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Discontinuous Galerkin Variational Integrators

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Motivation

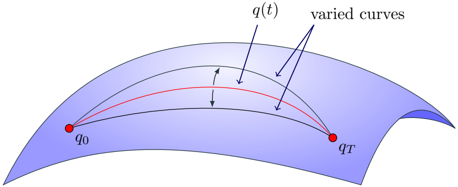
1. Variational spacetime discontinuous Galerkin methods
2. Unification and completion of Lagrangian and Hamiltonian variational integrators
3. Treatment of degenerate Lagrangian systems $L(q, \dot{q}) = \vartheta(q) \cdot \dot{q} - H(q)$ with nonlinear one-form $\vartheta(q)$
4. Treatment of Hamiltonian systems $H(q, p)$ subject to Dirac constraints $\phi(q, p) = 0$

Outline

1. Variational Integrators
2. Continuous Galerkin Variational Integrators
3. Discontinuous Galerkin Variational Integrators
4. Hamilton–Pontryagin–Galerkin Integrators
5. Summary and Outlook

Variational Integrators

Hamilton's Principle of Stationary Action



- action: functional of a trajectory q with Lagrangian $L : \mathrm{T}\mathcal{M} \to \mathbb{R}$

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

- Hamilton's principle of stationary action: among all possible trajectories q between two points q_0 and q_T, the physical trajectory makes the action integral $\mathcal{A}$ stationary
- variation and integration by parts (endpoints of q are fixed, such that $\delta q(0) = 0$ and $\delta q(T) = 0$)

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

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

$$\frac{\partial L}{\partial q}(q, \dot{q}) - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}(q, \dot{q}) \right) = 0 \qquad \text{(Euler-Lagrange equations)}$$

Discrete Lagrangian

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

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

- exact discrete Lagrangian, defined w.r.t. two points on a discrete solution 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}

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

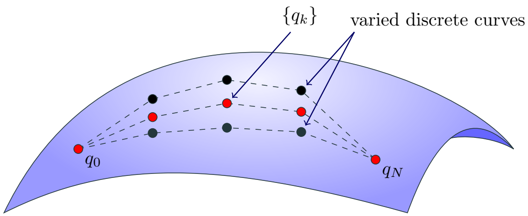
- approximate discrete Lagrangian with discrete quadrature formula (c_i, b_i)

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

- example: trapezoidal quadrature

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

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

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

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

$$p_n = \mathbb{F}^- L_d(q_n, q_{n+1}) = -D_1 L_d(q_n, q_{n+1}),$$

$$p_{n+1} = \mathbb{F}^+ L_d(q_n, q_{n+1}) = D_2 L_d(q_n, q_{n+1})$$

→ the discrete Lagrangian plays the role of a Type-I generating function

Hamilton's Phasespace Action Principle

- for regular Lagrangians the fibre derivative and Legendre transform can be used to introduce momenta p and the Hamiltonian $H: \mathrm{T}^* \mathcal{M} \to \mathbb{R}$,

$$p = \frac{\partial L}{\partial \dot{q}}(q, \dot{q}), \qquad H(q, p) = p \cdot \dot{q}(q, p) - L(q, \dot{q}(q, p))$$

- rewrite Hamilton's principle of stationary action as a so-called *phasespace action principle*,

$$\delta \int_0^T L(q, \dot{q}) \, dt = \delta \int_0^T \big[p \cdot \dot{q} - H(q, p) \big] \, dt = 0 \qquad \text{(Type-I phasespace action principle)}$$

- the same assumptions on the trajectory q as before are made, i.e., the endpoints $q(0) = q_0$ and $q(T) = q_T$ are fixed, while the endpoints of p are left free, thus $\delta q_0 = 0$ and $\delta q_N = 0$ but δp_0 and δp_N are arbitrary
- direct discretisation as before leads to an underdetermined system of equations (→ many extrema of the action exist), that needs to be suitably completed, for details see
    - Ellison, Finn, Burby, MK, Qin, Tang. Degenerate Variational Integrators for Magnetic Field Line Flow and Guiding Center Trajectories. Physics of Plasmas, Volume 25, 052502, 2018.
    - MK. On Action Principles and Degenerate Lagrangians: Continuous and Discrete. In preparation.

