Co-funded by
the European Union

Discontinuous Galerkin Variational Integrators

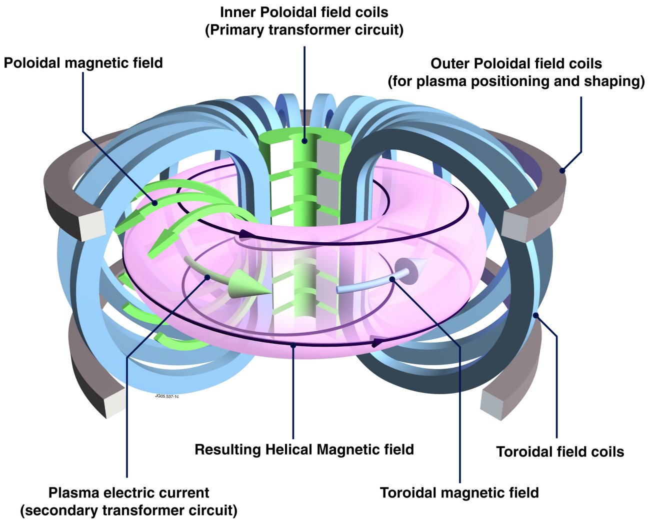
Towards the Geometric Discretisation of the Guiding Centre System

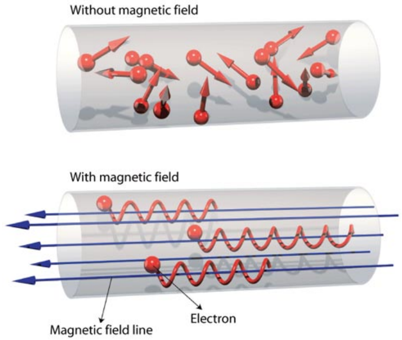
Michael Kraus[1,2,3] (michael.kraus@ipp.mpg.de)

In collaboration with Joshua Burby[4], Leland Ellison[5], Omar Maj[1,2], Hiroaki Yoshimura[3]

[1] Max-Planck-Institut für Plasmaphysik
[2] Technische Universität München, Zentrum Mathematik
[3] Waseda University, School of Science and Engineering
[4] Courant Institute of Mathematical Sciences, New York University
[5] Lawrence Livermore National Laboratory

Charged Particle Motion in Strong Magnetic Fields





Guiding Centre Dynamics

- split charged particle motion x into guiding centre motion X and gyro motion ρ

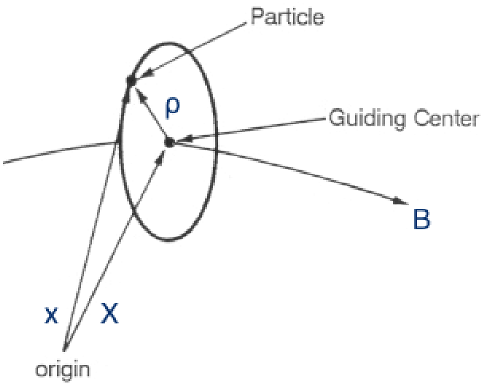
$$x = X + \rho$$

- strong magnetic fields: neglect finite gyroradius effects
- noncanonical Hamiltonian system

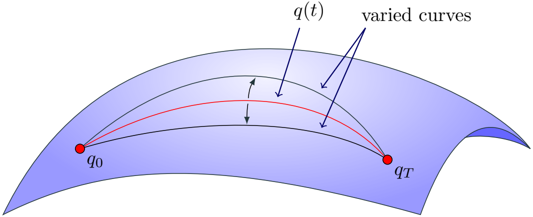
$$\dot{q} = \bar{\Omega}^{-1}(q)\,\nabla H(q)$$

- Lagrangian description: Euler–Lagrange equations

$$\frac{\partial L}{\partial q}(q, \dot{q}) - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}(q, \dot{q})\right) = 0, \qquad L(q, \dot{q}) = \vartheta(q) \cdot \dot{q} - H(q), \qquad \bar{\Omega}_{ij} = \frac{\partial \vartheta_j}{\partial z^i} - \frac{\partial \vartheta_i}{\partial z^j}$$



