Co-funded by
the European Union

Discontinuous Galerkin Variational Integrators for Degenerate Lagrangians

Michael Kraus[1,2,3] (michael.kraus@ipp.mpg.de)

[1] Max-Planck-Institut für Plasmaphysik
[2] Technische Universität München, Zentrum Mathematik
[3] Waseda University, School of Science and Engineering

Outline

1. Guiding Centre Dynamics and Variational Integrators
2. Projected Variational Integrators
3. Discontinuous Galerkin Variational Integrators
4. Summary and Outlook

Guiding Centre Dynamics and Variational Integrators

Guiding Centre Dynamics

- guiding centre Lagrangian with $q = (x^1, x^2, x^3, u)$ and μ a parameter

$$L(q, \dot{q}) = \big(A(x) + ub(x)\big) \cdot \dot{x} - \tfrac{1}{2} u^2 - \mu B(x) - \phi(x)$$

with

$$u = b \cdot \dot{x}, \quad v_\perp = v - ub, \quad \mu = v_\perp^2 / 2 \, |B| \, , \quad B = \nabla \times A, \quad b = B / \, |B|$$

- degenerate Lagrangian linear in velocities

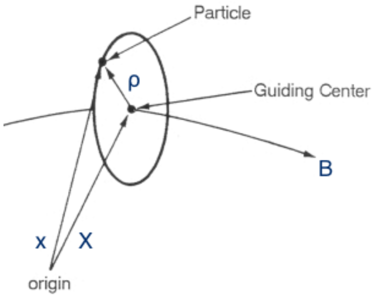
$$L(q, \dot{q}) = \vartheta(q) \cdot \dot{q} - H(q) \qquad \text{with} \qquad \det \left| \frac{\partial^2 L}{\partial \dot{q}^i \, \partial \dot{q}^j} \right| = 0$$

- Euler-Lagrange equations

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

→ 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 Variational Principle

- discrete Lagrangian, e.g., midpoint

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

- 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

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

→ leads to multi-step variational integrators

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

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

→ susceptible to parasitic modes driving simulations unstable

Variational Guiding Centre Integrators

- 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

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

→ provides an update rule of the form

$$\tilde{\Psi}_{L_d} : (q_n, p_n) \mapsto (q_{n+1}, p_{n+1})$$

- use continuous fibre derivative to obtain the second initial condition

$$p_0 = \frac{\partial L}{\partial \dot{q}}(q_0) = \vartheta(q_0), \qquad \vartheta(q) = A(x) + u b(x)$$

→ provides an exact initialisation mechanism given q_0

Variational Runge–Kutta Integrators

- discrete Hamilton–Pontryagin action principle

$$\mathcal{A}_d = \sum_{n=0}^{N-1} \left(h \sum_{i=1}^{s} b_i \left[L\big(Q_{n,i}, \dot{Q}_{n,i} \big) + \dot{P}_{n,i} \cdot \left(Q_{n,i} - q_n - h \sum_{j=1}^{s} a_{ij} \, \dot{Q}_{n,j} \right) \right] - p_{n+1} \cdot \left(q_{n+1} - q_n - h \sum_{i=1}^{s} b_i \, \dot{Q}_{n,i} \right) \right)$$

