General Techniques for Constructing Variational Integrators

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Joint work with James Hall, Cuicui Liao, Tatiana Shingel,
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Rough Paths and Combinatorics in Control Theory, UCSD, July, 2011.

arXiv:1001.1408 arXiv:1101.1995 arXiv:1102.2685

Supported in part by NSF DMS-0726263,
DMS-1001521, DMS-1010687 (CAREER).

Geometry and Numerical Methods

■ Dynamical equations preserve structure

- Many continuous systems of interest have properties that are conserved by the flow:
    - Energy
    - Symmetries, Reversibility, Monotonicity
    - Momentum - Angular, Linear, Kelvin Circulation Theorem.
    - Symplectic Form
    - Integrability
- At other times, the equations themselves are defined on a manifold, such as a Lie group, or more general configuration manifold of a mechanical system, and the discrete trajectory we compute should remain on this manifold, since the equations may not be well-defined off the surface.

Motivation: Geometric Integration

- **Main Goal of Geometric Integration:**

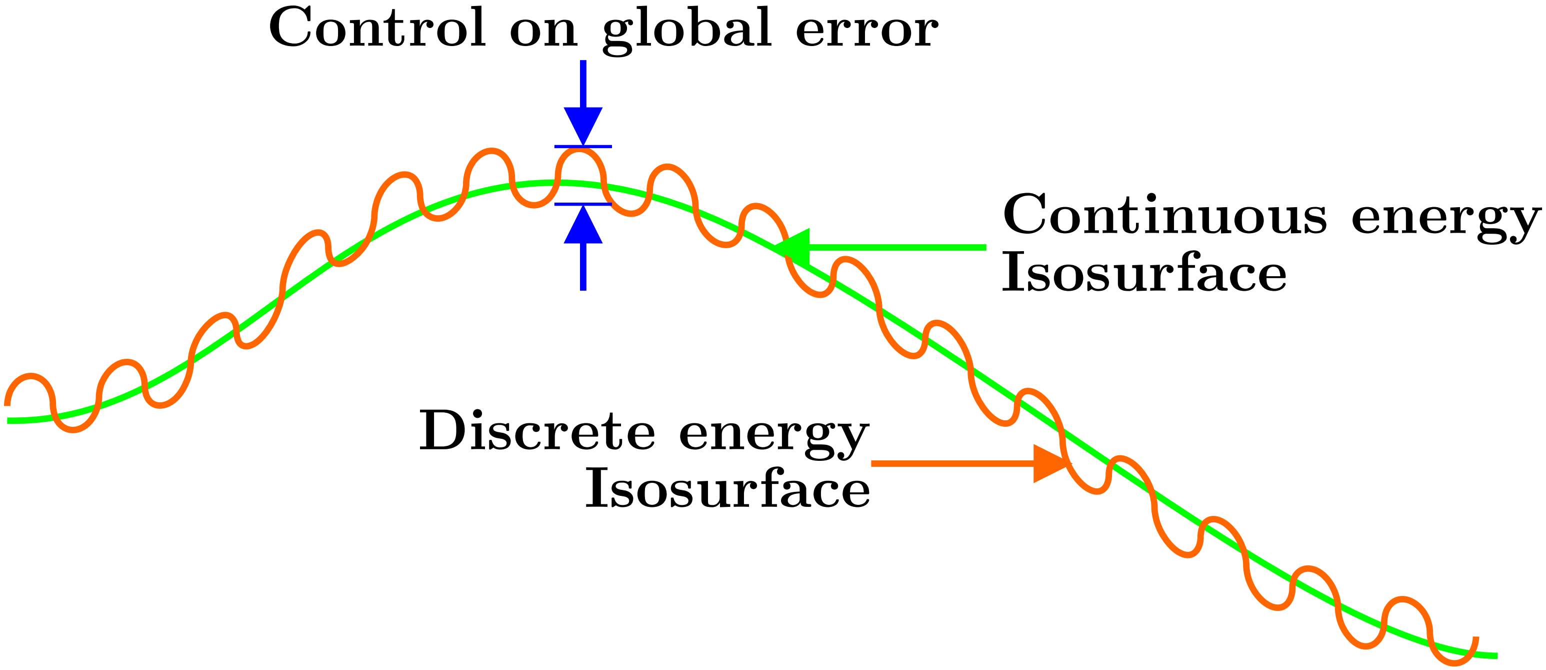
  Structure preservation in order to reproduce long time behavior.

- **Role of Discrete Structure-Preservation:**

  Discrete conservation laws impart long time numerical stability to computations, since the structure-preserving algorithm exactly conserves a discrete quantity that is always close to the continuous quantity we are interested in.

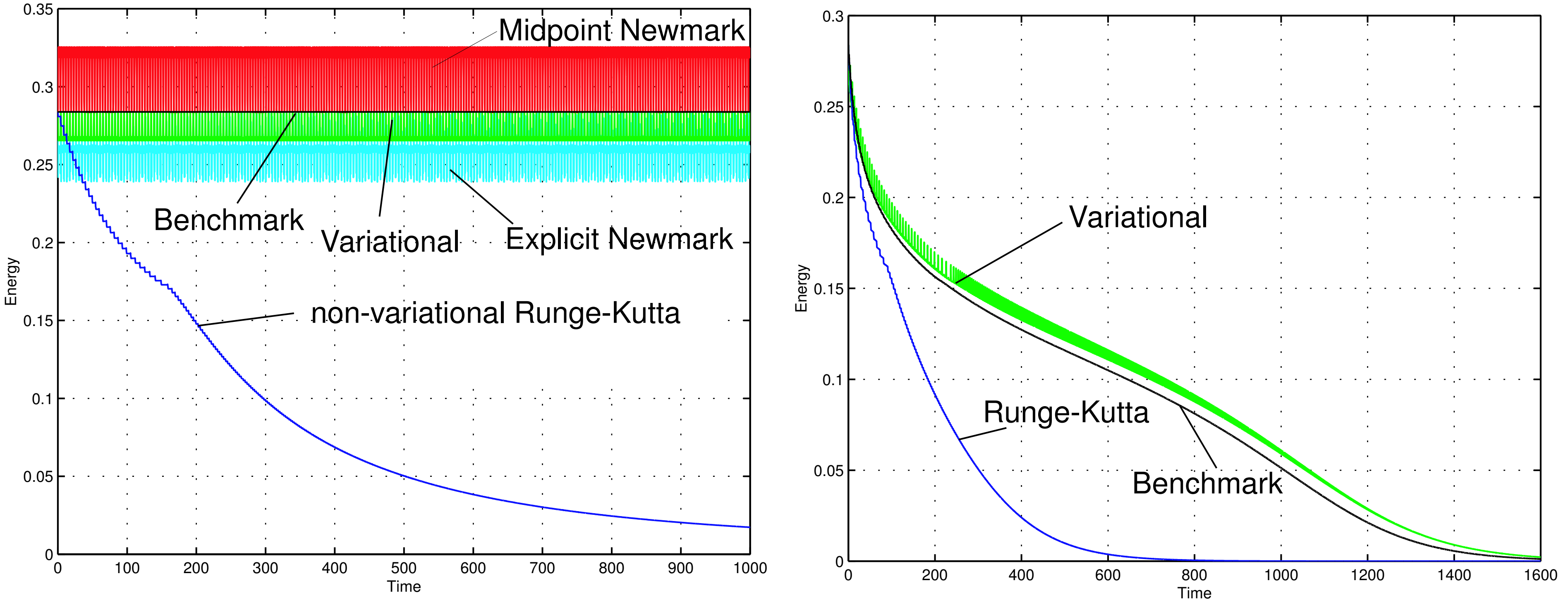
Geometric Integration: Energy Stability

- **Energy stability for symplectic integrators**



Geometric Integration: Energy Stability

🟧 Energy behavior for conservative and dissipative systems



(a) Conservative mechanics (b) Dissipative mechanics

Geometric Integration: Energy Stability

Solar System Simulation

- Forward Euler

$$\begin{aligned}\mathbf{q}_{k+1} &= \mathbf{q}_k + h\dot{\mathbf{q}}(\mathbf{q}_k, \mathbf{p}_k),\\ \mathbf{p}_{k+1} &= \mathbf{p}_k + h\dot{\mathbf{p}}(\mathbf{q}_k, \mathbf{p}_k).\end{aligned}$$

- Inverse Euler

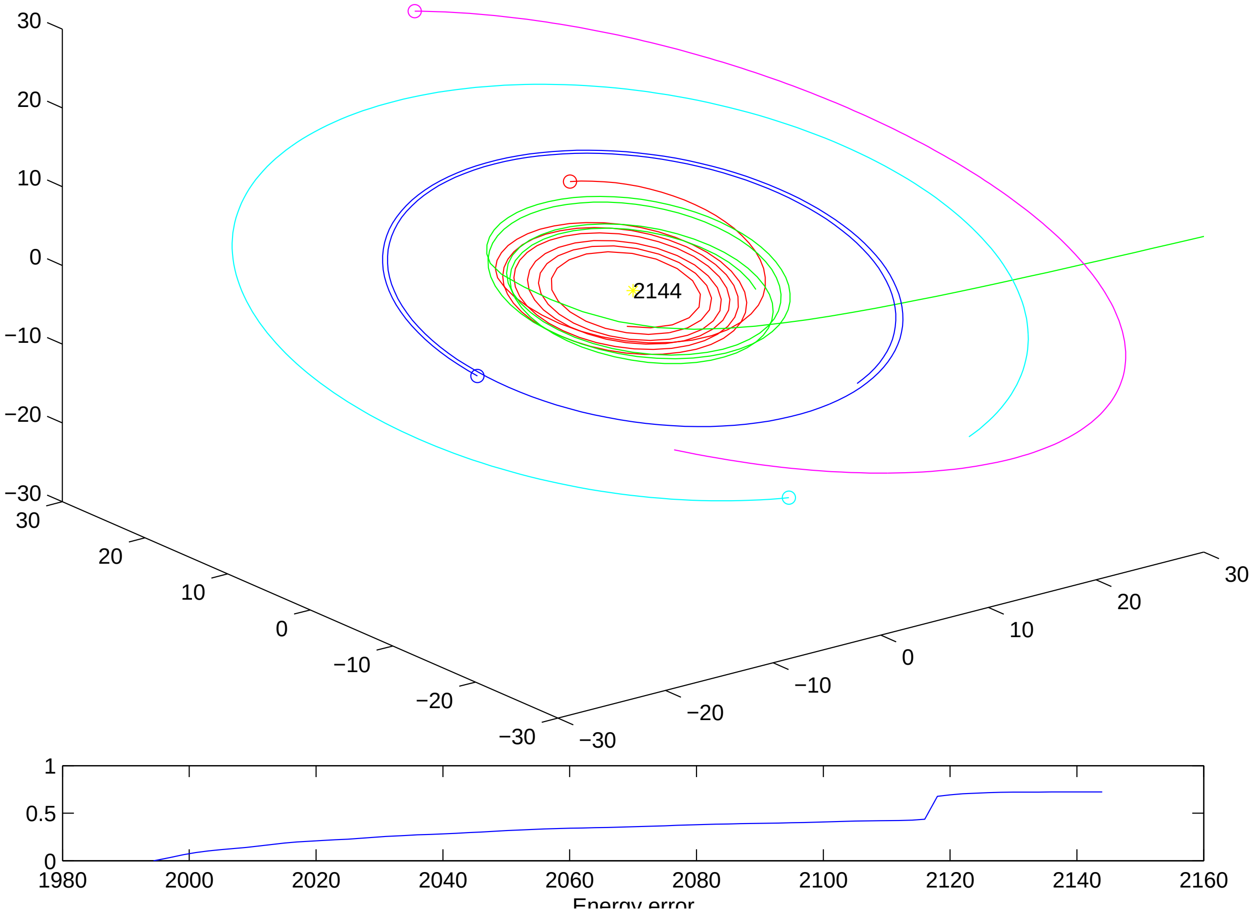
$$\begin{aligned}\mathbf{q}_{k+1} &= \mathbf{q}_k + h\dot{\mathbf{q}}(\mathbf{q}_{k+1}, \mathbf{p}_{k+1}),\\ \mathbf{p}_{k+1} &= \mathbf{p}_k + h\dot{\mathbf{p}}(\mathbf{q}_{k+1}, \mathbf{p}_{k+1}).\end{aligned}$$

- Symplectic Euler

$$\begin{aligned}\mathbf{q}_{k+1} &= \mathbf{q}_k + h\dot{\mathbf{q}}(\mathbf{q}_k, \mathbf{p}_{k+1}),\\ \mathbf{p}_{k+1} &= \mathbf{p}_k + h\dot{\mathbf{p}}(\mathbf{q}_k, \mathbf{p}_{k+1}).\end{aligned}$$

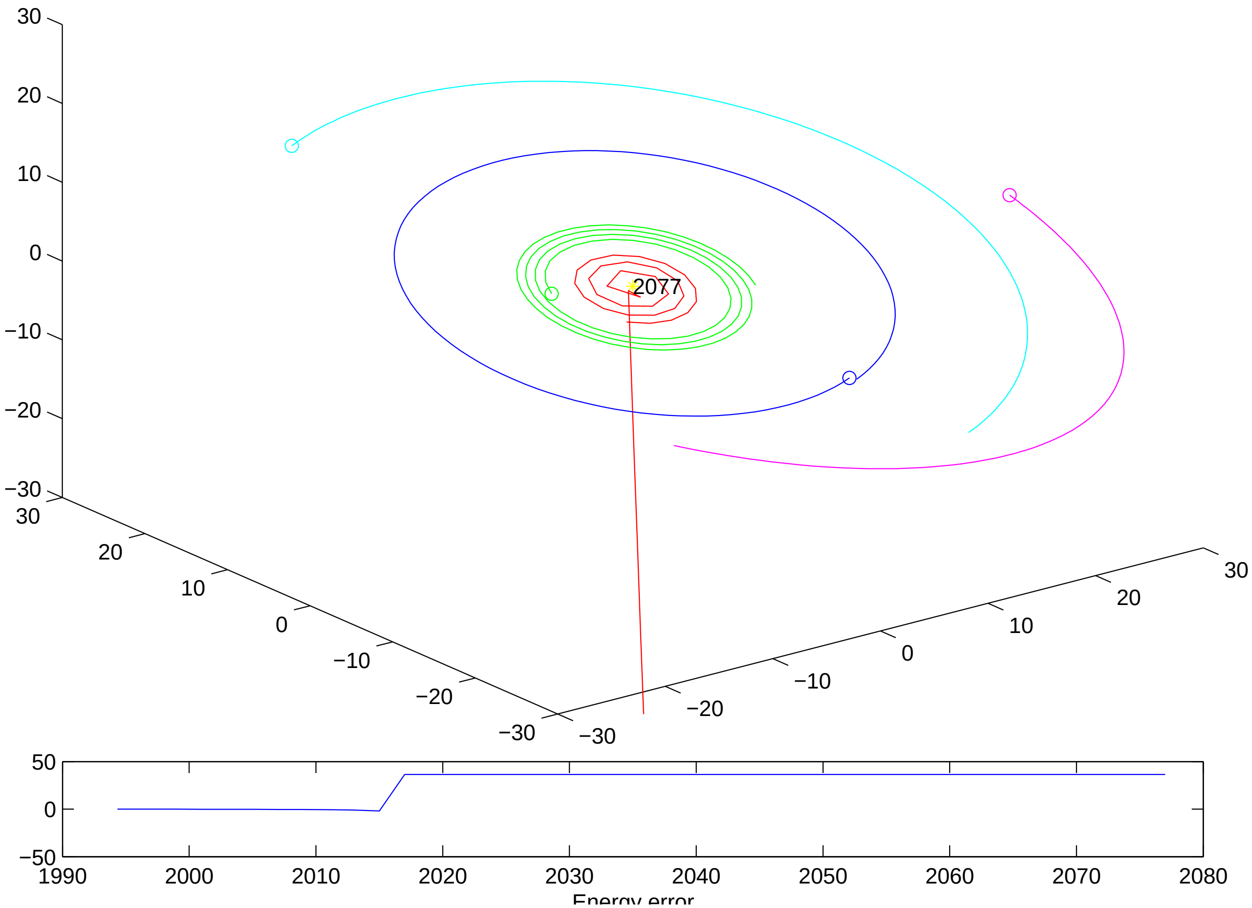
Geometric Integration: Energy Stability

■ Forward Euler



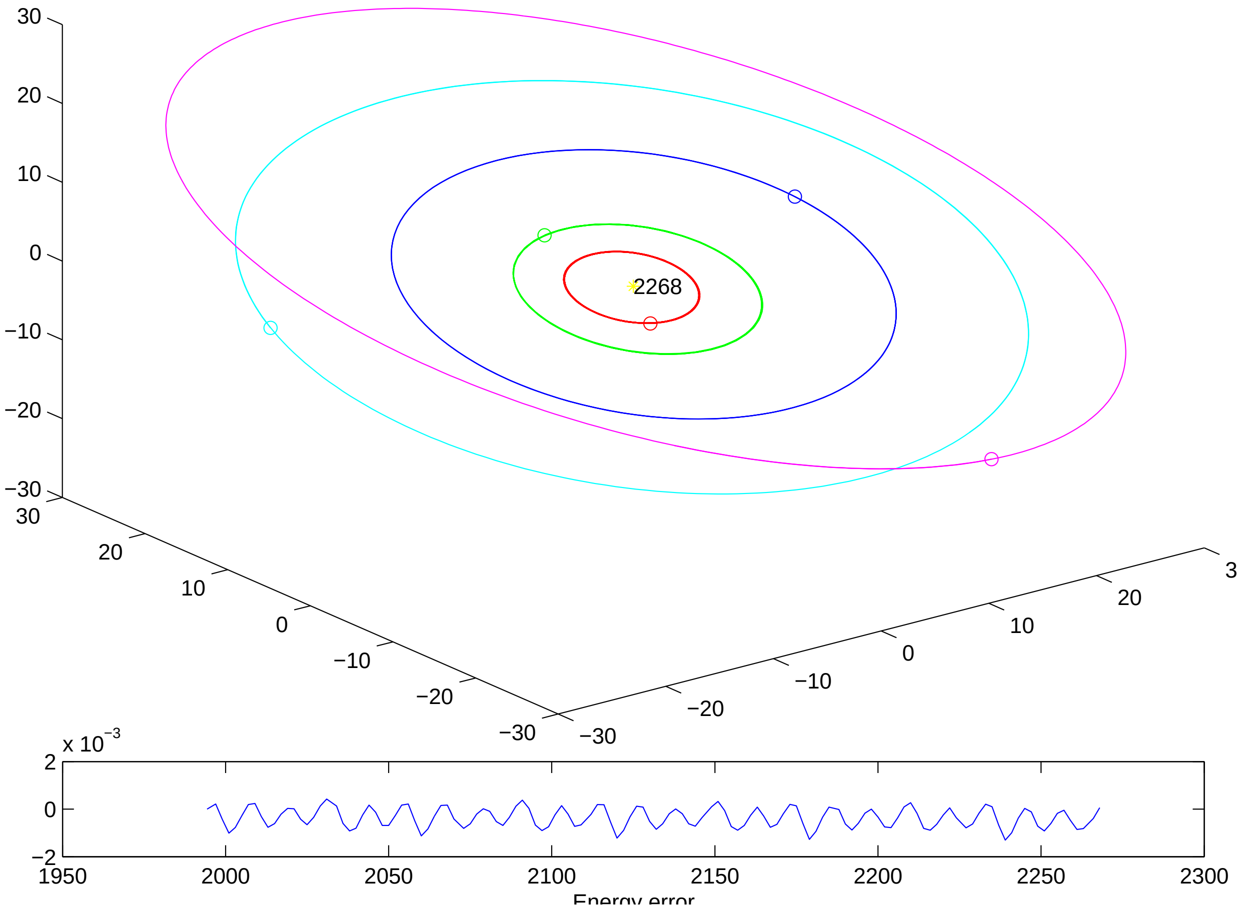
Geometric Integration: Energy Stability

- **Inverse Euler**



Geometric Integration: Energy Stability

Symplectic Euler



Introduction to Computational Geometric Mechanics

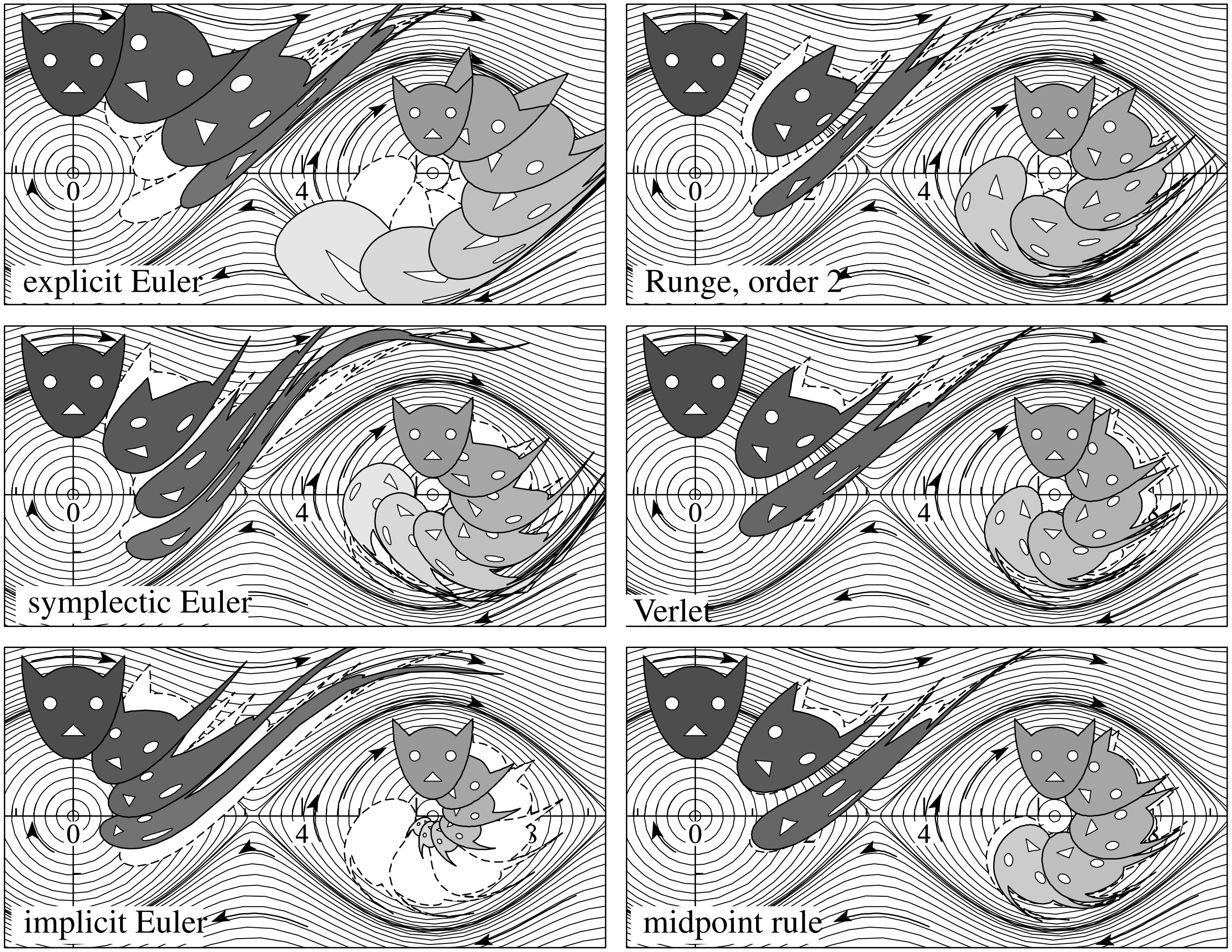
Geometric Mechanics

- Differential geometric and symmetry techniques applied to the study of Lagrangian and Hamiltonian mechanics.

Computational Geometric Mechanics

- Constructing computational algorithms using ideas from geometric mechanics.
- Variational integrators based on discretizing Hamilton's principle, automatically symplectic and momentum preserving.

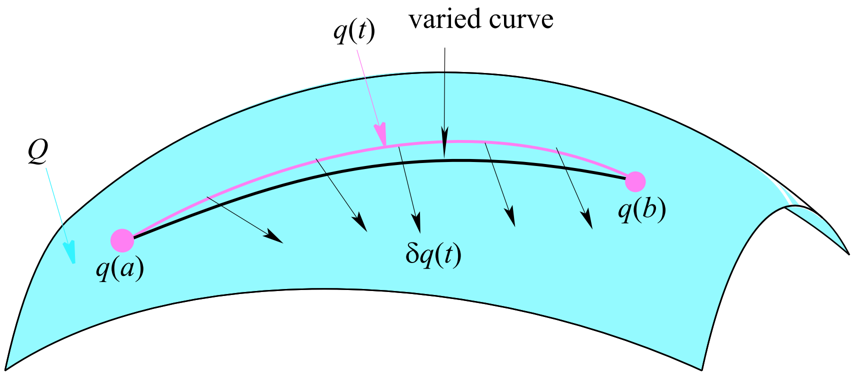
Symplecticity in the Planar Pendulum

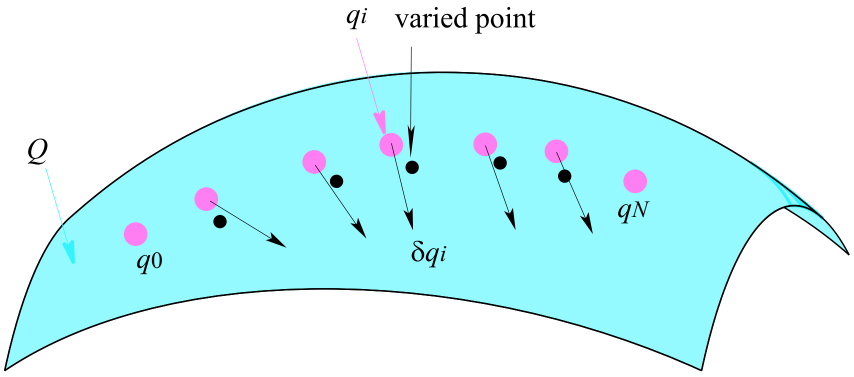


Images courtesy of Hairer, Lubich, Wanner, *Geometric Numerical Integration*, 2nd Edition, