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Hamilton–Pontryagin–Galerkin Integrators

Unifying Continuous and Discontinuous Galerkin Variational Integrators

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Outline

1. Variational Integrators
2. Hamilton–Pontryagin–Galerkin Integrators
3. Some Examples: Old and New
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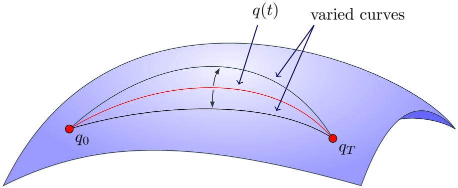
Variational Integrators

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 $q(t)$ between two points q_0 and 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

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

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 trajectory, e.g., via linear interpolation between q_n and q_{n+1}

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

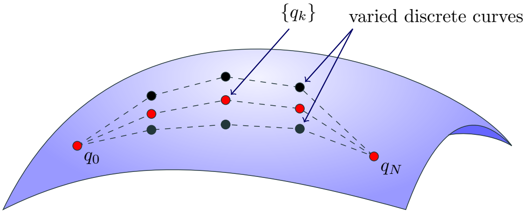
- approximate discrete Lagrangian with discrete quadrature formula (c_i, b_i)

$$L_d(q_n, q_{n+1}) = h \sum_{i=1}^{s} b_i\, L\big(q_h(t_n + c_i h), \dot{q}_h(t_n + c_i h)\big), \qquad h = t_{n+1} - t_n,$$

$$L_d^{\mathrm{tr}}(q_n, q_{n+1}) = \frac{h}{2}\left[L\left(q_n, \frac{q_{n+1} - q_n}{h}\right) + L\left(q_{n+1}, \frac{q_{n+1} - q_n}{h}\right)\right] \qquad \text{(trapezoidal)}$$

- ingredients: polynomial space for approximation of q or v and quadrature rule

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

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

- use discrete fibre derivatives $(\mathbb{F}^-, \mathbb{F}^+)$ to define momenta

$$\begin{aligned} p_n &= \mathbb{F}^- L_d(q_n, q_{n+1}) = -D_1 L_d(q_n, q_{n+1}), \\ p_{n+1} &= \mathbb{F}^+ L_d(q_n, q_{n+1}) = D_2 L_d(q_n, q_{n+1}) \end{aligned}$$

- note that the discrete Euler–Lagrange equations can be expressed as

$$\mathbb{F}^+ L_d(q_{n-1}, q_n) = \mathbb{F}^- L_d(q_n, q_{n+1})$$

Generating Functions

- position-momentum form of the variational integrator

$$
\begin{aligned}
p_n &= -D_1 L_d(q_n, q_{n+1}), \\
p_{n+1} &= D_2 L_d(q_n, q_{n+1})
\end{aligned}
$$

→ the discrete Lagrangian plays the role of a Type 1 generating function

- similarly, the discrete Hamiltonians H_d^+ and H_d^- in Hamiltonian variational integrators (Leok & Zhang, IMA JNA 2011) correspond to Type 2 or Type 3 generating functions

- generating function types

Type 1	$S(q, Q)$	$p = D_1 S(q, Q)$,	$P = D_2 S(q, Q)$	L_d
Type 2	$S(q, P)$	$p = D_1 S(q, P)$,	$Q = D_2 S(q, P)$	H_d^+
Type 3	$S(p, Q)$	$q = D_1 S(p, Q)$,	$P = D_2 S(p, Q)$	H_d^-
Type 4	$S(p, P)$	$q = D_1 S(p, P)$,	$Q = D_2 S(p, P)$	?

- gaps in current state of the theory
  - no unified treatment of discrete Lagrangian and Hamiltonian mechanics
  - no equivalent to Type 4 generating functions

Degenerate Lagrangians

- degenerate Lagrangian linear in velocities

$$L(q, \dot{q}) = \vartheta(q) \cdot \dot{q} - H(q) \qquad \text{with} \qquad \det \left| \frac{\partial^2 L}{\partial \dot{q}^i \, \partial \dot{q}^j} \right| = 0$$

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

$$\bar{\Omega}\big(q(t)\big)\, \dot{q}(t) = \nabla H\big(q(t)\big) \qquad \text{with} \qquad \bar{\Omega}_{ij} = \vartheta_{j,i} - \vartheta_{i,j}$$