- variational Runge–Kutta integrators with s stages

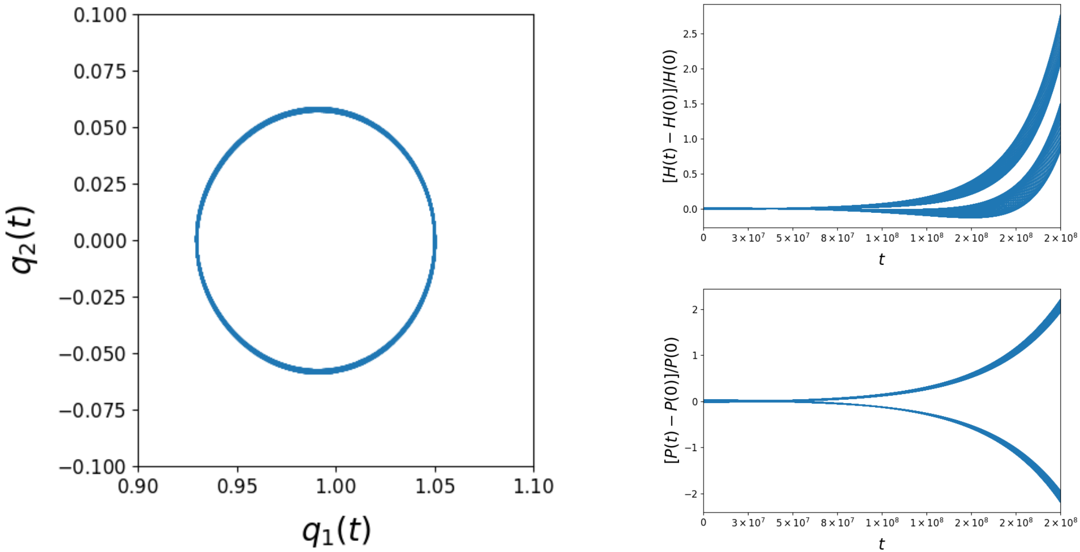
$$P_{n,i} = \frac{\partial L}{\partial \mathrm{v}} (Q_{n,i}, \dot{Q}_{n,i}), \qquad Q_{n,i} = q_n + h \sum_{j=1}^{s} a_{ij} \, \dot{Q}_{n,j}, \qquad q_{n+1} = q_n + h \sum_{i=1}^{s} b_i \, \dot{Q}_{n,i},$$

$$\dot{P}_{n,i} = \frac{\partial L}{\partial \mathrm{x}} (Q_{n,i}, \dot{Q}_{n,i}), \qquad P_{n,i} = p_n + h \sum_{j=1}^{s} \bar{a}_{ij} \, \dot{P}_{n,j}, \qquad p_{n+1} = p_n + h \sum_{i=1}^{s} \bar{b}_i \, \dot{P}_{n,i},$$

with coefficients satisfying the symplecticity conditions,

$$b_i \bar{a}_{ij} + \bar{b}_j a_{ji} = b_i \bar{b}_j \qquad \text{and} \qquad \bar{b}_i = b_i$$

Passing Particle (Variational Gauss–Legendre Runge–Kutta Integrator)



Passing Particle (Variational Gauss–Legendre Runge–Kutta Integrator)

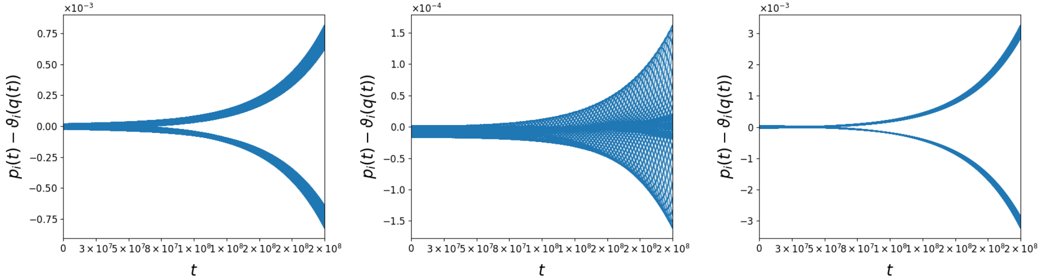
- position-momentum form: rewrite the equations of motion as an index 2 DAE

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

- the variational Runge–Kutta integrator satisfies these equations only at the internal stages

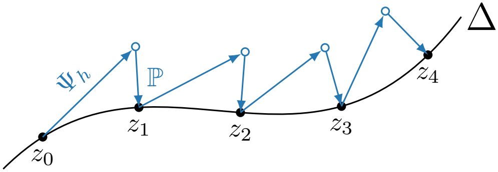
→ the numerical solution drifts away from the constraint submanifold defined by $\phi(q, p) = 0$

$$p_n \neq \vartheta(q_n) \quad \text{for } n \geq 1, \text{ even though} \quad p_0 = \vartheta(q_0)$$



