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Discontinuous Galerkin Variational Integrators and Discrete Dirac Mechanics

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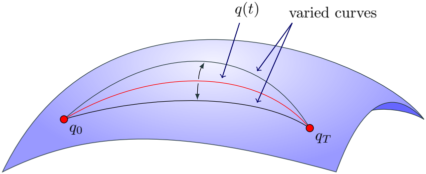
Outline

Variational Integrators

Hamilton's Principle of Stationary Action

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

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



- Hamilton's principle of stationary action: among all possible trajectories $q(t)$, the physical trajectory makes the action integral $\mathcal{A}$ stationary
- variation and integration by parts (endpoints fixed: $\delta q(0) = \delta q(T) = 0$)

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

- requiring stationarity of the action, $\delta\mathcal{A} = 0$ for arbitrary variations δq, leads to the Euler-Lagrange equations of motion

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

Discrete Lagrangian

- divide the interval $[0, T]$ into an equidistant, monotonic sequence $\{t_n\}_{n=0}^{N}$,

$$\mathcal{A}[q(t)] = \sum_{n=0}^{N-1} \int_{t_n}^{t_{n+1}} L\big(q(t), \dot{q}(t)\big)\, dt$$

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

$$L_d^{\mathrm{e}}(q_n, q_{n+1}) = \int_{t_n}^{t_{n+1}} L\big(q_{n,n+1}(t), \dot{q}_{n,n+1}(t)\big)\, dt$$

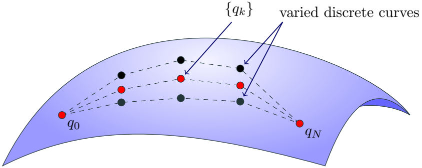
- approximate velocities $\dot{q}$ with finite differences (timestep h)

$$\dot{q} \to \frac{q_{n+1} - q_n}{h}$$

- approximate discrete Lagrangian with discrete quadrature formula

$$L_d(q_n, q_{n+1}) = h\, L\left(\frac{q_n + q_{n+1}}{2}, \frac{q_{n+1} - q_n}{h}\right) \qquad \text{(midpoint)}$$

Discrete Action and Discrete Variational Principle



- discrete action

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

- requiring stationarity of the discrete action,

$$\delta \mathcal{A}_d = \delta \sum_{n=0}^{N-1} L_d(q_n, q_{n+1}) = 0 \quad \text{for all} \quad \delta q_n$$

with $\delta q_0 = \delta q_N = 0$ leads to the discrete Euler-Lagrange equations

$$D_2 L_d(q_{n-1}, q_n) + D_1 L_d(q_n, q_{n+1}) = 0 \quad \text{for all} \quad n$$

$\rightarrow$ numerical integrator (update map)

$$\Psi_{L_d} : (q_{n-1}, q_n) \mapsto (q_n, q_{n+1})$$

- similar derivation leads to symplectic Runge-Kutta methods

Discontinuous Galerkin Variational Integrators

Hamilton-Pontryagin Principle

- Hamilton-Pontryagin principle: action principle on $\mathsf{T}\mathcal{M} \oplus \mathsf{T}^*\mathcal{M}$

$$\delta \int \Big[L(q, v) + \langle p, \dot{q} - v \rangle \Big] \, dt = 0$$

- variations of v are left free, a kinematic constraint ensures the second- order condition $v = \dot{q}$ with the momentum p as a Lagrange multiplier

  (Hamilton's action principle: variations δv are induced by variations δq)

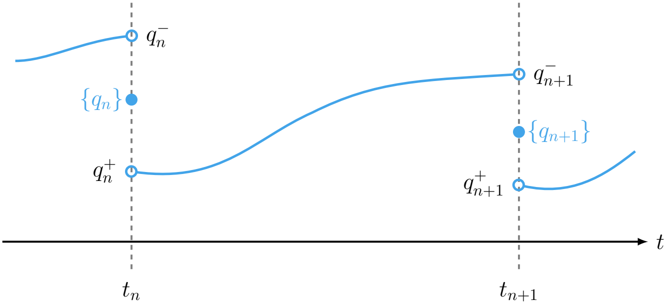
- requiring stationarity of the Hamilton-Pontryagin action,

$$\int \bigg[\frac{\partial L}{\partial q} \delta q + \frac{\partial L}{\partial v} \delta v + \langle \delta p, \dot{q} - v \rangle + \langle p, \delta \dot{q} - \delta v \rangle \bigg] \, dt = 0,$$

  leads to the implicit Euler–Lagrange equations (second-order condition, the Legendre transform, and the Euler-Lagrange equations),

$$\dot{q} = v, \qquad p = \frac{\partial L}{\partial v}, \qquad \dot{p} = \frac{\partial L}{\partial q}$$