Hamiltonian Variational Integrators

- similarly to the standard version of Hamilton's phasespace action principle, corresponding Type-II, III and IV principles can be constructed
- Type-II phasespace action principle

$$\delta\left[p_T \cdot q_T - \int_0^T \left[p \cdot \dot{q} - H(q,p)\right] dt\right] = 0, \qquad q(0) = q_0, \qquad p(T) = p_T,$$

with q fixed at the initial point, and p fixed at the final point, while $q(T)$ and $p(0)$ are left free

- Type-III phasespace action principle

$$\delta\left[p_0 \cdot q_0 + \int_0^T \left[p \cdot \dot{q} - H(q,p)\right] dt\right] = 0, \qquad q(T) = q_T, \qquad p(0) = p_0,$$

with q fixed at the final point and p fixed at the initial point, while $q(0)$ and $p(T)$ are left free

- Type-IV phasespace action principle

$$\delta\left[p_T \cdot q_T - p_0 \cdot q_0 - \int_0^T \left[p \cdot \dot{q} - H(q,p)\right] dt\right] = 0, \qquad p(0) = p_0, \qquad p(T) = p_T,$$

with the endpoints of q left free and both endpoints of p fixed

Generating Functions

- the discrete Lagrangian plays the role of a Type-I generating function [1]
- the discrete Hamiltonians H_d^+ and H_d^- play the role of Type-II and III generating functions [2,3]
- 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	$S(p, P)$	$q = D_1 S(p, P)$,	$Q = D_2 S(p, P)$	?

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

[1] Marsden, West: Discrete mechanics and variational integrators. Acta Numerica, Vol. 10, pp. 357–514, 2001.

[2] Leok, Zhang. Discrete Hamiltonian variational integrators. IMA J. of Numerical Analysis, Vol. 31, pp. 1497–1532, 2011.

[3] Leok, Ohsawa. Variational and Geometric Structures of Discrete Dirac Mechanics. Foundations of Computational Mathematics, Vol. 11, pp. 529–562, 2011.

Continuous Galerkin Variational Integrators

Continuous Galerkin Variational Integrators: Some References

- Marsden, West: Discrete mechanics and variational integrators. Acta Numerica, Vol. 10, pp. 357–514, 2001.
- Leok, Zhang. Discrete Hamiltonian variational integrators. IMA Journal of Numerical Analysis, Vol. 31, pp. 1497–1532, 2011.
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- Campos, Ober-Blöbaum, Trélat. High order variational integrators in the optimal control of mechanical systems. Discrete and Continuous Dynamical Systems, Vol. 35, pp. 4193–4223, 2015.
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- Ober-Blöbaum. Galerkin variational integrators and modified symplectic Runge–Kutta methods. IMA Journal of Numerical Analysis, drv062, 2016.
- Wenger, Ober-Blöbaum, Leyendecker. Construction and analysis of higher order variational integrators for dynamical systems with holonomic constraints. Advances in Computational Mathematics, Vol. 257, pp. 1–33, 2017.

- the time interval $\mathcal{I} = [0, T]$ is partitioned into N subintervals $\mathcal{I}_n = (t_n, t_{n+1})$ with $0 \leq n < N$, $t_n = nh$, time step h, and the corresponding closed intervals denoted by $\bar{\mathcal{I}}_n = [t_n, t_{n+1}]$
- on each time interval $\bar{\mathcal{I}}_n$ construct a polynomial approximation $q_h(t)\big|_{\bar{\mathcal{I}}_n} \in \mathbb{P}^r(\bar{\mathcal{I}}_n)$ such that $q_h(t) \approx q(t)$
- the approximate trajectories q_h on the configuration space $\mathcal{M}$ are elements of

$$\mathcal{Q}_h = \left\{ q_h \, : \, q_h\big|_{\bar{\mathcal{I}}_n} \in \mathbb{P}^r(\bar{\mathcal{I}}_n) \text{ for } n \in \{0, \dots, N-1\}, \; q_h(0) = q_0, \; q_h(T) = q_T \right\},$$

so that with appropriate basis functions $\varphi_{n,i}$ we can write

$$q_h(t)\big|_{\bar{\mathcal{I}}_n} = \sum_{i=1}^{r} Q_{n,i} \, \varphi_{n,i}(t)$$