Projected Variational Integrators

Standard Projection



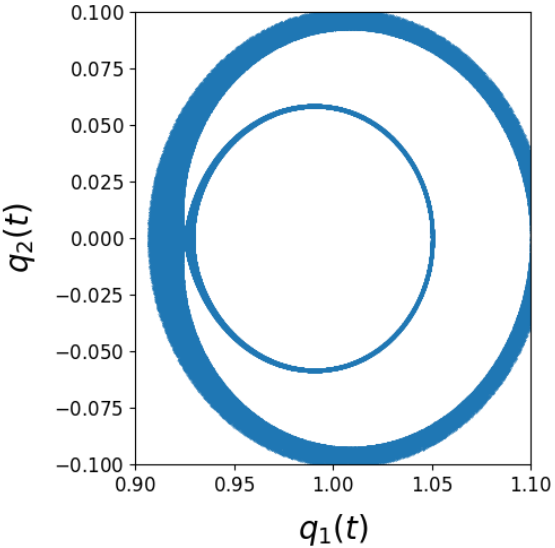
- index 2 DAE

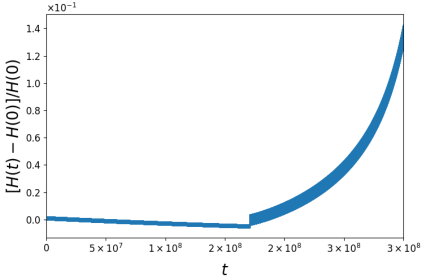
$$\dot{z} = \Omega^{-1}\big(\nabla H(z) + \nabla\phi^T(z)\,\lambda\big), \qquad z = (q, p), \qquad \Omega = \begin{pmatrix} \mathbb{0} & -\mathbb{1} \\ \mathbb{1} & \mathbb{0} \end{pmatrix}$$
$$0 = \phi(z),$$

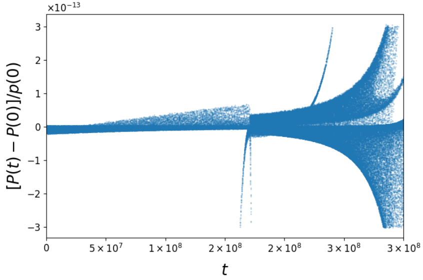
- standard projection of primary constraint

$$\tilde{z}_{n+1} = \Psi_h(z_n) \qquad \text{apply arbitrary one-step method}$$
$$z_{n+1} = \tilde{z}_{n+1} + h\Omega^{-1}\nabla\phi^T(z_{n+1})\lambda_{n+1} \qquad \text{project on constraint submanifold}$$
$$0 = \phi(z_{n+1}) \qquad \text{constraint}$$

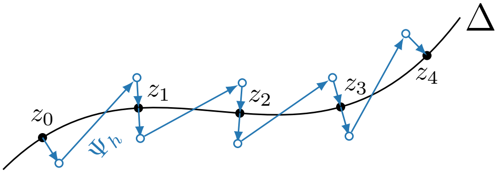
Passing Particle (Variational Gauss–Legendre Runge–Kutta Integrator)