Discontinuous Galerkin Approximation



- discrete trajectories $q_h(t)$ connecting q_0 and q_N in the time interval $[0, T]$ are elements of

$$\mathcal{Q}_h(q_0, q_N, [0, T]) = \left\{ q_h : [0, T] \to \mathcal{M} \;\middle|\; q_h|_{[t_n, t_{n+1}]} \in \mathbb{P}_s([t_n, t_{n+1}]) \right\}$$

- average operators of q_h are usually given by

$$\{q_{n+1}\} = \frac{1}{2}(q_{n+1}^- + q_{n+1}^+), \qquad \{q_{n+1}\} = q_{n+1}^-, \qquad \{q_{n+1}\} = q_{n+1}^+$$

Discrete Hamilton-Pontryagin Principle

- denote by $Q_n(t) = q_h|_{[t_n, t_{n+1}]}$, $V_n(t) = v_h|_{[t_n, t_{n+1}]}$, $P_n(t) = p_h|_{[t_n, t_{n+1}]}$
- choose quadrature rule with nodes c_i and weights b_i and set $t_{n,i} = t_n + c_i h$
- discrete Hamilton-Pontryagin principle

$$\delta \sum_{n=0}^{N-1} \left(\sum_{i=1}^{s} h b_i \Big[L\big(Q_n(t_{n,i}), V_n(t_{n,i})\big) + \big\langle P_n(t_{n,i}),\ \dot{Q}_n(t_{n,i}) - V_n(t_{n,i}) \big\rangle \Big] \right.$$
$$\left. + \text{continuity constraints or numerical flux} \right) = 0$$

- define generalised energy $E(q, v, p) = p \cdot v - L(q, v)$
- equivalent formulation of discrete Hamilton-Pontryagin principle

$$\delta \sum_{n=0}^{N-1} \left(\sum_{i=1}^{s} h b_i \Big[\big\langle P_n(t_{n,i}),\ \dot{Q}_n(t_{n,i}) \big\rangle - E\big(Q_n(t_{n,i}), V_n(t_{n,i}), P_n(t_{n,i})\big) \Big] \right.$$
$$\left. + \text{continuity constraints or numerical flux} \right) = 0$$

Discrete Hamilton-Pontryagin Principle

- discrete Hamilton-Pontryagin principle

$$\delta \sum_{n=0}^{N-1} \left(\sum_{i=1}^{s} h b_i \Big[L\big(Q_n(t_{n,i}),\, V_n(t_{n,i})\big) + \big\langle P_n(t_{n,i}),\, \dot{Q}_n(t_{n,i}) - V_n(t_{n,i}) \big\rangle \Big] + \text{continuity constraints or numerical flux} \right) = 0$$

$$\delta \sum_{n=0}^{N-1} \left(\sum_{i=1}^{s} h b_i \Big[\big\langle P_n(t_{n,i}),\, \dot{Q}_n(t_{n,i}) \big\rangle - E\big(Q_n(t_{n,i}),\, V_n(t_{n,i}),\, P_n(t_{n,i})\big) \Big] + \text{continuity constraints or numerical flux} \right) = 0$$

- continuity constraints: enforce continuity weakly via Lagrange multipliers
  → unifying framework for many existing variational integrators
- numerical flux: discontinuous Galerkin discretisation
  → new families of variational integrators

Weak Continuity

- possible continuity constraints

$$(q, Q) \qquad + \left\langle \bar{p}_n,\ q_n^+ - q_n \right\rangle + \left\langle \tilde{p}_{n+1},\ q_{n+1} - q_{n+1}^- \right\rangle$$

$$(q, P) \qquad + \left\langle \bar{p}_n,\ q_n^+ - q_n \right\rangle - \left\langle p_{n+1} - p_{n+1}^-,\ \tilde{q}_{n+1} \right\rangle$$

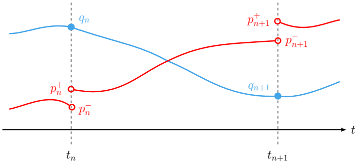
$$(p, Q) \qquad - \left\langle p_n^+ - p_n,\ \bar{q}_n \right\rangle + \left\langle \tilde{p}_{n+1},\ q_{n+1} - q_{n+1}^- \right\rangle$$

$$(p, P) \qquad - \left\langle p_n^+ - p_n,\ \bar{q}_n \right\rangle - \left\langle p_{n+1} - p_{n+1}^-,\ \tilde{q}_{n+1} \right\rangle$$

