac{q_k + q_{k+1}}{2}, \frac{q_{k+1} - q_k}{h_t} \right)$$

- discrete action

$$\mathcal{A}_d[q_d] = \sum_{k=0}^{N-1} L_d(q_k, q_{k+1})$$



Discrete Variational Principle

- discrete variational principle

$$\delta \mathcal{A}_d = \sum_{k=0}^{N-1} \Big[D_1 L_d(q_k, q_{k+1}) \cdot \delta q_k + D_2 L_d(q_k, q_{k+1}) \cdot \delta q_{k+1} \Big]$$

- discrete integration by parts (use $\delta q_0 = \delta q_N = 0$)

$$\begin{aligned} \delta \mathcal{A}_d = {} & D_1 L_d(q_0, q_1) \cdot \delta q_0 + \sum_{k=1}^{N-1} D_1 L_d(q_k, q_{k+1}) \cdot \delta q_k \\ & + \sum_{k=0}^{N-2} D_2 L_d(q_k, q_{k+1}) \cdot \delta q_{k+1} + D_2 L_d(q_{N-1}, q_N) \cdot \delta q_N \\ & = \sum_{k=1}^{N-1} \Big[D_1 L_d(q_k, q_{k+1}) + D_2 L_d(q_{k-1}, q_k) \Big] \cdot \delta q_k \end{aligned}$$

Discrete Variational Principle

- discrete variational principle

$$\delta \mathcal{A}_d = \sum_{k=0}^{N-1} \Big[D_1 L_d(q_k, q_{k+1}) \cdot \delta q_k + D_2 L_d(q_k, q_{k+1}) \cdot \delta q_{k+1} \Big]$$

$$= \sum_{k=1}^{N-1} \Big[D_1 L_d(q_k, q_{k+1}) + D_2 L_d(q_{k-1}, q_k) \Big] \cdot \delta q_k$$

- the variation of the discrete action $\delta \mathcal{A}_d$ has to vanish for all δq_k

→ for all k we get the Discrete Euler-Lagrange Equations

$$D_1 L_d(q_k, q_{k+1}) + D_2 L_d(q_{k-1}, q_k) = 0$$

- in general: fully nonlinear algebraic equation (in many cases implicit)
- often recovering well-known schemes (e.g. Störmer–Verlet, Newmark)

Continuous Variational Principle for Field Theories

- action (first order scalar field theory)

$$\mathcal{A} = \int L\big(y(t,x), y_t(t,x), y_x(t,x)\big)\, dt\, dx$$

- variation and integration by parts (variation vanishes at boundary)

$$\begin{aligned} \delta\mathcal{A} &= \int \left[\frac{\partial L}{\partial y} \cdot \delta y + \frac{\partial L}{\partial y_t} \cdot \delta y_t + \frac{\partial L}{\partial y_x} \cdot \delta y_x \right] dt\, dx \\ &= \int \left[\frac{\partial L}{\partial y} - \frac{d}{dt} \left(\frac{\partial L}{\partial y_t} \right) - \frac{d}{dx} \left(\frac{\partial L}{\partial y_x} \right) \right] \cdot \delta y\, dt\, dx \end{aligned}$$

- the variation of the action has to vanish for all δy, thus the integrand has to vanish, and we get the Euler-Lagrange Field Equations

$$\frac{\partial L}{\partial y} - \frac{d}{dt} \left(\frac{\partial L}{\partial y_t} \right) - \frac{d}{dx} \left(\frac{\partial L}{\partial y_x} \right) = 0$$

Discrete Lagrangian Density and Discrete Action

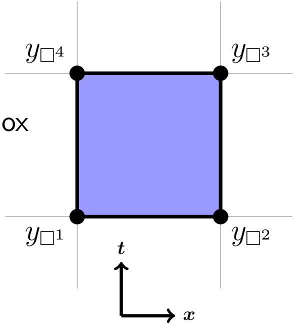
- average the fields over all vertices of a spacetime grid cell

$$y \to \frac{1}{4}\left(y_{\square^1} + y_{\square^2} + y_{\square^3} + y_{\square^4}\right)$$

- define derivatives along the edges of the grid box

$$\frac{\partial y}{\partial x} \to \frac{1}{2}\left(\frac{y_{\square^2} - y_{\square^1}}{h_x} + \frac{y_{\square^3} - y_{\square^4}}{h_x}\right)$$

$$\frac{\partial y}{\partial t} \to \frac{1}{2}\left(\frac{y_{\square^4} - y_{\square^1}}{h_t} + \frac{y_{\square^3} - y_{\square^2}}{h_t}\right)$$



- replace continuous Lagrangian and action with discrete counterparts

$$L(y, y_t, y_x) \;\to\; L_d(y_{\square^1}, y_{\square^2}, y_{\square^3}, y_{\square^4})$$

$$\mathcal{A} = \int L(y, y_t, y_x)\, dt\, dx \;\to\; \mathcal{A}_d = \sum_{\square} L_d(y_{\square^1}, y_{\square^2}, y_{\square^3}, y_{\square^4})$$

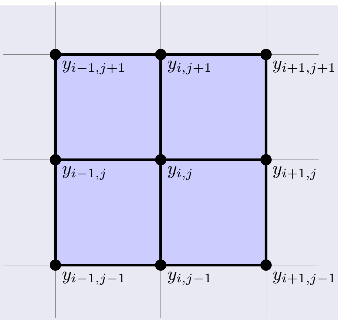
Discrete Variational Principle for Field Theories

- apply discrete variational principle

$$\delta \mathcal{A}_d = \sum_{\square} \sum_{l=1}^{4} \frac{\partial L_d}{\partial y_{\square^l}} (y_{\square^1}, y_{\square^2}, y_{\square^3}, y_{\square^4}) \cdot \delta y_{\square^l} = 0$$

to obtain the Discrete Euler-Lagrange Field Equations for all (i, j)

$$\begin{aligned} 0 = &\frac{\partial L_d}{\partial y_{\square^1}} \Big(y_{i,j}, y_{i+1,j}, y_{i+1,j+1}, y_{i,j+1} \Big) \\ + &\frac{\partial L_d}{\partial y_{\square^2}} \Big(y_{i-1,j}, y_{i,j}, y_{i,j+1}, y_{i-1,j+1} \Big) \\ + &\frac{\partial L_d}{\partial y_{\square^3}} \Big(y_{i-1,j-1}, y_{i,j-1}, y_{i,j}, y_{i-1,j} \Big) \\ + &\frac{\partial L_d}{\partial y_{\square^4}} \Big(y_{i,j-1}, y_{i+1,j-1}, y_{i+1,j}, y_{i,j} \Big) \end{aligned}$$



Discrete Variational Principle for Field Theories

- apply discrete variational principle

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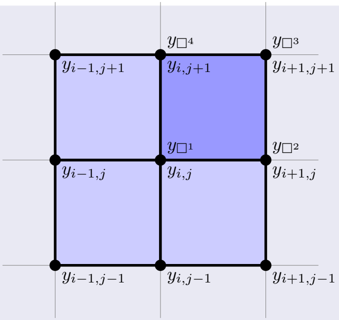

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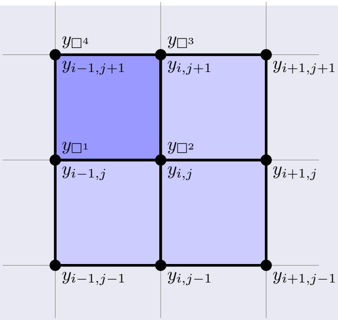