Hamilton's Principle of Stationary Action



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

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

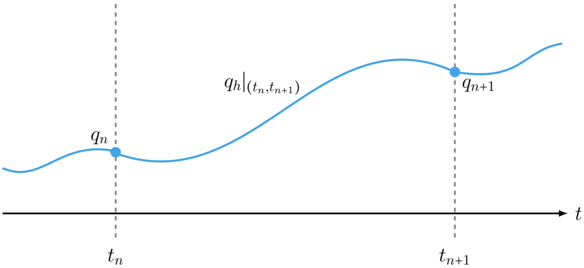
- Hamilton's principle of stationary action: among all possible trajectories q connecting q_0 and q_T, the physical trajectory makes the action integral $\mathcal{A}$ stationary
- variation and integration by parts (endpoints fixed: $\delta q(0) = \delta q(T) = 0$)

$$\delta \mathcal{A}[q] = \int_0^T \left[\frac{\partial L}{\partial q} \cdot \delta q + \frac{\partial L}{\partial \dot q} \cdot \delta \dot q\right] dt = \int_0^T \left[\frac{\partial L}{\partial q} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot q}\right)\right] \cdot \delta q\, dt + \cancelto{0}{\left[\frac{\partial L}{\partial \dot q} \cdot \delta q\right]_0^T} = 0 \text{ for all } \delta q$$

- requiring stationarity of the action leads to the Euler-Lagrange equations of motion

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

Continuous Galerkin Approximation



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

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

- approximate q such that discrete trajectories q_h in the time interval $[0, T]$ are elements of

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

Discrete Variational Principle

- upon choosing a quadrature rule (b_i, c_i), the discrete Lagrangian becomes

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

- discrete Action with discrete trajectory $q_d = \{ q_n = q_h(t_n) \}_{n=0}^{N}$

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

- 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

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

Guiding Centre Lagrangian

- the guiding centre Lagrangian is a special case of degenerate Lagrangian linear in velocities

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

  where ϑ is a general, usually nonlinear function of q

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

$$\frac{d}{dt}\vartheta(q) = \nabla\vartheta(q) \cdot \dot{q} - \nabla H(q)$$

- the discrete Euler–Lagrange equations correspond to multi-step variational integrators Ψ_{L_d}

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

→ susceptible to parasitic modes driving simulations unstable

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

Variational Guiding Centre Integrators

- analogously to the continuous Legendre-transform,

$$p = \frac{\partial L}{\partial \dot{q}}(q, \dot{q}) = \vartheta(q),$$

we use the discrete Legendre-transform to rewrite the DELEQs in position-momentum form

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

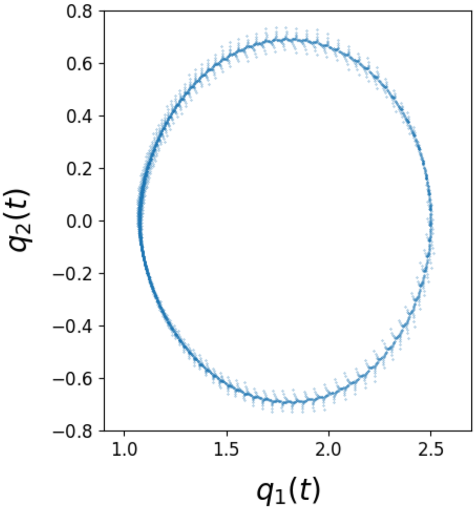
- can be solved as the discrete Lagrangian L_d is not degenerate, providing an update rule