- resulting continuity of p and q

	p	q	Gen. Func.
(q, Q)	double discontinuous	left-right-continuous	Type 1
(q, P)	right-continuous	left-continuous	Type 2
(p, Q)	left-continuous	right-continuous	Type 3
(p, P)	left-right-continuous	double discontinuous	Type 4

Lagrangian VIs (Type 1 Generating Functions)



- piecewise linear/constant discretisation of $q(t)$, $v(t)$, $p(t)$

$$q_h(t)|_{[t_n, t_{n+1}]} = \frac{t_{n+1} - t}{t_{n+1} - t_n} \, q_n^+ + \frac{t - t_n}{t_{n+1} - t_n} \, q_{n+1}^-,$$

$$v_h(t)|_{[t_n, t_{n+1}]} = v_{n+1/2},$$

$$p_h(t)|_{[t_n, t_{n+1}]} = p_{n+1/2}$$

- trapezoidal quadrature and (q, Q) continuity constraint

$$\delta \sum_{n=0}^{N-1} \left(\frac{h}{2} \Big[L\big(q_n^+, v_{n+1/2}\big) + L\big(q_{n+1}^-, v_{n+1/2}\big) \Big] + h \left\langle p_{n+1/2}, \, \frac{q_{n+1}^- - q_n^+}{h} - v_{n+1/2} \right\rangle + \big\langle \bar{p}_n \, , \, q_n^+ - q_n \big\rangle + \big\langle \tilde{p}_{n+1} \, , \, q_{n+1} - q_{n+1}^- \big\rangle \right) = 0$$

Lagrangian VIs (Type 1 Generating Functions)

- variations

$$
\begin{aligned}
\delta q_n^+ :& \qquad p_{n+1/2} = \bar{p}_n - \frac{h}{2}\frac{\partial L}{\partial q}(q_n, v_{n+1/2}), \\
\delta q_{n+1}^- :& \qquad \tilde{p}_{n+1} = p_{n+1/2} + \frac{h}{2}\frac{\partial L}{\partial q}(q_{n+1}^-, v_{n+1/2}), \\
\delta v_{n+1/2} :& \qquad p_{n+1/2} = \frac{1}{2}\left[\frac{\partial L}{\partial v}(q_n^+, v_{n+1/2}) + \frac{\partial L}{\partial v}(q_{n+1}^-, v_{n+1/2})\right], \\
\delta p_{n+1/2} :& \qquad q_{n+1}^- = q_n^+ + h\, v_{n+1/2}, \\
\delta \bar{p}_n :& \qquad q_n^+ = q_n, \\
\delta \tilde{p}_{n+1} :& \qquad q_{n+1} = q_{n+1}^-, \\
\delta q_n :& \qquad \bar{p}_n = \tilde{p}_n = p_n
\end{aligned}
$$

Lagrangian VIs (Type 1 Generating Functions)

- generalised Störmer-Verlet method

$$
\begin{aligned}
p_{n+1/2} &= \frac{1}{2}\left[\frac{\partial L}{\partial v}(q_n, v_{n+1/2}) + \frac{\partial L}{\partial v}(q_{n+1}, v_{n+1/2})\right], \\
p_{n+1/2} &= p_n - \frac{h}{2}\frac{\partial L}{\partial q}(q_n, v_{n+1/2}), \\
q_{n+1} &= q_n + h\, v_{n+1/2}, \\
p_{n+1} &= p_{n+1/2} + \frac{h}{2}\frac{\partial L}{\partial q}(q_{n+1}, v_{n+1/2})
\end{aligned}
$$

Lagrangian VIs (Type 1 Generating Functions)

- eliminating all auxiliary variables, we obtain

$$p_n = -\frac{h}{2}\Big[\frac{\partial L}{\partial q}\left(q_n, \frac{q_{n+1}-q_n}{h})\right) - \frac{1}{h}\frac{\partial L}{\partial v}\left(q_n, \frac{q_{n+1}-q_n}{h})\right) - \frac{1}{h}\frac{\partial L}{\partial v}\left(q_{n+1}, \frac{q_{n+1}-q_n}{h})\right)\Big],$$

$$p_{n+1} = \frac{h}{2}\Big[\frac{\partial L}{\partial q}\left(q_{n+1}, \frac{q_{n+1}-q_n}{h})\right) + \frac{1}{h}\frac{\partial L}{\partial v}\left(q_n, \frac{q_{n+1}-q_n}{h})\right) + \frac{1}{h}\frac{\partial L}{\partial v}\left(q_{n+1}, \frac{q_{n+1}-q_n}{h})\right)\Big],$$