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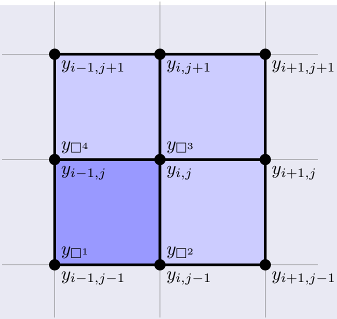

Discrete Variational Principle for Field Theories

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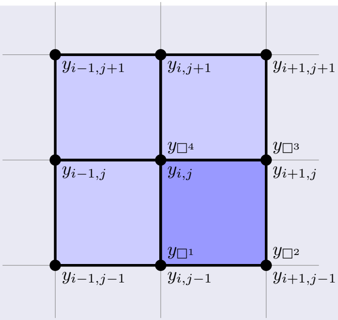

Discrete Variational Principle for Field Theories

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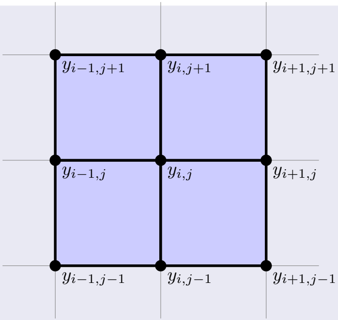


Continuous Noether Theorem (Classical Mechanics)

- infinitesimal transformation

$$q \to q^\epsilon(t) = \xi\big(q(t), \epsilon\big) = \xi^\epsilon\big(q(t)\big) \quad \text{with} \quad \xi^0 = \mathrm{id} \quad \text{and} \quad X = \left.\frac{d\xi^\epsilon}{d\epsilon}\right|_{\epsilon=0}$$

such that

$$\dot{q}^\epsilon(t) = \frac{d}{dt} q^\epsilon(t), \qquad q^0(t) = q(t), \qquad \dot{q}^0(t) = \dot{q}(t)$$

- symmetry: Lagrangian is invariant under this transformation

$$L\big(q^\epsilon(q,t), \dot{q}^\epsilon(q,t)\big) = L\big(q(t), \dot{q}(t)\big) \quad \leftrightarrow \quad \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} L\big(q^\epsilon(q,t), \dot{q}^\epsilon(q,t)\big) = 0$$

- explicitly

$$\left.\frac{d}{d\epsilon}\right|_{\epsilon=0} L\big(q^\epsilon, \dot{q}^\epsilon\big) = \frac{\partial L}{\partial q}(q, \dot{q}) \cdot \left.\frac{d\xi^\epsilon}{d\epsilon}\right|_{\epsilon=0} + \frac{\partial L}{\partial \dot{q}}(q, \dot{q}) \cdot \frac{d}{dt}\left[\left.\frac{d\xi^\epsilon}{d\epsilon}\right|_{\epsilon=0}\right] = 0$$

Continuous Noether Theorem (Classical Mechanics)

- symmetry: Lagrangian is invariant under this transformation

$$\frac{d}{d\epsilon}\bigg|_{\epsilon=0} L(q^\epsilon, \dot{q}^\epsilon) = \frac{\partial L}{\partial q}(q, \dot{q}) \cdot X + \frac{\partial L}{\partial \dot{q}}(q, \dot{q}) \cdot \dot{X} = 0$$

- if $q(t)$ solves the Euler-Lagrange equations, we can write

$$\left[\frac{d}{dt}\frac{\partial L}{\partial \dot{q}}(q, \dot{q})\right] \cdot X + \frac{\partial L}{\partial \dot{q}}(q, \dot{q}) \cdot \frac{d}{dt} X = 0$$

$\rightarrow$ this is a total time derivative

$\rightarrow$ conservation law corresponding to a symmetry generated by X for solutions q of the Euler-Lagrange equations

$$\frac{d}{dt}\left[\frac{\partial L}{\partial \dot{q}}(q, \dot{q}) \cdot X\right] = 0, \qquad X = \frac{d\xi^\epsilon}{d\epsilon}\bigg|_{\epsilon=0}$$

Continuous Noether Theorem (Classical Mechanics)

Example: Free Point Particle $\left(L(q,\dot{q}) = \frac{1}{2}\dot{q}^2\right)$

- transformation: translation

$$q^\epsilon(t) = q(t) + \epsilon X, \qquad \dot{q}^\epsilon(t) = \dot{q}(t)$$

- transformed Lagrangian

$$L\big(q^\epsilon(q,t), \dot{q}^\epsilon(q,t)\big) = \frac{1}{2}\left(\dot{q}(t)\right)^2 = L\big(q,\dot{q}\big)$$

- symmetry condition

$$\left.\frac{d}{d\epsilon}\right|_{\epsilon=0} L\big(q^\epsilon(q,t), \dot{q}^\epsilon(q,t)\big) = 0$$

- conservation law

$$\frac{d}{dt}\left[\frac{\partial L}{\partial \dot{q}}(q,\dot{q}) \cdot X\right] = \frac{d}{dt}\left[\dot{q} \cdot X\right] = 0$$

$\rightarrow$ momentum is preserved in direction of X

Discrete Noether Theorem (Discrete Mechanics)

- infinitesimal transformation

$$q_k \to q_k^\epsilon = \xi_k(q_k, \epsilon) = \xi_k^\epsilon(q_k) \quad \text{with} \quad \xi_k^0 = \mathrm{id} \quad \text{and} \quad X_k = \left. \frac{d\xi_k^\epsilon}{d\epsilon} \right|_{\epsilon=0}$$

- symmetry: Lagrangian is invariant under this transformation

$$L_d\big(q_k^\epsilon, q_{k+1}^\epsilon\big) = L_d\big(q_k, q_{k+1}\big) \quad \leftrightarrow \quad \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} L_d\big(q_k^\epsilon, q_{k+1}^\epsilon\big) = 0$$

- explicitly

$$0 = D_1 L_d\big(q_k, q_{k+1}\big) \cdot \left. \frac{d\xi_k^\epsilon}{d\epsilon} \right|_{\epsilon=0} + D_2 L_d\big(q_k, q_{k+1}\big) \cdot \left. \frac{d\xi_{k+1}^\epsilon}{d\epsilon} \right|_{\epsilon=0}$$

Discrete Noether Theorem (Discrete Mechanics)

- symmetry: Lagrangian is invariant under this transformation

$$0 = D_1 L_d\big(q_k, q_{k+1}\big) \cdot X_k + D_2 L_d\big(q_k, q_{k+1}\big) \cdot X_{k+1}$$

- if the q_k solve the discrete Euler-Lagrange equations, we can write

$$0 = -D_2 L_d\big(q_{k-1}, q_k\big) \cdot X_k + D_2 L_d\big(q_k, q_{k+1}\big) \cdot X_{k+1}$$

→ discrete conservation law corresponding to a symmetry generated by X_k for solutions q_k of the discrete Euler-Lagrange equations

$$D_2 L_d\big(q_{k-1}, q_k\big) \cdot X_k = D_2 L_d\big(q_k, q_{k+1}\big) \cdot X_{k+1}, \qquad X_k = \left. \frac{d\xi_k^\epsilon}{d\epsilon} \right|_{\epsilon=0}$$

Discrete Noether Theorem (Discrete Mechanics)

Example: Free Point Particle $\left(L_d(q_k, q_{k+1}) = \frac{h_t}{2} \left(\frac{q_{k+1} - q_k}{h_t} \right)^2 \right)$

- transformation: translation

$$q_k^\epsilon = q_k + \epsilon X$$

- discrete transformed Lagrangian

$$L_d(q_k^\epsilon, q_{k+1}^\epsilon) = \frac{h_t}{2} \left(\frac{q_{k+1} + \epsilon X - q_k - \epsilon X}{h_t} \right)^2 = \frac{h_t}{2} \left(\frac{q_{k+1} - q_k}{h_t} \right)^2 = L_d(q_k, q_{k+1})$$

- symmetry condition

$$\left. \frac{d}{d\epsilon} \right|_{\epsilon=0} L_d\big(q_k^\epsilon, q_{k+1}^\epsilon\big) = 0$$

- discrete conservation law

$$\left(\frac{q_k - q_{k-1}}{h_t} \right) \cdot X = \left(\frac{q_{k+1} - q_k}{h_t} \right) \cdot X$$

→ discrete momentum is preserved in direction of X

Discrete Noether Theorem (Discrete Mechanics) rev.