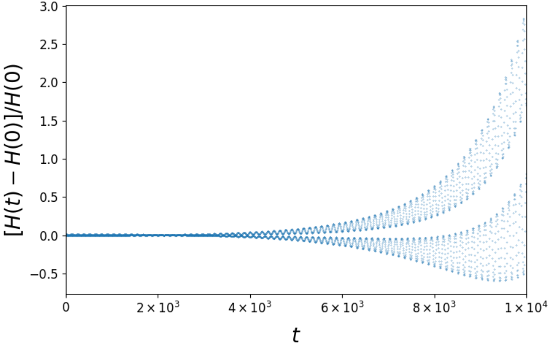
$$\tilde{\Psi}_{L_d} : (q_n, p_n) \mapsto (q_{n+1}, p_{n+1})$$

- use continuous Legendre-transform to obtain an exact second initial condition p_0 given q_0

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

Passing Guiding Centre Particle with Variational Integrator





[http://github.com/DDMGNI/GeometricIntegrators.jl]

Passing Guiding Centre Particle with Variational Integrator

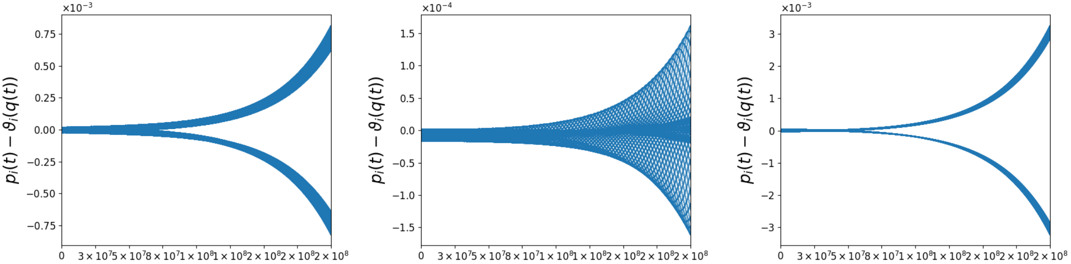
- position-momentum form: rewrite the equations of motion as an index-two DAE

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

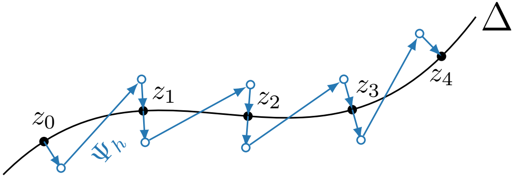
- the variational integrator does not preserve the constraint $\phi(q, p) = 0$

→ the numerical solution drifts away from the constraint submanifold

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



Symmetric Projection



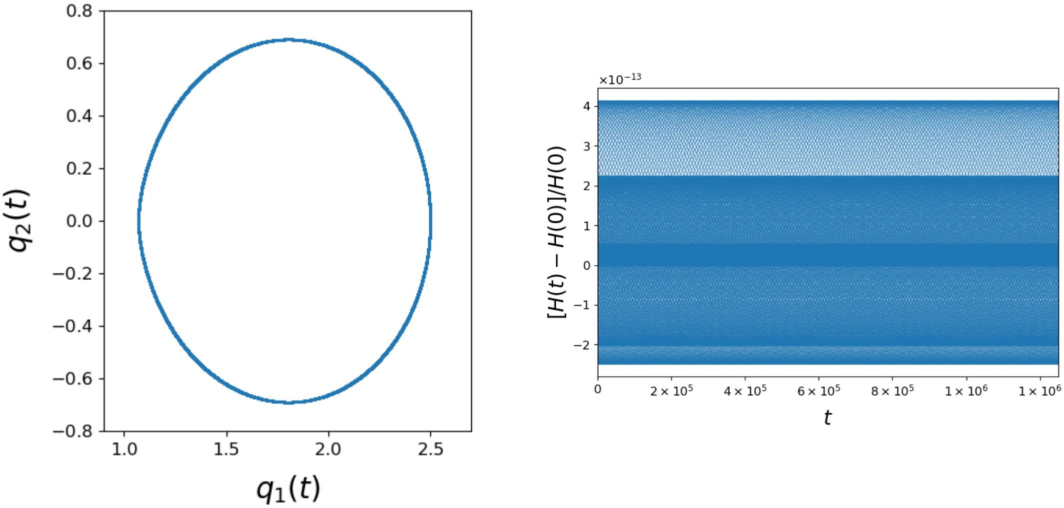
- index-two differential-algebraic equation

