Co-funded by
the European Union

Hamilton–Pontryagin–Galerkin Integrators

Unifying Continuous and Discontinuous Galerkin Variational Integrators

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Motivation

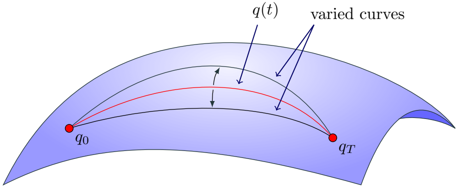
1. Variational spacetime discontinuous Galerkin methods
2. Treatment of degenerate Lagrangian systems $L(q, \dot{q}) = \vartheta(q) \cdot \dot{q} - H(q)$
3. Treatment of Hamiltonian systems $H(q, p)$ subject to Dirac constraints $\phi(q, p) = 0$
4. Unification and "*completion*" of Lagrangian and Hamiltonian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

Outline

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

Variational Integrators and Generating Functions

Hamilton's Principle of Stationary Action



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

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

- 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}

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

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

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

- 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

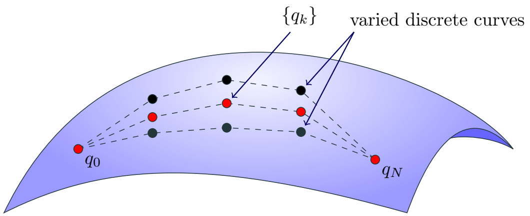
$$\mathcal{A}_d[q_d] = \sum_{n=0}^{N-1} L_d(q_n, q_{n+1})$$

- 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 $S_{(1)}(q, Q)$ determining (p, P)

Hamilton's Phasespace Action Principle

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

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

- 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 ($\to$ 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.

Hamilton's Phasespace Action Principle

- similarly to the standard (Type-I) version of Hamilton's phasespace action principle, corresponding Type-II, III and IV action 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

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

  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 [1,3]
- the discrete Hamiltonians H_d^+ and H_d^- play the role of Type-II and III generating functions [2,4,5]
- generating function types

Type I	$S_{(1)}(q, Q)$	$p = D_1 S_{(1)}(q, Q), \quad P = D_2 S_{(1)}(q, Q)$	L_d
Type II	$S_{(2)}(q, P)$	$p = D_1 S_{(2)}(q, P), \quad Q = D_2 S_{(2)}(q, P)$	H_d^+
Type III	$S_{(3)}(p, Q)$	$q = D_1 S_{(3)}(p, Q), \quad P = D_2 S_{(3)}(p, Q)$	H_d^-
Type IV	$S_{(4)}(p, P)$	$q = D_1 S_{(4)}(p, P), \quad Q = D_2 S_{(4)}(p, P)$	?

- 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:

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[3] Stern: Discrete Hamilton-Pontryagin mechanics and generating functions on Lie groupoids. J. Sympl. Geom. 8, pp. 225–238, 2010.
[4] Leok, Zhang. Discrete Hamiltonian variational integrators. IMA J. Numer. Anal. 31, pp. 1497–1532, 2011.
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Continuous Galerkin Variational Integrators

Continuous Galerkin Variational Integrators: Some References

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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 $0 \leq n < N$, $t_n = nh$, 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 $q_h\big|_{\bar{\mathcal{I}}_n} \in \mathbb{P}^r(\bar{\mathcal{I}}_n)$ so that with appropriate basis functions $\varphi_{n,i}$ we can write

$$q_h\big|_{\bar{\mathcal{I}}_n}(t) = \sum_{i=1}^{r} Q_{n,i}\,\varphi_{n,i}(t) \qquad \text{where} \qquad q_h\big|_{\bar{\mathcal{I}}_n}(t_n) = q_n \quad \text{and} \quad q_h\big|_{\bar{\mathcal{I}}_n}(t_{n+1}) = q_{n+1}$$

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

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

- requiring variations of $\mathcal{A}_d$ to vanish for arbitrary variations of $\{Q_{n,i}\}_{n=0,\dots,N,\, i=1,\dots,s}$ 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
- gap in the theory: not applicable to degenerate Lagrangians $L = \vartheta(q) \cdot \dot{q} - H(q)$ with nonlinear one-form ϑ and Hamiltonian systems subject to Dirac-constraints $\phi(q, p) = 0$