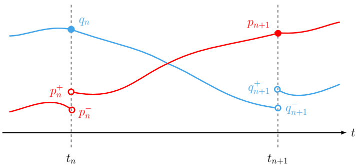
→ position-momentum form,

$$p_n = -D_1 L_d(q_n, q_{n+1}), \qquad p_{n+1} = D_2 L_d(q_n, q_{n+1}),$$

of the variational integrator corresponding to the discrete Lagrangian

$$L_d(q_n, q_{n+1}) = \frac{h}{2}\left[L\left(q_n, \frac{q_{n+1}-q_n}{h})\right) + L\left(q_{n+1}, \frac{q_{n+1}-q_n}{h})\right)\right]$$

Hamiltonian VIs (Type 2 Generating Functions)



- piecewise constant discretisation of $q(t)$, $v(t)$, $p(t)$

$$
\begin{aligned}
q_h(t)|_{[t_n, t_{n+1}]} &= q_n^+, \\
v_h(t)|_{[t_n, t_{n+1}]} &= v_n^+, \\
p_h(t)|_{[t_n, t_{n+1}]} &= p_{n+1}^-
\end{aligned}
$$

- trapezoidal quadrature and (q, P) continuity constraint

$$
\delta \sum_{n=0}^{N-1} \left(h \left[L\big(q_n^+, v_n^+\big) + \left\langle p_{n+1}^-, \, \frac{q_{n+1} - q_n^+}{h} - v_n^+ \right\rangle \right] + \big\langle p_n, \, q_n^+ - q_n \big\rangle \right) = 0
$$

Hamiltonian VIs (Type 2 Generating Functions)

- piecewise constant and (q, P) continuity constraint

$$\delta \sum_{n=0}^{N-1} \left(h \left[L(q_n^+, v_n^+) + \left\langle p_{n+1}^-, \, \frac{q_{n+1} - q_n^+}{h} - v_n^+ \right\rangle \right] + \left\langle p_n, \, q_n^+ - q_n \right\rangle \right) = 0$$

- variations

$$\begin{aligned}
\delta q_n^+ : &\qquad p_{n+1}^- = p_n + h \frac{\partial L}{\partial q}(q_n^+, v_n^+), \\
\delta v_n^+ : &\qquad p_{n+1}^- = \frac{\partial L}{\partial v}(q_n^+, v_n^+), \\
\delta p_{n+1}^- : &\qquad q_{n+1} = q_n^+ + h \, v_n^+, \\
\delta p_n : &\qquad q_n^+ = q_n, \\
\delta q_{n+1} : &\qquad p_{n+1} = p_{n+1}^-
\end{aligned}$$

Hamiltonian VIs (Type 2 Generating Functions)

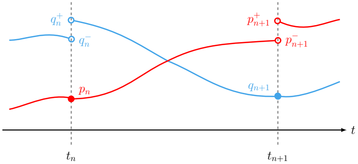
- discrete generalised energy (setting $v_n = v_n^+$)

$$E(q_n, v_n, p_{n+1}) = p_{n+1} v_n - L(q_n, v_n)$$

- generalised symplectic Euler-B method

$$\begin{aligned} p_{n+1} &= p_n + h \frac{\partial E}{\partial q}(q_n, v_n, p_{n+1}), \\ q_{n+1} &= q_n + h \frac{\partial E}{\partial p}(q_n, v_n, p_{n+1}), \\ 0 &= \frac{\partial E}{\partial v}(q_n, v_n, p_{n+1}), \end{aligned}$$

Hamiltonian VIs (Type 3 Generating Functions)



- piecewise constant discretisation of $q(t)$, $v(t)$, $p(t)$

$$q_h(t)|_{[t_n,t_{n+1}]} = q_{n+1}^-,$$
$$v_h(t)|_{[t_n,t_{n+1}]} = v_{n+1}^-,$$
$$p_h(t)|_{[t_n,t_{n+1}]} = p_n^+$$

- trapezoidal quadrature and (q, P) continuity constraint

$$\delta \sum_{n=0}^{N-1} \left(h \left[L(q_{n+1}^-, v_{n+1}^-) + \left\langle p_n^+, \, \frac{q_{n+1}^- - q_n}{h} - v_{n+1}^- \right\rangle \right] + \left\langle p_{n+1}, \, q_{n+1} - q_{n+1}^- \right\rangle \right) = 0$$