- discrete Lagrangian, e.g., trapezoidal

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

- the discrete Euler-Lagrange equations correspond to multi-step integrators

$$D_2 L_d(q_{n-1}, q_n) + D_1 L_d(q_n, q_{n+1}) = 0 \quad \Rightarrow \quad \Psi_{L_d} : (q_{n-1}, q_n) \mapsto (q_n, q_{n+1})$$

→ initialisation deficit: we need two sets of initial data even though we have first order ODEs

→ susceptible to parasitic modes driving simulations unstable

Position-Momentum Form

- use discrete fibre derivative to obtain position-momentum form

$$\begin{aligned} p_n &= -D_1 L_d(q_n, q_{n+1}), \\ p_{n+1} &= D_2 L_d(q_n, q_{n+1}) \end{aligned}$$

- can be solved as the discrete Lagrangian L_d is not degenerate

$$\det \left| \frac{\partial^2 L_d}{\partial q_n^i \, \partial q_{n+1}^j} \right| \neq 0$$

- the continuous fibre derivative provides an exact initialisation mechanism given q_0

$$p_0 = \frac{\partial L}{\partial \dot{q}}(q_0) = \vartheta(q_0)$$

- position-momentum form: rewrite the equations of motion as an index 2 DAE

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

- the numerical solution drifts away from the constraint submanifold defined by $\phi(q, p) = 0$

Position-Momentum Form

- position-momentum form: rewrite the equations of motion as an index 2 DAE

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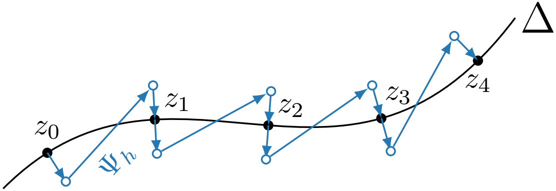
- the numerical solution drifts away from the constraint submanifold defined by $\phi(q, p) = 0$
- symmetric projection methods lead to long-time stable integrators, but are not variational



- gaps in current state of the theory
  - the Lagrangian framework is not susceptible to discontinuous Galerkin discretisations

Hamilton–Pontryagin–Galerkin Integrators

Hamilton–Pontryagin Principle

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

$$\delta \int_0^T \Big[L(q, v) + \langle p, \dot{q} - v \rangle \Big] \, dt = 0$$

- requiring stationarity of the Hamilton–Pontryagin action, leads to the implicit Euler–Lagrange equations (second-order condition, the fibre derivative, and the Euler-Lagrange equations)

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

- equivalently, we can introduce the generalised energy

$$E(q, v, p) = \langle p, v \rangle - L(q, v),$$

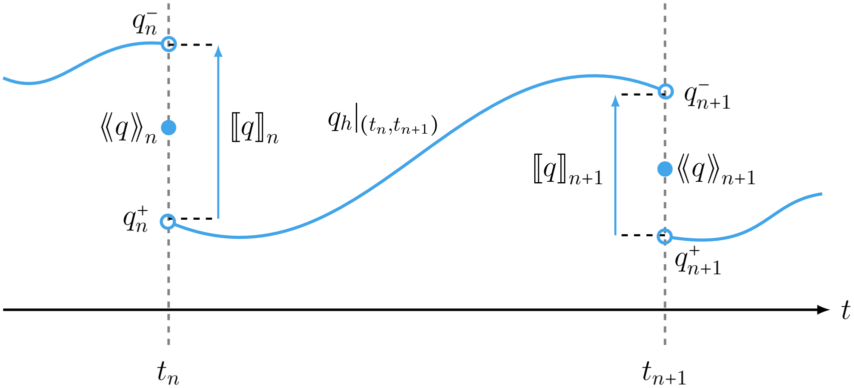
and rewrite the Hamilton–Pontryagin principle as

$$\delta \int_0^T \Big[\langle p, \dot{q} \rangle - E(q, v, p) \Big] \, dt = 0$$

- requiring stationarity leads to the generalised Hamilton equations

$$\dot{q} = \frac{\partial E}{\partial p}(q, v, p), \qquad \frac{\partial E}{\partial v} = 0, \qquad \dot{p} = -\frac{\partial E}{\partial q}(q, v, p)$$