Discontinuous Galerkin Variational Integrators

Discontinuous Galerkin Variational Integrators: Some References

- Tang, Sun. Time finite element methods: A unified framework for numerical discretizations of ODEs. Applied Mathematics and Computation, Vol. 219, pp. 2158–2179, 2012.
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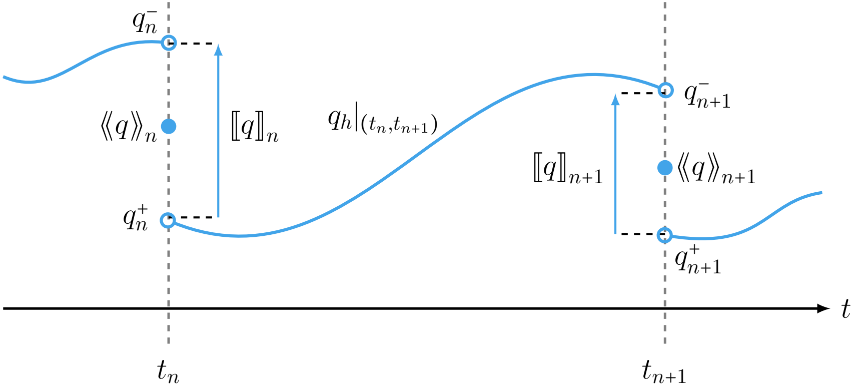
Discontinuous Galerkin Approximation



- piecewise-continuous polynomial basis $q_h\big|_{\mathcal{I}_n} \in \mathbb{P}^r(\mathcal{I}_n)$ with discontinuity at t_n and t_{n+1}
- the average and jump operators are usually given by

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

Discontinuous Galerkin Variational Integrators

- on each interval $\mathcal{I}_n = (t_n, t_{n+1})$ construct polynomials $q_h\big|_{\mathcal{I}_n} \in \mathbb{P}^r(\mathcal{I}_n)$ so that with appropriate basis functions $\varphi_{n,i}$ we can write

$$q_h\big|_{\mathcal{I}_n}(t) = \sum_{i=1}^{r} Q_{n,i}\,\varphi_{n,i}(t) \qquad \text{where} \qquad q_h\big|_{\mathcal{I}_n}(t_n) = q_n^+ \quad \text{and} \quad q_h\big|_{\mathcal{I}_n}(t_{n+1}) = q_{n+1}^-$$

  and analogously for p_h

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

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

  where $\langle\!\langle p \rangle\!\rangle_n \cdot [\![q]\!]_n$ is the jump discretisation of $p \cdot \dot{q}$ at t_n

- 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

- gap in the theory: discontinuous Galerkin discretisations not possible in the Lagrangian framework

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 by the Legendre transform

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

and rewrite the Hamilton–Pontryagin principle as a phasespace action princple

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

- 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

- discrete Hamilton–Pontryagin principles using piecewise-polynomial solutions (q_h, v_h, p_h) and quadrature (b, c)

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

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

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

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

- continuity constraints: enforce continuity weakly via Lagrange multipliers
  - → fills some holes in variational integrator framework (e.g., Type-I and Type-IV phasespace action principle)
  - → unifying framework for many existing variational integrators (Lagrangian and Hamiltonian)
- jump discretisation: discontinuous Galerkin discretisation
  - → new families of variational integrators, especially variational spacetime discontinuous Galerkin methods
  - → treatment of degenerate Lagrangian systems 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 I	(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 II	(q, P)	$+ \left\langle p_n,\, q^+_n - q_n \right\rangle + \left\langle p_{n+1} - p^-_{n+1},\, \hat{q}_{n+1} \right\rangle - \left\langle p^-_{n+1},\, q^-_{n+1} \right\rangle$
Type III	(p, Q)	$- \left\langle p^+_n - p_n,\, q_n \right\rangle + \left\langle \hat{p}_{n+1},\, q_{n+1} - q^-_{n+1} \right\rangle + \left\langle p^+_n,\, q^+_n \right\rangle$
Type IV	(p, P)	$- \left\langle p^+_n - p_n,\, q_n \right\rangle + \left\langle p_{n+1} - p^-_{n+1},\, \hat{q}_{n+1} \right\rangle + \left\langle p^+_n,\, q^+_n \right\rangle - \left\langle p^-_{n+1},\, q^-_{n+1} \right\rangle$

- resulting continuity of p and q

Continuity		q	p
Type I	(q, Q)	doubly continuous	doubly discontinuous
Type II	(q, P)	left-continuous	right-continuous
Type III	(p, Q)	right-continuous	left-continuous
Type IV	(p, P)	doubly discontinuous	doubly continuous

Summary and Outlook

Summary and Outlook

- Hamilton–Pontryagin–Galerkin integrators provide a common framework for many known but disparate variational integrator methods, unifying
  - Lagrangian and Hamiltonian action principles
  - Type I, II, III, IV action principles and generating functions
  - continuous and discontinuous Galerkin variational integrators
- 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/CGVIs in `GeometricIntegrators.jl`
  - discrete mechanics, discrete Noether theorem, discrete Dirac structures
  - extensions to holonomic and nonholonomic constraints, interconnected systems, multi-Dirac structures