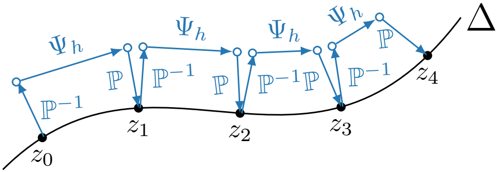






Symmetric Projection





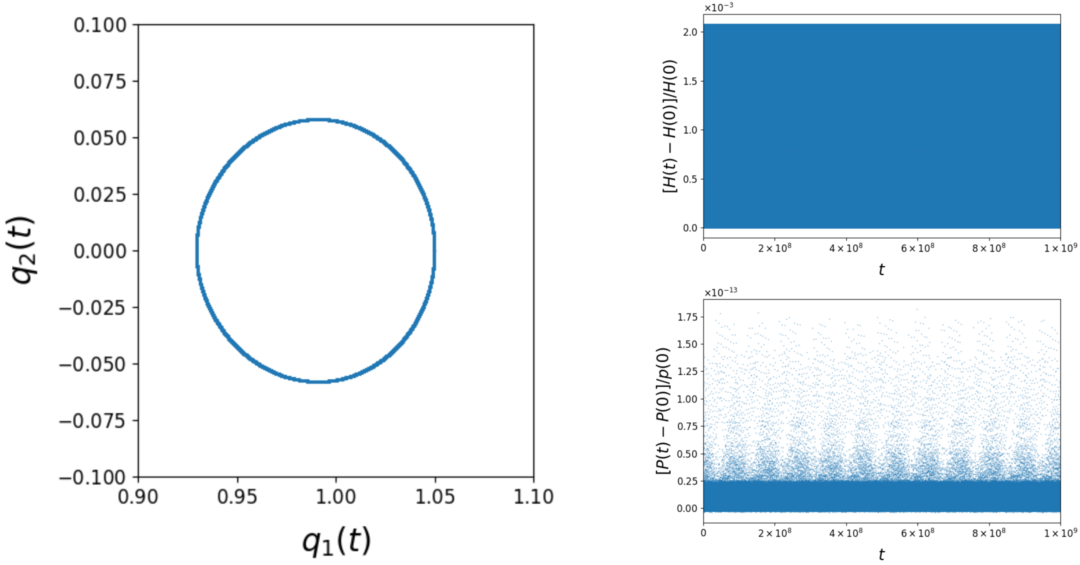
- index 2 DAE

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

- symmetric projection of primary constraint with $R(\infty) = \pm 1$ the stability function of Ψ_h

$$\begin{aligned} \tilde{z}_k &= z_k + h\,\Omega^{-1}\nabla\phi^T(z_k)\,\lambda_{k+1} && \text{perturb} \\ \tilde{z}_{k+1} &= \Psi_h(\tilde{z}_k) && \text{apply arbitrary one-step method} \\ z_{k+1} &= \tilde{z}_{k+1} + h\,R(\infty)\,\Omega^{-1}\nabla\phi^T(z_{k+1})\lambda_{k+1} && \text{project on constraint submanifold} \\ 0 &= \phi(z_{k+1}) && \text{constraint} \end{aligned}$$

Passing Particle (Variational Gauss–Legendre Runge–Kutta Integrator)



Symmetric Projection and Symplecticity

- symmetric projection of primary constraint

$$\begin{aligned}
\tilde{z}_n &= z_n + h\,\Omega^{-1} \nabla \phi^T(z_n)\,\lambda_{n+1} \\
\tilde{z}_{n+1} &= \Psi_h(\tilde{z}_n) \\
z_{n+1} &= \tilde{z}_{n+1} + h\,R(\infty)\,\Omega^{-1} \nabla \phi^T(z_{n+1}) \lambda_{n+1} \\
0 &= \phi(z_{n+1}).
\end{aligned}$$

- symplecticity condition

$$\begin{aligned}
&\mathrm{d} q_n^i \wedge \mathrm{d} p_n^i - \mathrm{d}\big(\lambda_{n+1}^T \phi_{q^i}(p_n, q_n)\big) \wedge \mathrm{d}\big(\lambda_{n+1}^T \phi_{p^i}(p_n, q_n)\big) = \\
&\qquad = \mathrm{d} q_{n+1}^i \wedge \mathrm{d} p_{n+1}^i - |R(\infty)|^2\, \mathrm{d}\big(\lambda_{n+1}^T \phi_{q^i}(p_{n+1}, q_{n+1})\big) \wedge \mathrm{d}\big(\lambda_{n+1}^T \phi_{p^i}(p_{n+1}, q_{n+1})\big)
\end{aligned}$$

→ assuming $|R(\infty)| = 1$, a variational integrator with symmetric projection is symplectic iff

$$\begin{aligned}
\lambda_{n+1}^T \phi_{p^i}(p_n, q_n) &= \lambda_{n+1}^T \phi_{p^i}(p_{n+1}, q_{n+1}) && \text{for all } i, \\
\lambda_{n+1}^T \phi_{q^i}(p_n, q_n) &= \lambda_{n+1}^T \phi_{q^i}(p_{n+1}, q_{n+1}) && \text{for all } i
\end{aligned}$$