Discontinuous Galerkin Approximation



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

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

and similarly $v_h(t)$ and $p_h(t)$

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

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

$$\left. + \text{continuity constraints or numerical flux} \right) = 0$$

- 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

Continuity Constraints

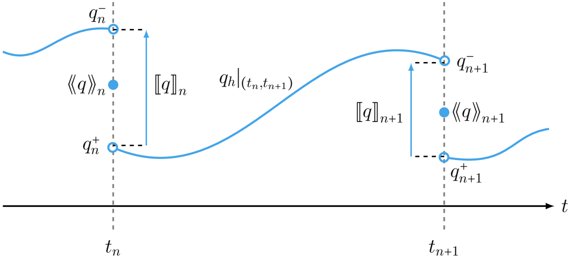
- possible continuity constraints ($q_{n+1}^- = \lim_{t \uparrow t_{n+1}} Q_n(t)$, $q_{n+1}^+ = \lim_{t \downarrow t_{n+1}} Q_{n+1}(t)$, etc.)

Type 1	(q, Q)	$+\langle p_n,\ q_n^+ - q_n \rangle + \langle \hat{p}_n,\ q_n - q_n^- \rangle$
Type 2	(q, P)	$+\langle p_n,\ q_n^+ - q_n \rangle + \langle p_n^-,\ q_n - q_n^- \rangle$
Type 3	(p, Q)	$+\langle p_n^+,\ q_n^+ - q_n \rangle + \langle p_n,\ q_n - q_n^- \rangle$
Type 4	(p, P)	$+\langle p_n^+,\ q_n^+ - q_n \rangle + \langle p_n^-,\ \hat{q}_n - q_n^- \rangle + \langle p_n,\ q_n - \hat{q}_n \rangle$

- resulting continuity of p and q

Continuity		q	p
Type 1	(q, Q)	doubly continuous	doubly discontinuous
Type 2	(q, P)	left-continuous	right-continuous
Type 3	(p, Q)	right-continuous	left-continuous
Type 4	(p, P)	doubly discontinuous	doubly continuous

Discontinuity and Numerical Fluxes



- discontinuous Hamilton–Pontryagin–Galerkin principle with numerical flux

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

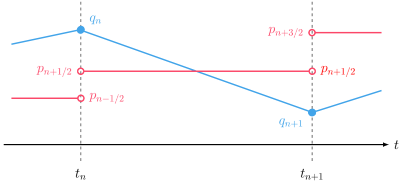
- numerical flux motivated by regularisation with average and jump operators

$$[\mathsf{flux}] = \big\langle \langle\!\langle p \rangle\!\rangle_n ,\, [\![q]\!]_n \big\rangle, \qquad \langle\!\langle p \rangle\!\rangle_n = (1-\alpha)\, p_n^- + \alpha\, p_n^+, \qquad [\![q]\!]_n = q_n^+ - q_n^-$$

→ new families of discontinuous Galerkin variational integrators

Some Examples: Old and New

Type 1 Continuity Constraints



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

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

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

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

- trapezoidal quadrature and Type 1 (q, Q) continuity constraint

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

$$+ \big\langle p_n \,,\, q_n^+ - q_n \big\rangle + \big\langle \hat{p}_{n+1} \,,\, q_{n+1} - q_{n+1}^- \big\rangle \Bigg) = 0$$

Type 1 Continuity Constraints

- Hamilton–Pontryagin–Galerkin principle with Type 1 continuity constraints

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

$$\left. + \left\langle p_n\,,\, q_n^+ - q_n\right\rangle + \left\langle \hat{p}_{n+1}\,,\, q_{n+1} - q_{n+1}^-\right\rangle \right) = 0$$

- generalised Störmer-Verlet method

$$p_{n+1/2} = \frac{1}{2}\left[\frac{\partial L}{\partial v}(q_n, v_{n+1/2}) + \frac{\partial L}{\partial v}(q_{n+1}, v_{n+1/2})\right],$$

$$p_{n+1/2} = p_n - \frac{h}{2}\frac{\partial L}{\partial q}(q_n, v_{n+1/2}),$$

$$q_{n+1} = q_n + h\, v_{n+1/2},$$

$$p_{n+1} = p_{n+1/2} + \frac{h}{2}\frac{\partial L}{\partial q}(q_{n+1}, v_{n+1/2})$$