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

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

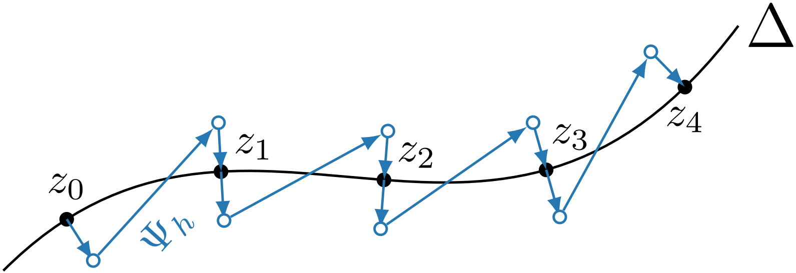
$$\tilde z_n = z_n + h\,\Omega^{-1}\nabla\phi^T(z_n)\,\lambda_{n+1} \qquad \text{perturb}$$
$$\tilde z_{n+1} = \Psi_h(\tilde z_n) \qquad \text{apply arbitrary one-step method}$$
$$z_{n+1} = \tilde z_{n+1} + h\,R(\infty)\,\Omega^{-1}\nabla\phi^T(z_{n+1})\lambda_{n+1} \qquad \text{project on constraint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

Passing Guiding Centre Particle with Projected Variational Integrator



[http://github.com/DDMGNI/GeometricIntegrators.jl]

Symmetric Projection



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

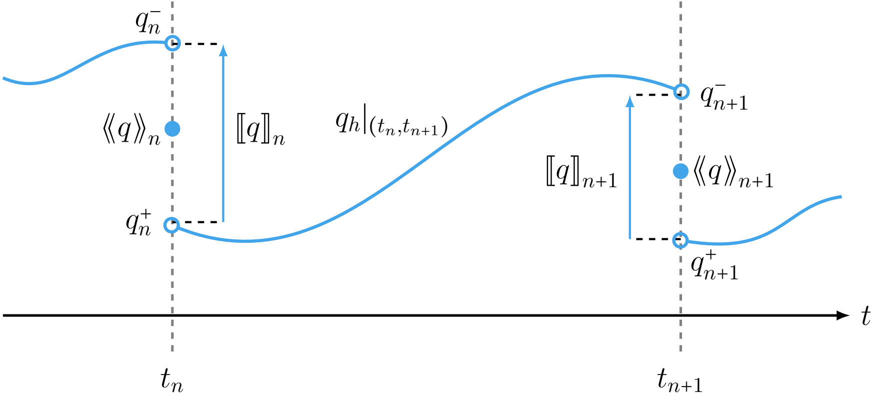
$$\tilde{z}_n = z_n + h\,\Omega^{-1}\nabla\phi^T(z_n)\,\lambda_{n+1} \qquad \text{perturb}$$

$$\tilde{z}_{n+1} = \Psi_h(\tilde{z}_n) \qquad \text{apply arbitrary one-step method}$$

$$z_{n+1} = \tilde{z}_{n+1} + h\,R(\infty)\,\Omega^{-1}\nabla\phi^T(z_{n+1})\lambda_{n+1} \qquad \text{project on constraint submanifold}$$

$$0 = \phi(z_{n+1}) \qquad \text{constraint}$$

Discontinuous Galerkin Approximation



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

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

with limits $q_n^+ = \lim_{t \downarrow t_n} q_h(t)$, $q_{n+1}^- = \lim_{t \uparrow t_n} q_h(t_{n+1})$, jumps $[\![q]\!]_n = q_n^+ - q_n^-$, averages $\langle\!\langle q \rangle\!\rangle_n = \frac{1}{2}(q_n^- + q_n^+)$