- example: Lagrange polynomials

$$\varphi_{n,i}(t) = \begin{cases} l^{r,i}\big((t - t_n)/(t_{n+1} - t_n)\big), & t_n \leq t \leq t_{n+1}, \\ 0, & \text{else}, \end{cases} \qquad l^{r,i}(\tau) = \prod_{\substack{1 \leq j \leq r, \\ j \neq i}} \frac{\tau - \tau_j}{\tau_i - \tau_j},$$

here $l^{r,i}(\tau)$ denotes the i-th Lagrange polynomial of order r

Continuous Galerkin Variational Integrators

- the time interval $\mathcal{I} = [0, T]$ is partitioned into N subintervals $\mathcal{I}_n = (t_n, t_{n+1})$ with $0 \le n < N$, $t_n = nh$, time step h, and the corresponding closed intervals denoted by $\bar{\mathcal{I}}_n = [t_n, t_{n+1}]$
- polynomial approximation $q_h(t)\big|_{\bar{\mathcal{I}}_n} \in \mathbb{P}^r(\bar{\mathcal{I}}_n)$ of the trajectory q in each time intervall $\bar{\mathcal{I}}_n = [t_n, t_{n+1}]$

$$q_h(t)\big|_{\bar{\mathcal{I}}_n} = \sum_{i=1}^{r} Q_{n,i} \, \varphi_{n,i}(t),$$

- choosing a quadrature rule (b_i, c_i) with $i = 1, \ldots, s$, the discrete action can be written as

$$\mathcal{A}_d = h \sum_{n=0}^{N-1} \sum_{i=1}^{s} b_i \, L\big(q_h(t_n + hc_i), \; \dot{q}_h(t_n + hc_i) \big)$$

- requiring variations of $\mathcal{A}_d$ to vanish for arbitrary variations of $\{ Q_{n,i} \}_{n=0,\ldots,N, \, i=1,\ldots,s}$ only restricted such that $\delta q_h(0) = 0$ and $\delta q_h(T) = 0$, leads to (continuous) Galerkin variational integrators
- similar constructions are possible for the Type-II and III phasespace action principles
- treatment of holonomic and nonholonomic constraints possible
- another gap in current state of the theory: treatment of degenerate Lagrangians $L = \vartheta(q) \cdot \dot{q} - H(q)$ with nonlinear one-form ϑ and Hamiltonian systems subject to Dirac-constraints $\phi(q, p) = 0$ not possible

Discontinuous Galerkin Variational Integrators

Discontinuous Galerkin Variational Integrators: Some References

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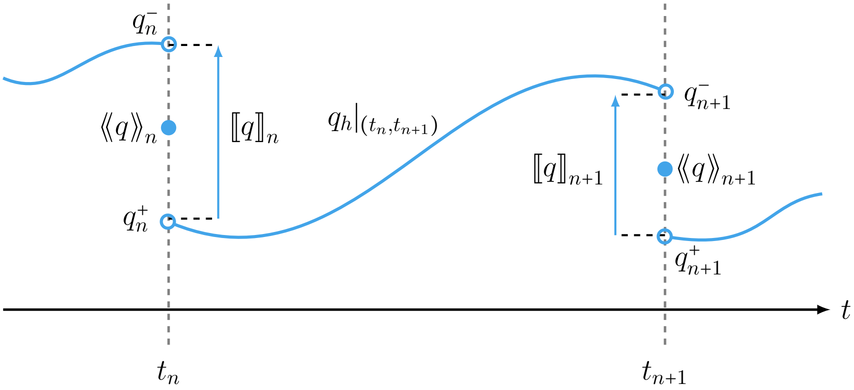
Discontinuous Galerkin Approximation



- 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 analogously $p_h(t)$

Discontinuous Galerkin Variational Integrators

- on each interval $\mathcal{I}_n = (t_n, t_{n+1})$ construct polynomials $q_h(t)\big|_{\mathcal{I}_n} \in \mathbb{P}^r(\mathcal{I}_n)$ such that $q_h(t)\big|_{\mathcal{I}_n} \approx q(t)\big|_{\mathcal{I}_n}$
- the approximate trajectories q_h on the configuration space $\mathcal{M}$ are elements of

$$\mathcal{Q}_h = \left\{ q_h \,:\, q_h\big|_{\mathcal{I}_n} \in \mathbb{P}^r(\mathcal{I}_n), \; n = 0, \ldots, N-1 \right\} \qquad \text{with} \qquad q_h(t)\big|_{\mathcal{I}_n} = \sum_{i=1}^{r} Q_{n,i}\, \varphi_{n,i}(t),$$