- symmetry: Lagrangian is invariant under this transformation

$$\frac{d}{d\epsilon}\bigg|_{\epsilon=0} L_d\big(q_k^\epsilon, q_{k+1}^\epsilon\big) = 0 \qquad \leftrightarrow \qquad \frac{d}{d\epsilon}\bigg|_{\epsilon=0} \mathcal{A}_d\big[q_d^\epsilon\big] = 0$$

→ symmetry: action is invariant under this transformation

$$\begin{aligned}\frac{d}{d\epsilon}\bigg|_{\epsilon=0} \mathcal{A}_d\big[q_d^\epsilon\big] &= \sum_{k=0}^{N-1} \Big[D_1 L_d(q_k, q_{k+1}) \cdot X_k + D_2 L_d(q_k, q_{k+1}) \cdot X_{k+1} \Big] \\ &= D_1 L_d(q_0, q_1) \cdot X_0 + \sum_{k=1}^{N-1} D_1 L_d(q_k, q_{k+1}) \cdot X_k \\ &+ \sum_{k=0}^{N-2} D_2 L_d(q_k, q_{k+1}) \cdot X_{k+1} + D_2 L_d(q_{N-1}, q_N) \cdot X_N \\ &= 0\end{aligned}$$

Discrete Noether Theorem (Discrete Mechanics) rev.

- symmetry: action is invariant under this transformation

$$\begin{aligned} \frac{d}{d\epsilon}\bigg|_{\epsilon=0} \mathcal{A}_d\big[q_d^\epsilon\big] &= D_1 L_d(q_0, q_1) \cdot X_0 + \sum_{k=1}^{N-1} D_1 L_d(q_k, q_{k+1}) \cdot X_k \\ &\quad + \sum_{k=0}^{N-2} D_2 L_d(q_k, q_{k+1}) \cdot X_{k+1} + D_2 L_d(q_{N-1}, q_N) \cdot X_N \\ &= \sum_{k=1}^{N-1} \Big[D_1 L_d(q_k, q_{k+1}) + D_2 L_d(q_{k-1}, q_k) \Big] \cdot X_k \\ &\quad + \Big[D_2 L_d(q_{N-1}, q_N) \cdot X_N - D_2 L_d(q_0, q_1) \cdot X_1 \Big] = 0 \end{aligned}$$

→ discrete conservation law for solutions q_k of the DELEQs

$$D_2 L_d(q_{N-1}, q_N) \cdot X_N = D_2 L_d(q_0, q_1) \cdot X_1$$

Continuous Noether Theorem (Classical Field Theory)

- vertical transformation (affects only fields, not coordinates)

$$y \to y^\epsilon(x) = \eta(x, y(x), \epsilon) = \eta^\epsilon(x, y(x)) \qquad \text{with} \qquad \eta^0 = \mathrm{id}$$

- infinitesimal generator

$$X = \frac{d\eta^\epsilon}{d\epsilon}\bigg|_{\epsilon=0} \quad \text{such that} \quad X = X^a \frac{\partial}{\partial y^a} \quad \text{with} \quad X^a = \frac{d}{d\epsilon}\bigg|_{\epsilon=0} \eta^a(x, y, \epsilon)$$

- prolongation

$$X_{\mathrm{pr}} = X^a \frac{\partial}{\partial y^a} + \left(\frac{\partial X^a}{\partial y^b} \frac{\partial y^b}{\partial x^\mu} + \frac{\partial X^a}{\partial x^\mu} \right) \frac{\partial}{\partial v^a_\mu}$$

- symmetry: Lagrangian $L(x, y, v)$ is invariant under this transformation

$$L\big(x^\mu, \eta^a, \eta^a_\mu\big) = L\big(x^\mu, y^a, v^a_\mu\big) \quad \leftrightarrow \quad X_{\mathrm{pr}}(L) = \frac{d}{d\epsilon}\bigg|_{\epsilon=0} L\big(x^\mu, \eta^a, \eta^a_\mu\big) = 0$$

Continuous Noether Theorem (Classical Field Theory)

- symmetry: Lagrangian $L(x, y, v)$ is invariant under this transformation

$$X_{\mathrm{pr}}(L) = \frac{\partial L}{\partial y^a}(x, y, v) \cdot X^a + \frac{\partial L}{\partial v^a_\mu}(x, y, v) \cdot X^a_\mu = 0$$

- if $y(x)$ solves the Euler-Lagrange field equations we can replace the first term on the RHS

$$X_{\mathrm{pr}}(L) = \left[\frac{d}{dx^\mu}\frac{\partial L}{\partial v^a_\mu}(x, y, v)\right] \cdot X^a + \frac{\partial L}{\partial v^a_\mu}(x, y, v) \cdot \left[\frac{d}{dx^\mu} X^a\right] = 0$$

→ this is a total divergence (of the Noether current J)

$$X_{\mathrm{pr}}(L) = \frac{d}{dx^\mu}\left[\frac{\partial L}{\partial v^a_\mu}(x, y, v) \cdot X^a\right] = \operatorname{div} J = 0$$

→ conservation law for solutions $y(x)$ of the Euler-Lagrange field eqs

$$\frac{d}{dt}\int \left[\frac{\partial L}{\partial v^a_t}(x, y, v) \cdot X^a\right] dx^i = 0$$

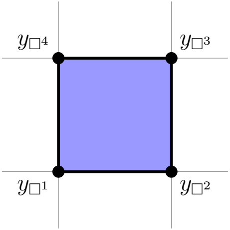
Discrete Noether Theorem (Discrete Field Theory)

- vertical transformation (affects only fields, not grid points)

$$y_{i,j} \to y^{\epsilon}_{i,j} = \eta^{\epsilon}_{i,j}(y_{i,j}) \quad \text{with} \quad \eta^{0}_{i,j} = \mathrm{id} \quad \text{and} \quad X_{i,j} = \frac{d}{d\epsilon}\bigg|_{\epsilon=0} \eta^{\epsilon}_{i,j}$$

- symmetry: discrete Lagrangian $L_d(y_{\square^1}, y_{\square^2}, y_{\square^3}, y_{\square^4})$ is invariant under this transformation

$$L_d\big(y^{\epsilon}_{\square^1}, y^{\epsilon}_{\square^2}, y^{\epsilon}_{\square^3}, y^{\epsilon}_{\square^4}\big) = L_d\big(y_{\square^1}, y_{\square^2}, y_{\square^3}, y_{\square^4}\big)$$