Variational Projection

- add the constraint via a Lagrange multiplier to the discrete action principle

$$\mathcal{A}_d = \sum_{n=0}^{N-1} \left(h \sum_{i=1}^{s} b_i \left[L\big(Q_{n,i}, \dot{Q}_{n,i} \big) + \dot{P}_{n,i} \cdot \left(Q_{n,i} - q_n - h \sum_{j=1}^{s} a_{ij} \, \dot{Q}_{n,j} \right) \right] \right.$$
$$\left. - \, p_{n+1} \cdot \left(q_{n+1} - q_n - h \sum_{i=1}^{s} b_i \, \dot{Q}_{n,i} \right) + \phi^T (q_{n+1}, p_{n+1}) \, \lambda_{n+1} \right)$$

- modified variational Runge-Kutta integrators with perturbation of p_n and projection of q_{n+1}

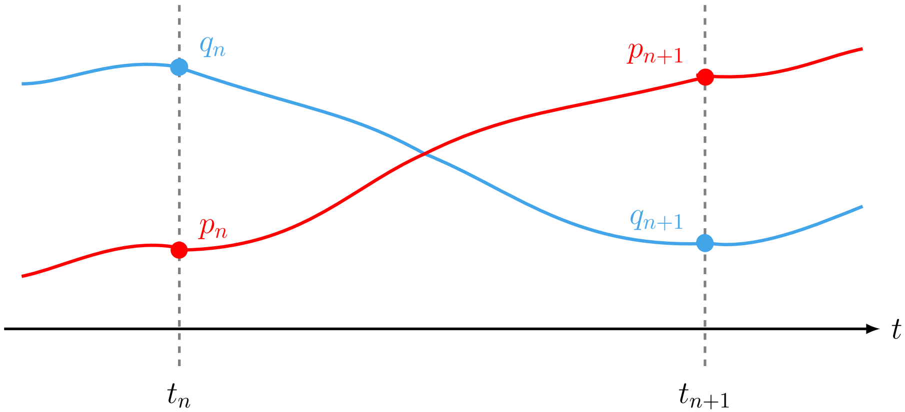
$$P_{n,i} = \tilde{p}_n + h \sum_{j=1}^{s} \bar{a}_{ij} \dot{P}_{n,j}, \qquad p_{n+1} = \tilde{p}_n + h \sum_{i=1}^{s} b_i \, \dot{P}_{n,i}, \qquad \tilde{p}_n = p_n - h \, \phi_q (q_n, p_n) \, \lambda_n$$

$$Q_{n,i} = q_n + h \sum_{j=1}^{s} a_{ij} \dot{Q}_{n,j}, \qquad \tilde{q}_{n+1} = q_n + h \sum_{i=1}^{s} b_i \, \dot{Q}_{n,i}, \qquad q_{n+1} = \tilde{q}_{n+1} + h \, \phi_p (q_{n+1}, p_{n+1}) \, \lambda_{n+1}$$

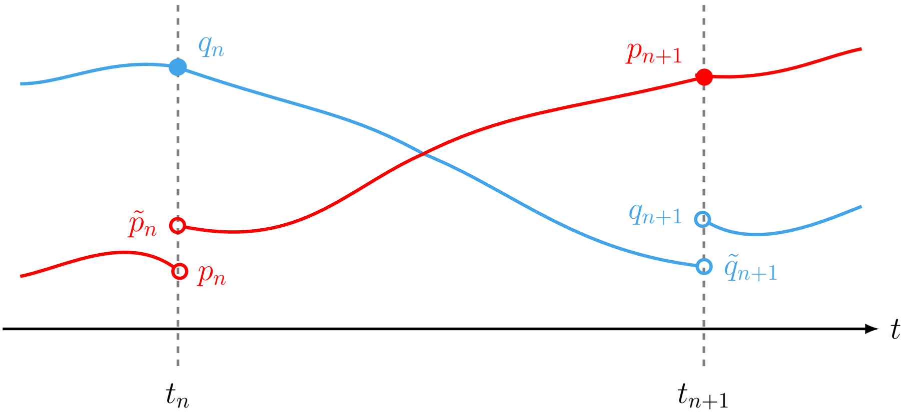
$$0 = \phi (q_{n+1}, p_{n+1})$$

Problem? Continuity!