- choosing a quadrature rule (b_i, c_i) with $i = 1, \ldots, s$, the discrete Type-I phasespace action can be written as

$$\mathcal{A}_d = h \sum_{n=0}^{N-1} \sum_{i=1}^{s} b_i \Big[p_h(t_n + hc_i) \cdot \dot{q}_h(t_n + hc_i) - H\big(q_h(t_n + hc_i),\, p_h(t_n + hc_i) \big) \Big] - \sum_{n=0}^{N} \langle\!\langle p \rangle\!\rangle_n \cdot [\![q]\!]_n ,$$

  where $\langle\!\langle p \rangle\!\rangle_n \cdot [\![q]\!]_n$ is the jump discretisation of $p \cdot \dot{q}$ at t_n
- simple discretisations for the average and jump operators are

$$\langle\!\langle p \rangle\!\rangle_n = (1 - \alpha)\, p_n^- + \alpha\, p_n^+, \quad 0 \le \alpha \le 1, \qquad [\![q]\!]_n = q_n^+ - q_n^-, \qquad q_n^- = \lim_{t \uparrow t_n} q_h(t), \qquad q_n^+ = \lim_{t \downarrow t_n} q_h(t)$$

- requiring variations of $\mathcal{A}_d$ to vanish for arbitrary variations of $\{Q_{n,i}\}_{n=0,\ldots,N,\, i=1,\ldots,s}$ only restricted such that $\delta q_h(0) = 0$ and $\delta q_h(T) = 0$, leads to discontinuous Galerkin variational integrators
- another gap in current state of the theory: discontinuous Galerkin discretisations not possible in the Lagrangian framework

Hamilton–Pontryagin–Galerkin Integrators

Hamilton–Pontryagin Principle

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

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

- 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

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

Discrete Hamilton–Pontryagin Principle

- choose quadrature rule with nodes c_i and weights b_i and set $t_{n,i} = t_n + c_i h$
- discrete Hamilton–Pontryagin principles

$$\delta \sum_{n=0}^{N-1} \left(h \sum_{i=1}^{s} b_i \left[L\big(q_h(t_{n,i}), v_h(t_{n,i})\big) + \big\langle p_h(t_{n,i}),\ \dot{q}_h(t_{n,i}) - v_h(t_{n,i}) \big\rangle \right] \right.$$

$$\left. + \text{continuity constraints or jump discretisation} \right) = 0$$

$$\delta \sum_{n=0}^{N-1} \left(h \sum_{i=1}^{s} b_i \left[\big\langle p_h(t_{n,i}),\ \dot{q}_h(t_{n,i}) \big\rangle - E\big(q_h(t_{n,i}), v_h(t_{n,i}), p_h(t_{n,i})\big) \right] \right.$$

$$\left. + \text{continuity constraints or jump discretisation} \right) = 0$$

- continuity constraints: enforce continuity weakly via Lagrange multipliers
  - → fills holes in variational integrator framework (Type-I and Type-IV phasespace action principle)
  - → unifying framework for many existing (Galerkin) variational integrators (Lagrangian and Hamiltonian)
- jump discretisation: discontinuous Galerkin discretisation
  - → new families of variational integrators, especially variational spacetime DG methods
  - → treatment of degenerate Lagrangian and Hamiltonian systems subject to Dirac constraints

Continuity Constraints

- possible continuity constraints ($q^-_{n+1} = \lim_{t\uparrow t_{n+1}} q_h(t)$, $q^+_{n+1} = \lim_{t\downarrow t_{n+1}} q_h(t)$, etc.)

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

- 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

Summary and Outlook

Summary and Outlook

- Hamilton–Pontryagin–Galerkin integrators provide a unifying 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
- outlook
  - complete implementation of HPGIs/DGVIs in `GeometricIntegrators.jl`
  - discrete mechanics, discrete Noether theorem, discrete Dirac structures
  - extension to holonomic and nonholonomic constraints
  - extension to interconnected systems and multi-Dirac structures (PDEs, spacetime DG)

Appendix

Degenerate Lagrangians

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

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

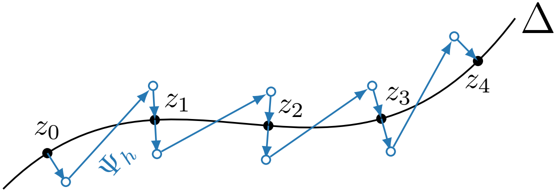
- the numerical solution drifts away from the constraint submanifold defined by $\phi(q, p) = 0$

Position-Momentum Form

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

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

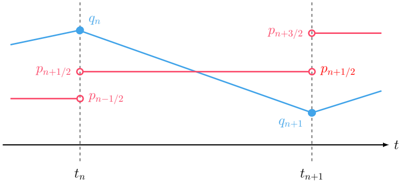
- the numerical solution drifts away from the constraint submanifold defined by $\phi(q,p) = 0$
- symmetric projection methods lead to long-time stable integrators, but are not variational, for details see
  - Michael Kraus. Projected Variational Integrators for Degenerate Lagrangian Systems. arXiv:1708.07356, 2017.