- this equivalent to

$$\begin{aligned} 0 &= \frac{d}{d\epsilon}\bigg|_{\epsilon=0} L_d\big(y^{\epsilon}_{\square^1}, y^{\epsilon}_{\square^2}, y^{\epsilon}_{\square^3}, y^{\epsilon}_{\square^4}\big) \\ &= \sum_{l=1}^{4} \frac{\partial L_d}{\partial y_{\square^l}}\big(y_{\square^1}, y_{\square^2}, y_{\square^3}, y_{\square^4}\big) \cdot X_{\square^l}(y_{\square^l}) \quad \text{with} \quad X_{\square^l} = \frac{d}{d\epsilon}\bigg|_{\epsilon=0} \eta^{\epsilon}_{\square^l}(y_{\square^l}) \end{aligned}$$

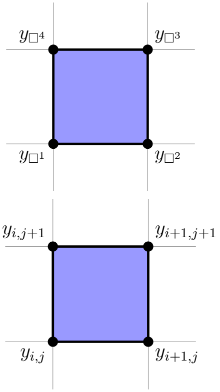
Discrete Noether Theorem (Discrete Field Theory)

- vertical transformation (affects only fields, not grid points)

$$y_{i,j} \to y^{\epsilon}_{i,j} = \eta^{\epsilon}_{i,j}(y_{i,j}) \quad \text{with} \quad \eta^0_{i,j} = \mathrm{id} \quad \text{and} \quad X_{i,j} = \frac{d}{d\epsilon}\bigg|_{\epsilon=0} \eta^{\epsilon}_{i,j}$$

- symmetry: discrete Lagrangian is invariant under this transformation

$$\begin{aligned}
0 &= \sum_{\substack{1 \le l \le 4,\\ \square^1 = (i,j)}} \frac{\partial L_d}{\partial y_{\square^l}} \left(y_{\square^1}, y_{\square^2}, y_{\square^3}, y_{\square^4} \right) \cdot X_{\square^l}(y_{\square^l}) \\
&= \frac{\partial L_d}{\partial y_{\square^1}} \Big(y_{i,j}, y_{i+1,j}, y_{i+1,j+1}, y_{i,j+1} \Big) \cdot X_{i,j} \\
&+ \frac{\partial L_d}{\partial y_{\square^2}} \Big(y_{i,j}, y_{i+1,j}, y_{i+1,j+1}, y_{i,j+1} \Big) \cdot X_{i+1,j} \\
&+ \frac{\partial L_d}{\partial y_{\square^3}} \Big(y_{i,j}, y_{i+1,j}, y_{i+1,j+1}, y_{i,j+1} \Big) \cdot X_{i+1,j+1} \\
&+ \frac{\partial L_d}{\partial y_{\square^4}} \Big(y_{i,j}, y_{i+1,j}, y_{i+1,j+1}, y_{i,j+1} \Big) \cdot X_{i,j+1}
\end{aligned}$$



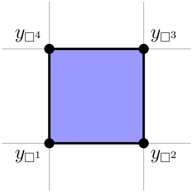
Discrete Noether Theorem (Discrete Field Theory)

- vertical transformation (affects only fields, not grid points)

$$y_{i,j} \to y^{\epsilon}_{i,j} = \eta^{\epsilon}_{i,j}(y_{i,j}) \quad \text{with} \quad \eta^0_{i,j} = \mathrm{id} \quad \text{and} \quad X_{i,j} = \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \eta^{\epsilon}_{i,j}$$

- symmetry: discrete Lagrangian is invariant under this transformation

$$0 = \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} L_d\big(y^{\epsilon}_{\Box^1}, y^{\epsilon}_{\Box^2}, y^{\epsilon}_{\Box^3}, y^{\epsilon}_{\Box^4}\big)$$

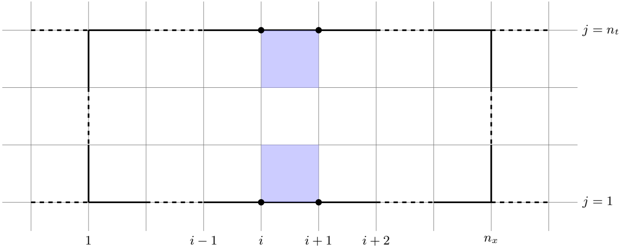


and thus is the discrete action

$$\left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \mathcal{A}_d\big[y^{\epsilon}_d\big] = \sum_{\Box} \sum_{l} \frac{\partial L_d}{\partial y_{\Box^l}}\big(y_{\Box^1}, y_{\Box^2}, y_{\Box^3}, y_{\Box^4}\big) \cdot X_{\Box^l}(y_{\Box^l}) = 0$$

→ interior contributions are zero for solutions $y_{i,j}$ of the discrete Euler-Lagrange field equations

Discrete Noether Theorem (Discrete Field Theory)



- discrete conservation law (sum over boundary)

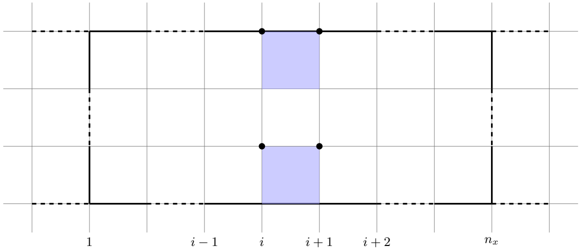
$$0 = \sum_{i=1}^{n_x-1} \Bigg[\frac{\partial L_d}{\partial y_{\Box^1}} \Big(y_{i,1}, y_{i+1,1}, y_{i+1,2}, y_{i,2} \Big) \cdot X_{i,1}$$

$$+ \frac{\partial L_d}{\partial y_{\Box^2}} \Big(y_{i,1}, y_{i+1,1}, y_{i+1,2}, y_{i,2} \Big) \cdot X_{i+1,1}$$

$$+ \frac{\partial L_d}{\partial y_{\Box^3}} \Big(y_{i,n_t-1}, y_{i+1,n_t-1}, y_{i+1,n_t}, y_{i,n_t} \Big) \cdot X_{i+1,n_t}$$

$$+ \frac{\partial L_d}{\partial y_{\Box^4}} \Big(y_{i,n_t-1}, y_{i+1,n_t-1}, y_{i+1,n_t}, y_{i,n_t} \Big) \cdot X_{i,n_t} \Bigg]$$

Discrete Noether Theorem (Discrete Field Theory)

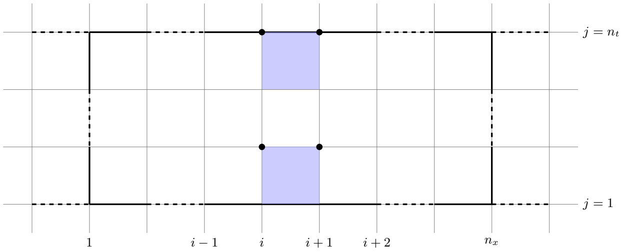


- use symmetry condition to replace first sum

$$\sum_{i=1}^{n_x-1} \Bigg[\frac{\partial L_d}{\partial y_{\square^3}} \Big(y_{i,1}, y_{i+1,1}, y_{i+1,2}, y_{i,2} \Big) \cdot X_{i+1,2} + \frac{\partial L_d}{\partial y_{\square^4}} \Big(y_{i,1}, y_{i+1,1}, y_{i+1,2}, y_{i,2} \Big) \cdot X_{i,2} \Bigg]$$

$$= \sum_{i=1}^{n_x-1} \Bigg[\frac{\partial L_d}{\partial y_{\square^3}} \Big(y_{i,n_t-1}, y_{i+1,n_t-1}, y_{i+1,n_t}, y_{i,n_t} \Big) \cdot X_{i+1,n_t} + \frac{\partial L_d}{\partial y_{\square^4}} \Big(y_{i,n_t-1}, y_{i+1,n_t-1}, y_{i+1,n_t}, y_{i,n_t} \Big) \cdot X_{i,n_t} \Bigg]$$