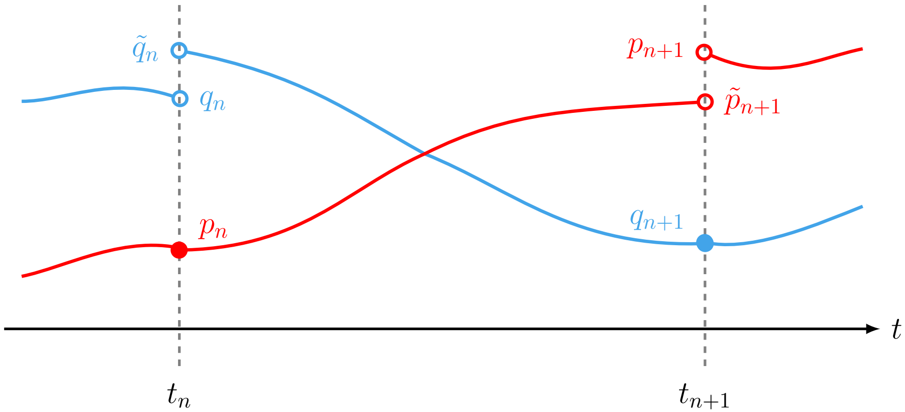
Position-Momentum Form of Lagrangian Variational Integrators



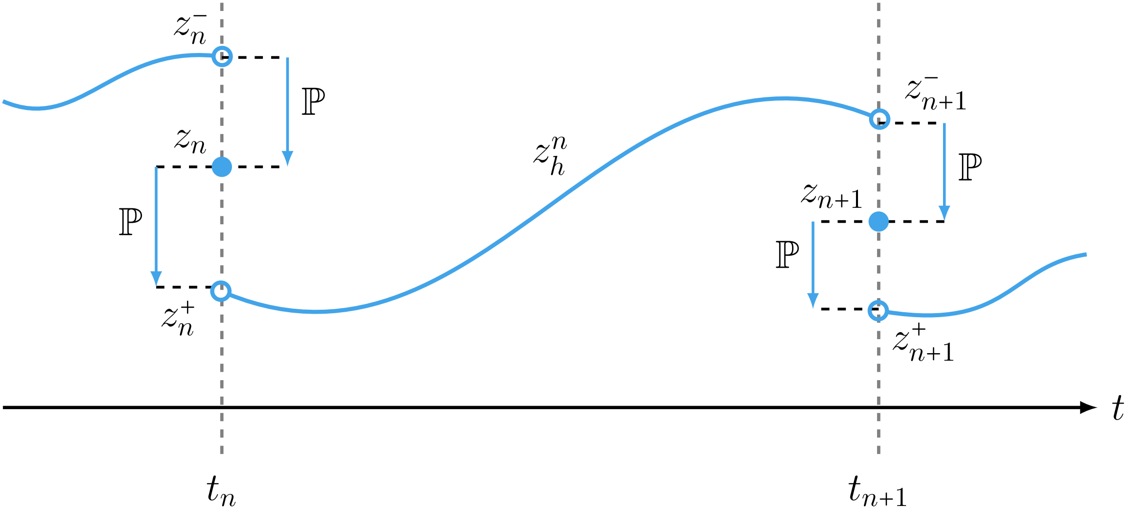
Variational Projection I



Variational Projection II



Symmetric Projection



Discontinuous Galerkin Variational Integrators

Discontinuous Galerkin Variational Integrators

- continuous action with degenerate Lagrangian $L : \mathsf{T}\mathcal{M} \to \mathbb{R}$

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

- 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 $\bar{\mathcal{I}}_n = [t_n, t_{n+1}]$
- on each interval $\mathcal{I}_n$, construct polynomials $q_h^n(t) \in \mathbb{P}^r(\mathcal{I}_n)$, which approximate the trajectory