Hamiltonian VIs (Type 3 Generating Functions)

- piecewise constant and (q, P) continuity constraint

$$\delta \sum_{n=0}^{N-1} \left(h \left[L\big(q_{n+1}^-, v_{n+1}^-\big) + \left\langle p_n^+, \, \frac{q_{n+1}^- - q_n}{h} - v_{n+1}^- \right\rangle \right] + \left\langle p_{n+1}, \, q_{n+1} - q_{n+1}^- \right\rangle \right) = 0$$

- variations

$$\delta q_{n+1}^- : \qquad p_{n+1} = p_n^+ + h \, \frac{\partial L}{\partial q}(q_{n+1}^-, v_{n+1}^-),$$

$$\delta v_{n+1}^- : \qquad p_n^+ = \frac{\partial L}{\partial v}(q_{n+1}^-, v_{n+1}^-),$$

$$\delta p_n^+ : \qquad q_{n+1}^- = q_n + h \, v_{n+1}^-,$$

$$\delta p_{n+1} : \qquad q_{n+1}^- = q_{n+1},$$

$$\delta q_n : \qquad p_n = p_n^+$$

Hamiltonian VIs (Type 3 Generating Functions)

- discrete generalised energy (setting $v_{n+1} = v_{n+1}^-$)

$$E(q_{n+1}, v_{n+1}, p_n) = p_n v_{n+1} - L(q_{n+1}, v_{n+1})$$

- generalised symplectic Euler-A method

$$\begin{aligned} p_{n+1} &= p_n + h \frac{\partial E}{\partial q}(q_{n+1}, v_{n+1}, p_n), \\ q_{n+1} &= q_n + h \frac{\partial E}{\partial p}(q_{n+1}, v_{n+1}, p_n), \\ 0 &= \frac{\partial E}{\partial v}(q_{n+1}, v_{n+1}, p_n) \end{aligned}$$

Momentum VIs (Type 4 Generating Functions)

- piecewise linear/constant discretisation of $q(t)$, $v(t)$, $p(t)$

$$
\begin{aligned}
q_h(t)\big|_{[t_n, t_{n+1}]} &= q_{n+1/2}, \\
v_h(t)\big|_{[t_n, t_{n+1}]} &= \frac{t_{n+1} - t}{t_{n+1} - t_n}\, v_n^+ + \frac{t - t_n}{t_{n+1} - t_n}\, v_{n+1}^-, \\
p_h(t)\big|_{[t_n, t_{n+1}]} &= \frac{t_{n+1} - t}{t_{n+1} - t_n}\, p_n^+ + \frac{t - t_n}{t_{n+1} - t_n}\, p_{n+1}^-
\end{aligned}
$$

- trapezoidal quadrature and (q, Q) continuity constraint

$$
\begin{aligned}
\delta \sum_{n=0}^{N-1} \Bigg(& \frac{h}{2} \Big[L\big(q_{n+1/2}, v_n^+\big) + \left\langle p_n^+, \, \frac{q_{n+1/2} - \bar{q}_n}{h/2} - v_n^+ \right\rangle \\
& + L\big(q_{n+1/2}, v_{n+1}^-\big) + \left\langle p_{n+1}^-, \, \frac{\tilde{q}_{n+1} - q_{n+1/2}}{h/2} - v_{n+1}^- \right\rangle \Big] \\
& + \langle p_n \,, \, \bar{q}_n \rangle - \langle p_{n+1} \,, \, \tilde{q}_{n+1} \rangle \Bigg) = 0
\end{aligned}
$$

Momentum VIs (Type 4 Generating Functions)

$$\delta q_{n+1/2}: \quad p_{n+1}^- = p_n^+ + \frac{h}{2}\left[\frac{\partial L}{\partial q}(q_{n+1/2}, v_n^+) + \frac{\partial L}{\partial q}(q_{n+1/2}, v_{n+1}^-)\right],$$

$$\delta v_n^+: \quad p_n^+ = \frac{\partial L}{\partial v}(q_{n+1/2}, v_n^+),$$

$$\delta v_{n+1}^-: \quad p_{n+1}^- = \frac{\partial L}{\partial v}(q_{n+1/2}, v_{n+1}^-),$$

$$\delta p_n^+: \quad q_{n+1/2} = \bar{q}_n + \frac{h}{2}\, v_n^+,$$

$$\delta p_{n+1}^-: \quad \tilde{q}_{n+1} = q_{n+1/2} + \frac{h}{2}\, v_{n+1}^-,$$

$$\delta \bar{q}_n: \quad p_n^+ = p_n,$$

$$\delta \tilde{q}_{n+1}: \quad p_{n+1} = p_{n+1}^-,$$

$$\delta p_n: \quad \bar{q}_n = \tilde{q}_n = q_n$$

Momentum VIs (Type 4 Generating Functions)