Discrete Noether Theorem (Discrete Field Theory)



- as n_t is arbitrary, the discrete conservation law can be written as

$$\sum_{i=1}^{n_x - 1} \Bigg[\frac{\partial L_d}{\partial y_{\square^3}} \Big(y_{i,j}, y_{i+1,j}, y_{i+1,j+1}, y_{i,j+1} \Big) \cdot X_{i+1,j+1} + \frac{\partial L_d}{\partial y_{\square^4}} \Big(y_{i,j}, y_{i+1,j}, y_{i+1,j+1}, y_{i,j+1} \Big) \cdot X_{i,j+1} \Bigg] = const$$

Nonvariational PDEs and Extended Lagrangians

- prerequisite for the derivation of variational integrators: existence of a Lagrangian formulation for the considered dynamical system

→ nonvariational PDEs: embed any dynamical system into a Lagrangian system by doubling the number of variables

→ extended Lagrangian for a system of differential equations $F[u] = 0$

$$L = v \cdot F[u] \qquad \text{with action} \qquad \mathcal{A}[u, v] = \int L \, dx$$

- variational principle: original and adjoint equation

$$F[u] = \frac{\delta \mathcal{A}}{\delta v} = 0, \qquad F^{*}[u, v] = \frac{\delta \mathcal{A}}{\delta u} = 0$$

- symmetries of original equation are transferred to adjoint equation
  - → application of Noether's theorem to extended Lagrangian results in conservation laws of the extended system
  - → fixing compatible solutions of the auxiliary fields by a map

$$\Phi : \big(u(x) \big) \mapsto \big(u(x), \phi(u)(x) \big)$$

allows us to recover conservation laws of the original system

Linear Advection Equation

- linear advection equation

$$\partial_t u + c\,\partial_x u = 0 \qquad\qquad c\text{: velocity (parameter, constant)}$$

- extended Lagrangian with auxiliary field $v(x, t)$

$$L(v, u_x, u_t) = v\big(u_t + c u_x\big)$$

- Euler-Lagrange equations

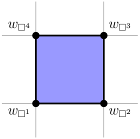
$$\frac{\delta L}{\delta v} = +u_t + c u_x = 0 \qquad\qquad \rightarrow \text{advection equation}$$

$$\frac{\delta L}{\delta u} = -v_t - c v_x = 0 \qquad\qquad \rightarrow \text{adjoint equation}$$

- the adjoint equation has the same solution as the original equation

→ if u is a solution of the advection equation, then $w = (u, u)$ solves the Euler-Lagrange equations of the above adjoint Lagrangian

Variational Integrators for the Advection Equation



- straight forward discretisation with midpoint rule
- discrete Lagrangian ($w_{\Box^l} = (u_{\Box^l}, v_{\Box^l})$, $1 \leq l \leq 4$):

$$L_d(w_{\Box^1}, w_{\Box^2}, w_{\Box^3}, w_{\Box^4}) = h_t h_x \frac{1}{4} \Big(v_{\Box^1} + v_{\Box^2} + v_{\Box^3} + v_{\Box^4} \Big) \times$$

$$\times \left[\frac{1}{2} \left(\frac{u_{\Box^4} - u_{\Box^1}}{h_t} + \frac{u_{\Box^3} - u_{\Box^2}}{h_t} \right) + \frac{c}{2} \left(\frac{u_{\Box^2} - u_{\Box^1}}{h_x} + \frac{u_{\Box^3} - u_{\Box^4}}{h_x} \right) \right]$$

- discrete Euler-Lagrange Field Equations ($w_{i,j} = (u_{i,j}, v_{i,j})$)

$$0 = \frac{\partial L_d}{\partial v_{\Box^1}} \Big(w_{i,j}, w_{i+1,j}, w_{i+1,j+1}, w_{i,j+1} \Big) + \frac{\partial L_d}{\partial v_{\Box^2}} \Big(w_{i-1,j}, w_{i,j}, w_{i,j+1}, w_{i-1,j+1} \Big)$$

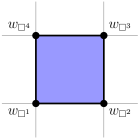
$$+ \frac{\partial L_d}{\partial v_{\Box^3}} \Big(w_{i-1,j-1}, w_{i,j-1}, w_{i,j}, w_{i-1,j} \Big) + \frac{\partial L_d}{\partial v_{\Box^4}} \Big(w_{i,j-1}, w_{i+1,j-1}, w_{i+1,j}, w_{i,j} \Big)$$

result in (i spatial index, j time index)

$$0 = \frac{1}{4} \left[\frac{u_{i+1,j+1} - u_{i+1,j-1}}{2h_t} + 2 \frac{u_{i,j+1} - u_{i,j-1}}{2h_t} + \frac{u_{i-1,j+1} - u_{i-1,j-1}}{2h_t} \right]$$

$$+ \frac{c}{4} \left[\frac{u_{i+1,j+1} - u_{i-1,j+1}}{2h_x} + 2 \frac{u_{i+1,j} - u_{i-1,j}}{2h_x} + \frac{u_{i+1,j-1} - u_{i-1,j-1}}{2h_x} \right]$$

Variational Integrators for the Advection Equation



- first simplification: two timesteps instead of three
- discrete Lagrangian ($w_{\square^l} = (u_{\square^l}, v_{\square^l})$, $1 \leq l \leq 4$):

$$L_d(w_{\square^1}, w_{\square^2}, w_{\square^3}, w_{\square^4}) = h_t h_x \, \frac{1}{2} \Big(v_{\square^1} + v_{\square^2} \Big) \times$$

$$\times \left[\frac{1}{2} \left(\frac{u_{\square^4} - u_{\square^1}}{h_t} + \frac{u_{\square^3} - u_{\square^2}}{h_t} \right) + \frac{c}{2} \left(\frac{u_{\square^2} - u_{\square^1}}{h_x} + \frac{u_{\square^3} - u_{\square^4}}{h_x} \right) \right]$$

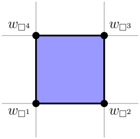
- discrete Euler-Lagrange Field Equations ($w_{i,j} = (u_{i,j}, v_{i,j})$)

$$0 = \frac{\partial L_d}{\partial v_{\square^1}} \Big(w_{i,j}, w_{i+1,j}, w_{i+1,j+1}, w_{i,j+1} \Big) + \frac{\partial L_d}{\partial v_{\square^2}} \Big(w_{i-1,j}, w_{i,j}, w_{i,j+1}, w_{i-1,j+1} \Big)$$
$$+ \frac{\partial L_d}{\partial v_{\square^3}} \Big(w_{i-1,j-1}, w_{i,j-1}, w_{i,j}, w_{i-1,j} \Big) + \frac{\partial L_d}{\partial v_{\square^4}} \Big(w_{i,j-1}, w_{i+1,j-1}, w_{i+1,j}, w_{i,j} \Big)$$

result in (i spatial index, j time index)

$$0 = \frac{1}{4} \left[\frac{u_{i+1,j+1} - u_{i+1,j}}{h_t} + 2 \, \frac{u_{i,j+1} - u_{i,j}}{h_t} + \frac{u_{i-1,j+1} - u_{i-1,j}}{h_t} \right]$$
$$+ \frac{c}{2} \left[\frac{u_{i+1,j} - u_{i-1,j}}{2h_x} + \frac{u_{i+1,j+1} - u_{i-1,j+1}}{2h_x} \right]$$