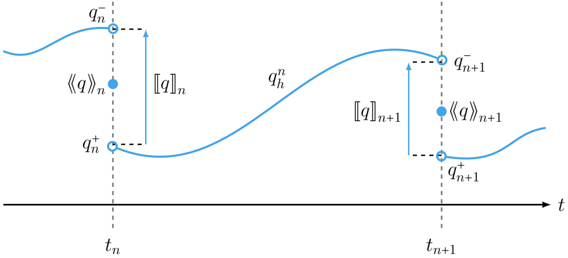
$$q_h^n(t) \approx q(t) \big|_{(t_n, t_{n+1})}$$

- the approximated trajectories q_h on the configuration space $\mathcal{M}$ are elements of

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

and appropriate basis functions $\varphi_{n,i}$ (e.g., Lagrange polynomials)

Jump and Average Operators



- denote the values of the polynomials q_h^n and q_h^{n+1} at the node t_{n+1} by q_{n+1}^- and q_{n+1}^+, given by

$$q_{n+1}^- = \lim_{t \uparrow t_{n+1}} q_h^n(t), \qquad q_{n+1}^+ = \lim_{t \downarrow t_{n+1}} q_h^{n+1}(t)$$

- denote the average operator by $\langle\!\langle q \rangle\!\rangle$ and the jump operator by $[\![q]\!]$, given by

$$\langle\!\langle q \rangle\!\rangle_n = \begin{cases} q_0, & n = 0, \\ \alpha q_n^- + (1-\alpha) q_n^+, & 0 < n < N, \\ q_N, & n = N, \end{cases} \qquad [\![q]\!]_n = \begin{cases} q_0^+ - q_0, & n = 0, \\ q_n^+ - q_n^-, & 0 < n < N, \\ q_N - q_N^-, & n = N, \end{cases}$$

Discontinuous Galerkin Variational Integrators

- together, the average operator and the jump operator define the numerical flux $\vartheta(\langle\!\langle q \rangle\!\rangle_n) \cdot [\![q]\!]_n$
- choosing a quadrature rule (b_i, c_i) with $i = 1, ..., s$, the discrete action can be written as

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

- the solutions q_n at each time t_n define the discrete phasespace trajectory $q_d = \{ q_n \}_{n=0}^{N}$
- these solutions are obtained via the average operator by setting $q_n = \langle\!\langle q \rangle\!\rangle_n$
- discrete Lagrangian

$$L_d(\langle\!\langle q \rangle\!\rangle_n , \langle\!\langle q \rangle\!\rangle_{n+1} , [\![q]\!]_n , [\![q]\!]_{n+1}) = \underset{\substack{Q_{n,i}, \\ \langle\!\langle q \rangle\!\rangle_n = q_n^+ - \frac{1}{2} [\![q]\!]_n , \\ \langle\!\langle q \rangle\!\rangle_{n+1} = q_{n+1}^- + \frac{1}{2} [\![q]\!]_{n+1}}}{\text{ext}} \Bigg\{ h \sum_{i=1}^{s} b_i \Big[\vartheta(q_h^n(t_n + c_i h)) \cdot \dot{q}_h^n(t_n + c_i h) - H(q_h^n(t_n + c_i h)) \Big] + \frac{1}{2} \Big[\vartheta(\langle\!\langle q \rangle\!\rangle_n) \cdot [\![q]\!]_n + \vartheta(\langle\!\langle q \rangle\!\rangle_{n+1}) \cdot [\![q]\!]_{n+1} \Big] \Bigg\}$$

Example: Linear Lagrange Polynomials and Trapezoidal Quadrature

- piecewise linear discretisation of $q(t)$, given by

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

  so that the corresponding discrete velocity becomes

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

- approximate the action integral by the trapezoidal rule to obtain the discrete action

$$\mathcal{A}_d[q_d] = \frac{h}{2} \sum_{n=0}^{N-1} \left[L\left(q_n^+, \frac{q_{n+1}^- - q_n^+}{h} \right) + L\left(q_{n+1}^-, \frac{q_{n+1}^- - q_n^+}{h} \right) \right] + \sum_{n=1}^{N-1} \left[\vartheta\left(\frac{q_n^- + q_n^+}{2} \right) \cdot \left(q_n^+ - q_n^- \right) \right] + \vartheta(q_0) \cdot (q_0^+ - q_0) + \vartheta(q_N) \cdot (q_N - q_N^-)$$