- generalised Störmer-Verlet method

$$
\begin{aligned}
p_n &= \frac{\partial L}{\partial v}(q_{n+1/2}, v_n^+), \\
q_{n+1/2} &= q_n + \frac{h}{2}\, v_n^+, \\
p_{n+1} &= p_n + \frac{h}{2}\left[\frac{\partial L}{\partial q}(q_{n+1/2}, v_n^+) + \frac{\partial L}{\partial q}(q_{n+1/2}, v_{n+1}^-)\right], \\
p_{n+1} &= \frac{\partial L}{\partial v}(q_{n+1/2}, v_{n+1}^-), \\
q_{n+1} &= q_{n+1/2} + \frac{h}{2}\, v_{n+1}^-,
\end{aligned}
$$

Degenerate Lagrangians and Dirac Constraints

Degenerate Lagrangian Systems

- consider degenerate Lagrangian systems linear in velocities

$$L(q, \dot{q}) = \alpha(q) \cdot \dot{q} - H(q), \qquad\qquad L : \mathsf{T}\mathcal{M} \to \mathbb{R},$$

  where α is a general, possibly nonlinear function of q

- Euler-Lagrange equations: ordinary differential equations of first order

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

  explicitly,

$$\alpha_{j,i}(q)\, \dot{q}^j - H_{,i}(q) - \frac{d}{dt}\alpha_i(q) = 0$$

- computing the time-derivative of α, the system can be rewritten with the noncanonical symplectic matrix,

$$\frac{d}{dt}\alpha_i(q) = \alpha_{i,j}(q)\, \dot{q}^j, \qquad \bar{\Omega}(q)\, \dot{q} = \nabla H(q), \qquad \bar{\Omega}_{ij}(q) = \alpha_{j,i}(q) - \alpha_{i,j}(q)$$

Constrained Dynamical Systems

- consider an extended dynamical system (q, p) whose dynamics is constrained to a subspace defined by

$$\phi(q, p) = p - \alpha(q) = 0$$

- constitutes an index 2 DAE

$$\begin{aligned} \dot{z} &= \Omega^{-1} \big(\nabla H(z) + \nabla \phi^T(z) \, \lambda \big), \\ 0 &= \phi(z), \end{aligned} \qquad z = (q, p), \qquad \Omega = \begin{pmatrix} \mathbb{0} & -\mathbb{1} \\ \mathbb{1} & \mathbb{0} \end{pmatrix}$$

- this system of DAEs is obtained from a Hamilton-Pontryagin principle

$$\delta \int \Big[L(q, \lambda) + p \, \big(\dot{q} - \lambda \big) \Big] \, dt = 0$$

- if the constraint $\phi(q, p) = 0$ is satisfied, the canonical symplectic form $\mathsf{d}q^i \wedge \mathsf{d}p_i$ is equivalent to the noncanonical symplectic form $\bar{\Omega}_{ij}(q) \, \mathsf{d}q^i \wedge \mathsf{d}q^j$

- embedding of noncanonical Lagrangian or Hamiltonian systems into canonical Hamiltonian systems of twice the size subject to a constraint

Constrained Dynamical Systems

- standard variational integrators will in general not satisfy the constraint

$$\phi(q, p) = p - \alpha(q)$$

- Dirac constraints $\phi(q, p) = 0$ (primary constraint)
  - symplectic projection of unconstrained integrators (generating functions, SPARK methods, discrete Lagrange-d'Alembert-Pontryagin principle)
  - variational integrators for formal Lagrangians of noncanonical Hamiltonian systems (gauge-invariant but not symplectic)
  - gauge-invariant variational integrators with exact or approximate quadrature
  - truly discrete tangent bundle based on Galerkin discretisation, preserving degeneracy of Lagrangian (generalisation / more systematic version of difference discrete variational principle with summation by parts rule)
  - discontinuous Galerkin variational integrators (Lagrangian one-step methods, Hamiltonian integrators with projection, Hamilton-Pontryagin integrators)