Variational Integrators for the Advection Equation



- second simplification: no spatial average of time derivative
- discrete Lagrangian ($w_{\Box^l} = (u_{\Box^l}, v_{\Box^l})$, $1 \leq l \leq 4$):

$$L_d(w_{\Box^1}, w_{\Box^2}, w_{\Box^3}, w_{\Box^4}) = h_t h_x \frac{1}{2} \left[v_{\Box^1} \frac{u_{\Box^4} - u_{\Box^1}}{h_t} + v_{\Box^2} \frac{u_{\Box^3} - u_{\Box^2}}{h_t} \right] + h_t h_x \frac{c}{4} \left[v_{\Box^1} + v_{\Box^2} \right] \left[\frac{u_{\Box^2} - u_{\Box^1}}{h_x} + \frac{u_{\Box^3} - u_{\Box^4}}{h_x} \right]$$

- discrete Euler-Lagrange Field Equations ($w_{i,j} = (u_{i,j}, v_{i,j})$)

$$0 = \frac{\partial L_d}{\partial v_{\Box^1}} \left(w_{i,j}, w_{i+1,j}, w_{i+1,j+1}, w_{i,j+1} \right) + \frac{\partial L_d}{\partial v_{\Box^2}} \left(w_{i-1,j}, w_{i,j}, w_{i,j+1}, w_{i-1,j+1} \right) + \frac{\partial L_d}{\partial v_{\Box^3}} \left(w_{i-1,j-1}, w_{i,j-1}, w_{i,j}, w_{i-1,j} \right) + \frac{\partial L_d}{\partial v_{\Box^4}} \left(w_{i,j-1}, w_{i+1,j-1}, w_{i+1,j}, w_{i,j} \right)$$

result in (i spatial index, j time index)

$$0 = \frac{u_{i,j+1} - u_{i,j}}{h_t} + \frac{c}{2} \left[\frac{u_{i+1,j+1} - u_{i-1,j+1}}{2h_x} + \frac{u_{i+1,j} - u_{i-1,j}}{2h_x} \right]$$

Conservation Laws of the Advection Equation

- extended Lagrangian with auxiliary field $v(t, x)$

$$L(v, u_t, u_x) = v \left(u_t + c u_x \right)$$

- infinitesimal generator of the transformation

$$X^u = 1, \qquad X^v = 0, \qquad X_{\mathrm{pr}} = \frac{\partial}{\partial u}$$

- invariance of the Lagrangian

$$X_{\mathrm{pr}}(L) = \frac{\partial L}{\partial u} = 0$$

- conservation of the L^1 norm of u

$$\frac{d}{dt} \int \frac{\partial L}{\partial u_t} \, X^u \, dx = \frac{d}{dt} \int v \, dx = \frac{d}{dt} \int u \, dx = 0$$

- discrete Lagrangian

$$L_d = h_t h_x \frac{1}{2}\left[v_{\square^1} \frac{u_{\square^4} - u_{\square^1}}{h_t} + v_{\square^2} \frac{u_{\square^3} - u_{\square^2}}{h_t} \right] + h_t h_x \frac{c}{4}\left[v_{\square^1} + v_{\square^2} \right]\left[\frac{u_{\square^2} - u_{\square^1}}{h_x} + \frac{u_{\square^3} - u_{\square^4}}{h_x} \right]$$

- infinitesimal generator of the transformation

$$X^u_{\square^l} = 1, \qquad X^v_{\square^l} = 0$$

- invariance of the Lagrangian

$$\sum_{\substack{1 \leq l \leq 4,\\ \square^1 = (i,j)}} \frac{\partial L_d}{\partial u_{\square^l}} (w_{\square^1}, w_{\square^2}, w_{\square^3}, w_{\square^4}) \cdot X^u_{\square^l} + \sum_{\substack{1 \leq l \leq 4,\\ \square^1 = (i,j)}} \frac{\partial L_d}{\partial v_{\square^l}} (w_{\square^1}, w_{\square^2}, w_{\square^3}, w_{\square^4}) \cdot X^v_{\square^l}$$

$$= \frac{h_t h_x}{2}\left[- \frac{v_{i,j}}{h_t} - \frac{c}{2} \frac{v_{i,j} + v_{i,j+1}}{h_x} \right] \cdot X^u_{i,j}$$

$$+ \frac{h_t h_x}{2}\left[- \frac{v_{i+1,j}}{h_t} + \frac{c}{2} \frac{v_{i,j} + v_{i,j+1}}{h_x} \right] \cdot X^u_{i+1,j}$$

$$+ \frac{h_t h_x}{2}\left[+ \frac{v_{i+1,j}}{h_t} + \frac{c}{2} \frac{v_{i,j} + v_{i,j+1}}{h_x} \right] \cdot X^u_{i+1,j+1}$$

$$+ \frac{h_t h_x}{2}\left[+ \frac{v_{i,j}}{h_t} - \frac{c}{2} \frac{v_{i,j} + v_{i,j+1}}{h_x} \right] \cdot X^u_{i,j+1} = 0$$

Discrete Conservation Laws of the Advection Equation

- discrete Lagrangian

$$L_d = h_t h_x \frac{1}{2} \left[v_{\square^1} \frac{u_{\square^4} - u_{\square^1}}{h_t} + v_{\square^2} \frac{u_{\square^3} - u_{\square^2}}{h_t} \right] + h_t h_x \frac{c}{4} \left[v_{\square^1} + v_{\square^2} \right] \left[\frac{u_{\square^2} - u_{\square^1}}{h_x} + \frac{u_{\square^3} - u_{\square^4}}{h_x} \right]$$

- infinitesimal generator of the transformation

$$X^u_{\square^l} = 1, \qquad\qquad X^v_{\square^l} = 0$$

- discrete conservation law

$$\sum_{i=1}^{n_x-1} \left[\frac{\partial L_d}{\partial u_{\square^3}} \Big(w_{i,j}, w_{i+1,j}, w_{i+1,j+1}, w_{i,j+1} \Big) \cdot X^u_{i+1,j+1} + \frac{\partial L_d}{\partial u_{\square^4}} \Big(w_{i,j}, w_{i+1,j}, w_{i+1,j+1}, w_{i,j+1} \Big) \cdot X^u_{i,j+1} \right] = const \text{ for all } j$$

upon explicit computation becomes

$$\frac{h_t h_x}{2} \sum_{i=1}^{n_x-1} \left[\frac{v_{i+1,j}}{h_t} + \frac{c}{2} \frac{v_{i,j} + v_{i+1,j}}{h_x} \right] \cdot X^u_{i+1,j+1} + \frac{h_t h_x}{2} \sum_{i=1}^{n_x-1} \left[\frac{v_{i,j}}{h_t} - \frac{c}{2} \frac{v_{i,j} + v_{i+1,j}}{h_x} \right] \cdot X^u_{i,j+1} = const \text{ for all } j$$

Discrete Conservation Laws of the Advection Equation

- discrete Lagrangian

$$L_d = h_t h_x \frac{1}{2} \left[v_{\square^1} \frac{u_{\square^4} - u_{\square^1}}{h_t} + v_{\square^2} \frac{u_{\square^3} - u_{\square^2}}{h_t} \right] + h_t h_x \frac{c}{4} \left[v_{\square^1} + v_{\square^2} \right] \left[\frac{u_{\square^2} - u_{\square^1}}{h_x} + \frac{u_{\square^3} - u_{\square^4}}{h_x} \right]$$