Discontinuous Galerkin Action Principle

- discontinuous Galerkin action principle for the Lagrangian $L(q, \dot{q}) = \vartheta(q) \cdot \dot{q} - H(q)$

$$\delta \sum_{n=0}^{N-1} \left(h \sum_{i=1}^{s} b_i \, L\big(q_h(t_n + c_i h), \; \dot{q}_h(t_n + c_i h) \big) + [\text{numerical flux}] \right) = 0$$

  with discontinuous trajectories $q_h|_{(t_n, t_{n+1})}$ and a quadrature rule with weights b_i and nodes c_i

- discrete solution: $q_d = \{ q_n = \langle\!\langle q \rangle\!\rangle_n \}_{n=0}^{N}$ with the averages $\langle\!\langle q \rangle\!\rangle_n = \frac{1}{2}(q_n^- + q_n^+)$

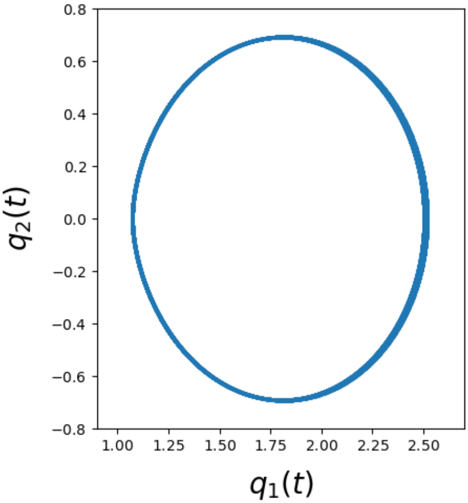
- the numerical flux is crucial for the stability and conservation properties of the integrator

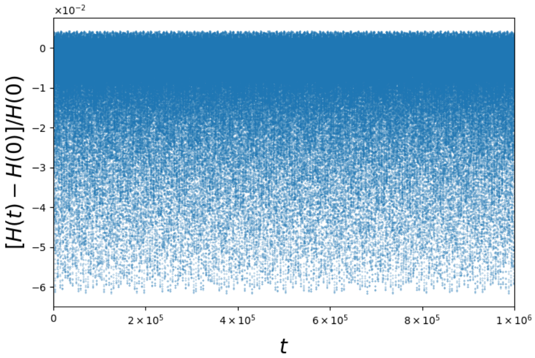
- candidate fluxes: approximations of the nonconservative product $\vartheta(q) \cdot \dot{q}$ of the form

$$\int_0^1 \vartheta\big(\phi(\tau; q_n^-, q_n^+)\big) \, \frac{d\phi}{d\tau}(\tau; q_n^-, q_n^+) \, d\tau \quad \approx \quad \sum_{i=1}^{\sigma} \beta_i \, \vartheta\big(\phi(\gamma_i; q_n^-, q_n^+)\big) \, \phi'(\gamma_i; q_n^-, q_n^+)$$

  with ϕ a path connecting q_n^- and q_n^+ and (β_i, γ_i) the weights and nodes of a quadrature rule

Passing Guiding Centre Particle with DG Variational Integrator





[http://github.com/DDMGNI/GeometricIntegrators.jl]

Summary and Outlook

- variational integrators
  - obtained from a variational principle applied to a discrete action
  - automatically preserve conservation laws originating from symmetries of the Lagrangian as well as a discrete symplectic structure, leading to good long-time energy behaviour
  - for degenerate Lagrangian systems VIs usually constitute multi-step methods, subject to parasitic modes
- projected variational integrators for degenerate Lagrangians
  - very good long-time stability, approximate conservation of energy, exact conservation of momenta
  - either not flexible or not symplectic or not conserving the constraint submanifold exactly

  [Projected Variational Integrators for Degenerate Lagrangian Systems, arXiv:1708.07356]
- discontinuous Galerkin variational integrators
  - one-step methods for degenerate Lagrangians obtained directly from a discrete action principle
  - careful and rigorous derivation of numerical fluxes using LeFloch's theory of nonconservative products

  [Hamilton-Pontryagin-Galerkin Integrators, in preparation]

  [Discontinuous Galerkin Variational Integrators for Degenerate Lagrangians, in preparation]