Example: Linear Lagrange Polynomials and Trapezoidal Quadrature

- discrete Euler–Lagrange equations obtained from $\delta \mathcal{A}_d = 0$ with $\delta q_0 = \delta q_N = 0$

$$\vartheta\left(\frac{q_n^- + q_n^+}{2}\right) = \frac{\vartheta(q_n^+) + \vartheta(q_{n+1}^-)}{2} - \frac{h}{2}\left[\nabla\vartheta(q_n^+) \cdot \frac{q_{n+1}^- - q_n^+}{h} - \nabla H(q_n^+)\right] - \nabla\vartheta^T\left(\frac{q_n^- + q_n^+}{2}\right) \cdot (q_n^+ - q_n^-),$$

$$\vartheta\left(\frac{q_{n+1}^- + q_{n+1}^+}{2}\right) = \frac{\vartheta(q_n^+) + \vartheta(q_{n+1}^-)}{2} + \frac{h}{2}\left[\nabla\vartheta(q_{n+1}^-) \cdot \frac{q_{n+1}^- - q_n^+}{h} - \nabla H(q_{n+1}^-)\right] - \nabla\vartheta^T\left(\frac{q_{n+1}^- + q_{n+1}^+}{2}\right) \cdot (q_{n+1}^+ - q_{n+1}^-)$$

- introducing additional variables p_n^+ and p_{n+1}^-

$$\begin{aligned}
q_n^+ &= \langle\!\langle q \rangle\!\rangle_n + \tfrac{1}{2} [\![q]\!]_n , \\
p_n^+ &= \vartheta(\langle\!\langle q \rangle\!\rangle_n) - \tfrac{1}{2} [\![q]\!]_n \cdot \nabla\vartheta^T(\langle\!\langle q \rangle\!\rangle_n), \\
p_n^+ &= \tfrac{1}{2}(\vartheta(q_n^+) + \vartheta(q_{n+1}^-)) - \tfrac{1}{2}\nabla\vartheta(q_n^+) \cdot (q_{n+1}^- - q_n^+) + \tfrac{h}{2}\nabla H(q_n^+), \\
p_{n+1}^- &= \tfrac{1}{2}(\vartheta(q_n^+) + \vartheta(q_{n+1}^-)) + \tfrac{1}{2}\nabla\vartheta(q_{n+1}^-) \cdot (q_{n+1}^- - q_n^+) - \tfrac{h}{2}\nabla H(q_{n+1}^-), \\
\langle\!\langle q \rangle\!\rangle_{n+1} &= q_{n+1}^- + \tfrac{1}{2} [\![q]\!]_{n+1} , \\
\vartheta(\langle\!\langle q \rangle\!\rangle_{n+1}) &= p_{n+1}^- - \tfrac{1}{2} [\![q]\!]_{n+1} \cdot \nabla\vartheta^T(\langle\!\langle q \rangle\!\rangle_{n+1}).
\end{aligned}$$

$\rightarrow$ similar to symmetric projection with the jump operator $[\![q]\!]$ taking the place of the Lagrange multiplier λ

Summary and Outlook

Summary and Outlook

- variational integrators for degenerate Lagrangians
  - intrinsic: multi-step methods susceptible to parasitic modes
  - extrinsic: position-momentum form violates constraint submanifold
- projected variational integrators
  - embed degenerate Lagrangian systems into larger canonical Hamiltonian systems
  - use constraints to restrict the dynamics to the original space by symmetric projection
  - very good long-time stability, approximate conservation of energy, exact conservation of momenta
  - either not symplectic or not conserving the constraint submanifold exactly
- discontinuous Galerkin variational integrators
  - one-step methods directly from the discrete action principle (no need for treating an extended system)
  - careful and rigorous derivation of jump operator using LeFloch's theory of nonconservative products
- ongoing work
  - discrete mechanics (symplectic structure, Noether theorem)
  - discontinuous Galerkin variational integrators for Hamiltonian systems subject to Dirac constraints
  - Hamilton–Pontryagin–Galerkin integrators (unifying framework for many known variational integrators)