- infinitesimal generator of the transformation

$$X^u_{\square^l} = 1, \qquad X^v_{\square^l} = 0$$

- discrete conservation law

$$\frac{h_t h_x}{2} \sum_{i=1}^{n_x - 1} \left[\frac{v_{i+1,j}}{h_t} + \frac{c}{2} \frac{v_{i,j} + v_{i+1,j}}{h_x} \right] \cdot 1 + \frac{h_t h_x}{2} \sum_{i=1}^{n_x - 1} \left[\frac{v_{i,j}}{h_t} - \frac{c}{2} \frac{v_{i,j} + v_{i+1,j}}{h_x} \right] \cdot 1 = const \text{ for all } j$$

- identifying $v = u$

$$h_x \sum_{i=1}^{n_x - 1} \left[\frac{v_{i,j} + v_{i+1,j}}{2} \right] = h_x \sum_{i=1}^{n_x - 1} u_{i,j} = const \text{ for all } j$$

Conservation Laws of the Advection Equation

- extended Lagrangian with auxiliary field $v(t, x)$

$$L(v, u_t, u_x) = v\left(u_t + c u_x\right)$$

- infinitesimal generator of the transformation

$$X^u = u, \qquad X^v = -v, \qquad X_{\mathrm{pr}} = u\,\frac{\partial}{\partial u} - v\,\frac{\partial}{\partial v} + u_\mu\,\frac{\partial}{\partial u_\mu} - v_\mu\,\frac{\partial}{\partial v_\mu}$$

- invariance of the Lagrangian

$$X_{\mathrm{pr}}(L) = -v\,\frac{\partial L}{\partial v} + u_\mu\,\frac{\partial L}{\partial u_\mu} = -v\left(u_t + c u_x\right) + v\left(u_t + c u_x\right) = 0$$

- conservation of the L^2 norm of u

$$\frac{d}{dt}\int \frac{\partial L}{\partial u_t}\,X^u\,dx = \frac{d}{dt}\int vu\,dx = \frac{d}{dt}\int u^2\,dx = 0$$

Discrete Conservation Laws of the Advection Equation

- discrete Lagrangian

$$L_d = h_t h_x \frac{1}{2} \left[v_{\square^1} \frac{u_{\square^4} - u_{\square^1}}{h_t} + v_{\square^2} \frac{u_{\square^3} - u_{\square^2}}{h_t} \right] + h_t h_x \frac{c}{4} \left[v_{\square^1} + v_{\square^2} \right] \left[\frac{u_{\square^2} - u_{\square^1}}{h_x} + \frac{u_{\square^3} - u_{\square^4}}{h_x} \right]$$

- infinitesimal generator of the transformation

$$X^u_{\square^l} = u_{\square^l}, \qquad X^v_{\square^l} = -v_{\square^l}$$

- invariance of the Lagrangian

$$\sum_{\substack{1 \leq l \leq 4, \\ \square^1 = (i,j)}} \frac{\partial L_d}{\partial u_{\square^l}} \left(w_{\square^1}, w_{\square^2}, w_{\square^3}, w_{\square^4} \right) \cdot X^u_{\square^l} + \sum_{\substack{1 \leq l \leq 4, \\ \square^1 = (i,j)}} \frac{\partial L_d}{\partial v_{\square^l}} \left(w_{\square^1}, w_{\square^2}, w_{\square^3}, w_{\square^4} \right) \cdot X^v_{\square^l}$$

$$= \frac{h_t h_x}{2} \left[- \frac{v_{i,j}}{h_t} - \frac{c}{2} \frac{v_{i,j} + v_{i,j+1}}{h_x} \right] \cdot u_{i,j} + \frac{h_t h_x}{2} \left[- \frac{v_{i+1,j}}{h_t} + \frac{c}{2} \frac{v_{i,j} + v_{i,j+1}}{h_x} \right] \cdot u_{i+1,j}$$

$$+ \frac{h_t h_x}{2} \left[+ \frac{v_{i+1,j}}{h_t} + \frac{c}{2} \frac{v_{i,j} + v_{i,j+1}}{h_x} \right] \cdot u_{i+1,j+1} + \frac{h_t h_x}{2} \left[+ \frac{v_{i,j}}{h_t} - \frac{c}{2} \frac{v_{i,j} + v_{i,j+1}}{h_x} \right] \cdot u_{i,j+1}$$

$$- \frac{h_t h_x}{2} \left[\frac{u_{i,j+1} - u_{i,j}}{h_t} + \frac{c}{2} \frac{u_{i+1,j} - u_{i,j}}{h_x} + \frac{c}{2} \frac{u_{i+1,j+1} - u_{i,j+1}}{h_x} \right] \cdot v_{i,j}$$

$$- \frac{h_t h_x}{2} \left[\frac{u_{i+1,j+1} - u_{i+1,j}}{h_t} + \frac{c}{2} \frac{u_{i+1,j} - u_{i,j}}{h_x} + \frac{c}{2} \frac{u_{i+1,j+1} - u_{i,j+1}}{h_x} \right] \cdot v_{i+1,j} = 0$$

Discrete Conservation Laws of the Advection Equation

- discrete Lagrangian

$$L_d = h_t h_x \frac{1}{2} \left[v_{\Box 1} \frac{u_{\Box 4} - u_{\Box 1}}{h_t} + v_{\Box 2} \frac{u_{\Box 3} - u_{\Box 2}}{h_t} \right] + h_t h_x \frac{c}{4} \left[v_{\Box 1} + v_{\Box 2} \right] \left[\frac{u_{\Box 2} - u_{\Box 1}}{h_x} + \frac{u_{\Box 3} - u_{\Box 4}}{h_x} \right]$$

- infinitesimal generator of the transformation

$$X^u_{\Box l} = u_{\Box l}, \qquad X^v_{\Box l} = -v_{\Box l}$$

- discrete conservation law

$$\sum_{a \in (u,v)} \sum_{i=1}^{n_x - 1} \left[\frac{\partial L_d}{\partial w^a_{\Box 3}} \left(w_{i,j}, w_{i+1,j}, w_{i+1,j+1}, w_{i,j+1} \right) \cdot X^a_{i+1,j+1} + \frac{\partial L_d}{\partial w^a_{\Box 4}} \left(w_{i,j}, w_{i+1,j}, w_{i+1,j+1}, w_{i,j+1} \right) \cdot X^a_{i,j+1} \right] = const \text{ for all } j$$

upon explicit computation becomes

$$\frac{h_x h_t}{2} \sum_{i=1}^{n_x - 1} \left[\frac{v_{i+1,j}}{h_t} + \frac{c}{2} \frac{v_{i,j} + v_{i+1,j}}{h_x} \right] \cdot u_{i+1,j+1} + \frac{h_x h_t}{2} \sum_{i=1}^{n_x - 1} \left[\frac{v_{i,j}}{h_t} - \frac{c}{2} \frac{v_{i,j} + v_{i+1,j}}{h_x} \right] \cdot u_{i,j+1} = const \text{ for all } j$$

Discrete Conservation Laws of the Advection Equation

- discrete conservation law

$$\frac{h_x h_t}{2} \sum_{i=1}^{n_x-1} \left(\left[\frac{v_{i+1,j}}{h_t} + \frac{c}{2} \frac{v_{i,j} + v_{i+1,j}}{h_x} \right] \cdot u_{i+1,j+1} + \left[\frac{v_{i,j}}{h_t} - \frac{c}{2} \frac{v_{i,j} + v_{i+1,j}}{h_x} \right] \cdot u_{i,j+1} \right) = c \; \forall j$$