Dynamics on the Configuration Bundle

- degenerate Lagrangian linear in velocities

$$L(q, \dot{q}) = \alpha(q) \cdot \dot{q} - H(q),$$

- simple (piecewise linear) discretisation of the trajectory $q(t)$

$$q_h(t)|_{(t_n, t_{n+1})} = \frac{t_{n+1} - t}{t_{n+1} - t_n} \, q_n^+ + \frac{t - t_n}{t_{n+1} - t_n} \, q_{n+1}^-,$$

- discrete velocity

$$\dot{q}_h(t)|_{(t_n, t_{n+1})} = \frac{q_{n+1}^- - q_n^+}{t_{n+1} - t_n},$$

- jump and average operators

$$[\![q_{n+1}]\!] = \tfrac{1}{h}(q_{n+1}^+ - q_{n+1}^-), \qquad \{ q_{n+1} \} = \tfrac{1}{2}(q_{n+1}^- + q_{n+1}^+),$$

- numerical flux

$$[\![q_{n+1}]\!] \, \alpha(\{ q_{n+1} \})$$

Dynamics on the Configuration Bundle (Midpoint Rule)

- discrete action (midpoint rule)

$$\mathcal{A}_d[q_h] = h \sum_{n=0}^{N-1} \Big[\alpha\big(\tfrac{1}{2}(q_n^+ + q_{n+1}^-)\big) \cdot \frac{q_{n+1}^- - q_n^+}{h} - h\big(\tfrac{1}{2}(q_n^+ + q_{n+1}^-)\big) + \tfrac{1}{h}(q_{n+1}^+ - q_{n+1}^-) \cdot \alpha\big(\tfrac{1}{2}(q_{n+1}^- + q_{n+1}^+)\big) \Big]$$

- discrete Euler-Lagrange equations

$$\alpha(q_{n+1/2}) = \alpha(\{q_n\}) + \tfrac{h}{2} \nabla\alpha(q_{n+1/2}) \cdot \frac{q_{n+1}^- - q_n^+}{h} - \tfrac{h}{2} \nabla H(q_{n+1/2}) - \tfrac{h}{2} [\![q_n]\!] \cdot \nabla\alpha^T(\{q_n\}),$$

$$\alpha(\{q_{n+1}\}) = \alpha(\{q_n\}) + h\nabla\alpha(q_{n+1/2}) \cdot \frac{q_{n+1}^- - q_n^+}{h} - h\nabla H(q_{n+1/2}) - \tfrac{h}{2} [\![q_n]\!] \cdot \nabla\alpha^T(\{q_n\}) - \tfrac{h}{2} [\![q_{n+1}]\!] \cdot \nabla\alpha^T(\{q_{n+1}\}),$$

with

$$q_{n+1/2} = \tfrac{1}{2}(q_n^+ + q_{n+1}^-), \quad q_n^+ = \{q_n\} + \tfrac{h}{2} [\![q_n]\!], \quad \{q_{n+1}\} = q_{n+1}^- + \tfrac{h}{2} [\![q_{n+1}]\!]$$

Dynamics on the Configuration Bundle (Midpoint Rule)

→ projection with the jump operator acting like a Lagrange multiplier

- setting $p_n = \alpha(q_n)$, the algorithm can be expressed as

$$
\begin{aligned}
q_n^+ &= q_n + \tfrac{h}{2} [\![q_n]\!] , \\
p_n^+ &= p_n - \tfrac{h}{2} [\![q_n]\!] \cdot \nabla\alpha^T(q_n), \\
p_{n+1/2} &= p_n^+ + \tfrac{h}{2} \nabla\alpha(q_{n+1/2}) \cdot \frac{q_{n+1}^- - q_n^+}{h} - \tfrac{h}{2} \nabla H(q_{n+1/2}), \\
p_{n+1}^- &= p_n^+ + h\nabla\alpha(q_{n+1/2}) \cdot \frac{q_{n+1}^- - q_n^+}{h} - h\nabla H(q_{n+1/2}), \\
q_{n+1} &= q_{n+1}^- + \tfrac{h}{2} [\![q_{n+1}]\!] , \\
p_{n+1} &= p_{n+1}^- - \tfrac{h}{2} [\![q_{n+1}]\!] \cdot \nabla\alpha^T(q_{n+1}),
\end{aligned}
$$

with

$$
q_{n+1/2} = \tfrac{1}{2}(q_n^+ + q_{n+1}^-), \qquad p_{n+1/2} = \alpha(q_{n+1/2}), \qquad p_{n+1} = \alpha(q_{n+1})
$$