- projection methods are discontinuous in nature → are there variational projection methods?

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

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

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

Type 1 Continuity Constraints

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

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

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

- generalised Störmer-Verlet method

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

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

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

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

Type 1 Continuity Constraints

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

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

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

- eliminating all auxiliary variables, we obtain

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

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

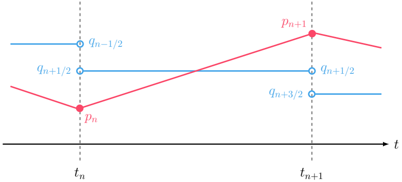
→ position-momentum form,

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

of the variational integrator corresponding to the trapezoidal Lagrangian

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

Type 4 Continuity Constraints



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

$$q_h(t)|_{(t_n,t_{n+1})} = q_{n+1/2},$$

$$v_h(t)|_{(t_n,t_{n+1})} = \frac{t_{n+1}-t}{t_{n+1}-t_n}\, v_n^+ + \frac{t-t_n}{t_{n+1}-t_n}\, v_{n+1}^-$$

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

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

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

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

Type 4 Continuity Constraints

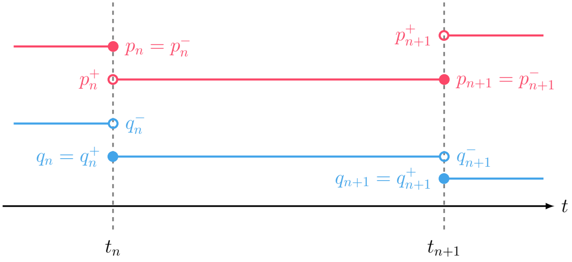
- Hamilton–Pontryagin–Galerkin principle with Type 4 continuity constraints

$$\delta \sum_{n=0}^{N-1} \left(\frac{h}{2} \left[L\big(q_{n+1/2}, \overset{+}{v}_n\big) + L\big(q_{n+1/2}, \overset{-}{v}_{n+1}\big) \right] + \frac{h}{2} \left[\left\langle \overset{+}{p}_n, \frac{q_{n+1/2} - q_n}{h/2} - \overset{+}{v}_n \right\rangle + \left\langle \overset{-}{p}_{n+1}, \frac{q_{n+1} - q_{n+1/2}}{h/2} - \overset{-}{v}_{n+1} \right\rangle \right] + \big\langle p_n, q_n \big\rangle - \big\langle p_{n+1}, \hat{q}_{n+1} \big\rangle \right) = 0$$

- generalised Störmer-Verlet method

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

Type 2 Continuity Constraints



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

$$q_h(t)|_{(t_n,t_{n+1})} = q_n^+,$$
$$v_h(t)|_{(t_n,t_{n+1})} = v_n^+,$$
$$p_h(t)|_{(t_n,t_{n+1})} = p_{n+1}^-$$

- trapezoidal quadrature and (q, P) continuity constraint

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

Type 2 Continuity Constraints

- Hamilton–Pontryagin–Galerkin principle with Type 2 (q, P) continuity constraints

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

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

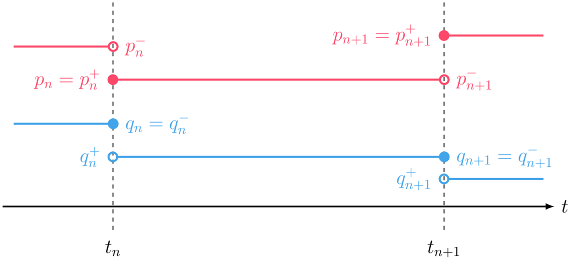
- discrete Legendre transform

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

- generalised symplectic Euler-B method (replacing $q_n = q_n^+$, $v_n = v_n^+$, $p_n = p_n^-$)

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

Type 3 Continuity Constraints



- 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

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

Type 3 Continuity Constraints

- Hamilton–Pontryagin–Galerkin principles with Type 3 (Q, p) continuity constraints

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

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

- discrete Legendre transform

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

- generalised symplectic Euler-A method(replacing $q_{n+1} = q_{n+1}^-,\ v_{n+1} = v_{n+1}^-,\ p_n = p_n^+$)

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