- index shift in first sum: $i + 1 \to i$

$$h_x h_t \sum_{i=1}^{n_x-1} \left[\frac{v_{i,j}}{h_t} - \frac{c}{2} \frac{v_{i+1,j} - v_{i-1,j}}{2h_x} \right] \cdot u_{i,j+1} = c \; \forall j$$

- use discrete Euler-Lagrange field equations to replace first term

$$h_x h_t \sum_{i=1}^{n_x-1} \left[\frac{v_{i,j+1}}{h_t} + \frac{c}{2} \frac{v_{i+1,j+1} - v_{i-1,j+1}}{2h_x} + \frac{c}{2} \frac{v_{i+1,j} - v_{i-1,j}}{2h_x} - \frac{c}{2} \frac{v_{i+1,j} - v_{i-1,j}}{2h_x} \right] u_{i,j+1} = c$$

- more index shifting and identifying $v = u$

$$h_x \sum_{i=1}^{n_x-1} v_{i,j+1} \, u_{i,j+1} + h_x h_t \frac{c}{2} \sum_{i=1}^{n_x-1} \left[\frac{v_{i+1,j+1} \, u_{i,j+1} - v_{i,j+1} \, u_{i+1,j+1}}{2h_x} \right] = h_x \sum_{i=1}^{n_x-1} u_{i,j+1}^2 = c \; \forall j$$

Ideal Magnetohydrodynamics

- incompressible ideal MHD

$$\frac{\partial V}{\partial t} + (V \cdot \nabla) V = (B \cdot \nabla) B - \nabla P, \qquad \nabla \cdot V = 0, \qquad P = p + \frac{1}{2} B^2$$
$$\frac{\partial B}{\partial t} + (V \cdot \nabla) B = (B \cdot \nabla) V, \qquad \nabla \cdot B = 0$$

B magnetic field $\quad$ V velocity field $\quad$ p gas pressure

- extended Lagrangian with auxiliary fields (α, β, γ)

$$L = \alpha \cdot \left(V_t + \psi(V, B) + \nabla \tilde{P} \right) + \beta \cdot \left(B_t + \phi(V, B) \right) + \gamma \nabla \cdot V$$

with

$$\psi(V, B) = V \times (\nabla \times V) - B \times (\nabla \times B),$$
$$\phi(V, B) = \nabla \times (V \times B),$$
$$\tilde{P} = p + \frac{1}{2} V^2$$

Ideal Magnetohydrodynamics

- conservation of energy

$$E = \int \left(V^2 + B^2 \right) dx$$

- infinitesimal generator of the transformation

$$X^V = V, \quad X^B = B, \quad X^{\tilde{P}} = \tilde{P}, \quad X^\alpha = -\alpha, \quad X^\beta = -\beta, \quad X^\gamma = -\gamma$$

- prolonged vector field

$$\begin{aligned} X_{\text{pr}} = {} & V_x \frac{\partial}{\partial V_x} + V_{x,t} \frac{\partial}{\partial V_{x,t}} + V_{x,x} \frac{\partial}{\partial V_{x,x}} + V_{x,y} \frac{\partial}{\partial V_{x,y}} + V_y \frac{\partial}{\partial V_y} + V_{y,t} \frac{\partial}{\partial V_{y,t}} + V_{y,x} \frac{\partial}{\partial V_{y,x}} + V_{y,y} \frac{\partial}{\partial V_{y,y}} \\ & + B_x \frac{\partial}{\partial B_x} + B_{x,t} \frac{\partial}{\partial B_{x,t}} + B_{x,x} \frac{\partial}{\partial B_{x,x}} + B_{x,y} \frac{\partial}{\partial B_{x,y}} + B_y \frac{\partial}{\partial B_y} + B_{y,t} \frac{\partial}{\partial B_{y,t}} + B_{y,x} \frac{\partial}{\partial B_{y,x}} + B_{y,y} \frac{\partial}{\partial B_{y,y}} \\ & - \alpha_x \frac{\partial}{\partial \alpha_x} - \alpha_{x,t} \frac{\partial}{\partial \alpha_{x,t}} - \alpha_{x,x} \frac{\partial}{\partial \alpha_{x,x}} - \alpha_{x,y} \frac{\partial}{\partial \alpha_{x,y}} - \alpha_y \frac{\partial}{\partial \alpha_y} - \alpha_{y,t} \frac{\partial}{\partial \alpha_{y,t}} - \alpha_{y,x} \frac{\partial}{\partial \alpha_{y,x}} - \alpha_{y,y} \frac{\partial}{\partial \alpha_{y,y}} \\ & - \beta_x \frac{\partial}{\partial \beta_x} - \beta_{x,t} \frac{\partial}{\partial \beta_{x,t}} - \beta_{x,x} \frac{\partial}{\partial \beta_{x,x}} - \beta_{x,y} \frac{\partial}{\partial \beta_{x,y}} - \beta_y \frac{\partial}{\partial \beta_y} - \beta_{y,t} \frac{\partial}{\partial \beta_{y,t}} - \beta_{y,x} \frac{\partial}{\partial \beta_{y,x}} - \beta_{y,y} \frac{\partial}{\partial \beta_{y,y}} \\ & + P \frac{\partial}{\partial P} + P_{,t} \frac{\partial}{\partial P_{,t}} + P_{,x} \frac{\partial}{\partial P_{,x}} + P_{,y} \frac{\partial}{\partial P_{,y}} - \gamma \frac{\partial}{\partial \gamma} - \gamma_{,t} \frac{\partial}{\partial \gamma_{,t}} - \gamma_{,x} \frac{\partial}{\partial \gamma_{,x}} - \gamma_{,y} \frac{\partial}{\partial \gamma_{,y}} \end{aligned}$$

→ symmetry condition $X_{\text{pr}}(L) = 0$ upon identifying $\alpha = V$, $\beta = B$, $\gamma = \tilde{P}$

The Hamiltonian Point of View

- Stephen Omohundro: Geometric Perturbation Theory in Physics, 1986

→ any dynamical system can be imbedded into a Hamiltonian system by doubling the variables

- example: Vlasov equation
  - extended Hamiltonian

$$H = g\,[h, f]$$

  - equations of motion

$$\dot{f} = +\frac{\partial H}{\partial g} - \frac{d}{dx}\frac{\partial H}{\partial g_x} - \frac{d}{dv}\frac{\partial H}{\partial g_v} = [h, f]$$

$$\dot{g} = -\frac{\partial H}{\partial f} + \frac{d}{dx}\frac{\partial H}{\partial f_x} + \frac{d}{dv}\frac{\partial H}{\partial f_v} = [h, g]$$

  - Legendre transform

$$L = \dot{f}g - H = g\,(f_t + [f, h])$$

(f: distribution function, h: particle Hamiltonian, g: adjoint variable)

Summary

- variational integrators
  - obtain discrete equations of motion by applying a discrete action principle to a discrete Lagrangian instead of discretising equations of motion directly
  - automatic preservation of multisymplectic structure and discrete momenta
  - good long-time energy behaviour, no numerical dissipation

- discrete conservation laws
  - discrete Noether theorem relates variational symmetries of the discrete Lagrangian to discrete conservation laws
  - discrete momenta are preserved exactly (in practise up to machine precision)

- embedding of dynamical systems
  - embed any dynamical system into a Lagrangian or Hamiltonian system by doubling the number of variables
  - allows for derivation of variational integrators for arbitrary systems
  - rigorous theory for determining conservation laws via extended Noether theorem
  - conservation of momentum and energy follow from invariance with respect to vertical transformations, not from transformations with respect to space and time