Type 1 Continuity Constraints

- eliminating all auxiliary variables, we obtain

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

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

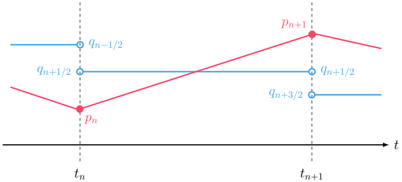
→ position-momentum form,

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

of the variational integrator corresponding to the trapezoidal Lagrangian

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

Type 4 Continuity Constraints



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

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

- trapezoidal quadrature and Type 4 (p, P) continuity constraint

$$
\delta \sum_{n=0}^{N-1} \Bigg(\frac{h}{2} \left[L\big(q_{n+1/2}, v_n^+\big) + L\big(q_{n+1/2}, v_{n+1}^-\big) \right] - \frac{h}{2} \left[\big\langle p_n^+,\, v_n^+ \big\rangle + \big\langle p_{n+1}^-,\, v_{n+1}^- \big\rangle \right]
$$

$$
+ \big\langle p_n^+,\, q_{n+1/2} - q_n \big\rangle + \big\langle p_{n+1}^-,\, \hat{q}_{n+1} - q_{n+1/2} \big\rangle + \big\langle p_n,\, q_n - \hat{q}_n \big\rangle \Bigg) = 0
$$

Type 4 Continuity Constraints

- Hamilton–Pontryagin–Galerkin principle with Type 4 continuity constraints

$$\delta \sum_{n=0}^{N-1} \Bigg(\frac{h}{2} \Big[L\big(q_{n+1/2}, \overset{+}{v}_n\big) + L\big(q_{n+1/2}, \overset{-}{v}_{n+1}\big) \Big] - \frac{h}{2} \Big[\big\langle \overset{+}{p}_n,\ \overset{+}{v}_n \big\rangle + \big\langle \overset{-}{p}_{n+1},\ \overset{-}{v}_{n+1} \big\rangle \Big]$$

$$+ \big\langle \overset{+}{p}_n,\ q_{n+1/2} - q_n \big\rangle + \big\langle \overset{-}{p}_{n+1},\ \hat{q}_{n+1} - q_{n+1/2} \big\rangle + \big\langle p_n,\ q_n - \hat{q}_n \big\rangle \Bigg) = 0$$

- generalised Störmer-Verlet method

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

One-step Variational Integrator for Degenerate Lagrangian $L(q, v) = \langle \vartheta(q), v \rangle - H(q)$

- 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 numerical flux $\langle \vartheta(\langle\!\langle q \rangle\!\rangle_n), [\![q]\!]_n \rangle$

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

- discrete Euler–Lagrange equations: one-step method with variational projection

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

$$p_{n+1/2} = \vartheta(q_n) + \frac{h}{2} \frac{\partial L}{\partial q} \left(q_n^+, \frac{q_n^+ - q_n^-}{h} \right) + \frac{h}{2} \nabla \vartheta \left(\frac{q_n^- + q_n^+}{2} \right) \cdot \left(q_n^+ - q_n^- \right),$$

$$\vartheta(q_{n+1}) = p_{n+1/2} + \frac{h}{2} \frac{\partial L}{\partial q} \left(q_{n+1}^-, \frac{q_n^+ - q_n^-}{h} \right) + \frac{h}{2} \nabla \vartheta \left(\frac{q_{n+1}^- + q_{n+1}^+}{2} \right) \cdot \left(q_{n+1}^+ - q_{n+1}^- \right)$$

Summary and Outlook

Summary and Outlook

- Hamilton–Pontryagin–Galerkin integrators provide a unified framework for several known but disparate methods as well as new methods
- ingredients: polynomial space, quadrature rule, continuity constraint or jump condition
- open up new horizons for structure preserving discretisation
  - variational one-step methods for degenerate Lagrangian systems
  - symplectic projection methods for Hamiltonian systems subject to Dirac constraints (special family of index 2 DAEs)
- next steps
  - implementation of HPGIs/DGVIs in `GeometricIntegrators.jl` (see `https://github.com/ddmgni/`)
  - discrete mechanics, discrete Dirac structures, discrete Noether theorem
  - extension to interconnected systems and multi-Dirac structures (PDEs)