Dynamics on the Cotangent Bundle

- phasespace action $\mathcal{A}[q,p]$ subject to the constraint $\phi(q,p)=0$

$$\mathcal{A}[q,p] = \int_0^T \left[p \cdot \dot{q} - H(q,p) - \lambda^T \phi(q,p) \right] dt,$$

- simple (piecewise linear) discretisation of the generalised coordinates $q(t)$ and conjugate momenta $p(t)$

$$q_h(t)|_{(t_n,t_{n+1})} = \frac{t_{n+1}-t}{t_{n+1}-t_n}\, q_n^+ + \frac{t-t_n}{t_{n+1}-t_n}\, q_{n+1}^-,$$
$$p_h(t)|_{(t_n,t_{n+1})} = \frac{t_{n+1}-t}{t_{n+1}-t_n}\, p_n^+ + \frac{t-t_n}{t_{n+1}-t_n}\, p_{n+1}^-,$$

- jump and average operators for q and p

$$[\![q_{n+1}]\!] = (q_{n+1}^+ - q_{n+1}^-), \qquad \{q_{n+1}\} = \tfrac{1}{2}(q_{n+1}^- + q_{n+1}^+),$$
$$[\![p_{n+1}]\!] = (p_{n+1}^+ - p_{n+1}^-), \qquad \{p_{n+1}\} = \tfrac{1}{2}(p_{n+1}^- + p_{n+1}^+),$$

- numerical flux and constraint

$$[\![q_{n+1}]\!] \{p_{n+1}\}, \qquad \phi(\{q_{n+1}\}, \{p_{n+1}\}) = 0$$

Dynamics on the Cotangent Bundle (Midpoint Rule)

- discrete phasespace action (trapezoidal rule)

$$\mathcal{A}_d[q_h, p_h, \lambda_h] = h \sum_{n=0}^{N-1} \Bigg[\frac{p_n^+ + p_{n+1}^-}{2} \cdot \frac{q_{n+1}^- - q_n^+}{h} - H\bigg(\frac{q_n^+ + q_{n+1}^-}{2}, \frac{p_n^+ + p_{n+1}^-}{2} \bigg) + [\![q_{n+1}]\!] \left\{ p_{n+1} \right\} - \lambda_{n+1}^T \phi(\left\{ q_{n+1} \right\}, \left\{ p_{n+1} \right\}) \Bigg]$$

- discrete Hamilton's equations

$$\begin{aligned}
q_{n+1/2} &= \{ q_n \} + h\, H_p(q_{n+1/2}, p_{n+1/2}) + h\, \lambda_n^T \phi_p(\{ q_n \}, \{ p_n \}), \\
p_{n+1/2} &= \{ p_n \} - h\, H_q(q_{n+1/2}, p_{n+1/2}) - h\, \lambda_n^T \phi_q(\{ q_n \}, \{ p_n \}), \\
\{ q_{n+1} \} &= q_{n+1/2} + h\, H_p(q_{n+1/2}, p_{n+1/2}) + h\, \lambda_{n+1}^T \phi_p(\{ q_{n+1} \}, \{ p_{n+1} \}), \\
\{ p_{n+1} \} &= p_{n+1/2} - h\, H_q(q_{n+1/2}, p_{n+1/2}) - h\, \lambda_{n+1}^T \phi_q(\{ q_{n+1} \}, \{ p_{n+1} \}), \\
0 &= \phi(\{ q_{n+1} \}, \{ p_{n+1} \}), \\
q_{n+1/2} &= \tfrac{1}{2}(q_n^+ + q_{n+1}^-), \\
p_{n+1/2} &= \tfrac{1}{2}(p_n^+ + p_{n+1}^-)
\end{aligned}$$

Summary and Outlook

Summary and Outlook

- discontinuous Galerkin variational integrators provide a unified framework for many known but disparate methods
- ingredients: polynomial space, quadrature rule, continuity/jump condition
- open up new horizons for structure preserving discretisation
  - one-step methods for degenerate Lagrangians
  - projection methods for Hamiltonian systems subject to Dirac constraints
  - Lagrangian splitting methods
- next steps
  - implementation in GeomDAE.jl and verification of conservation properties
  - analysis of discrete Dirac structure (generalisation of symplectic structure)
  - extension to interconnected systems and multi-Dirac structures (PDEs)
- ongoing and complementary work
  - gauge-invariant variational integrators with exact and approximate quadrature
  - Isogeometric Euler-Poincaré and Lie-Dirac reduction (Eulerian discretisations)
  - Isogeometric/Galerkin discretisation of tangent and jet bundles (multispaces)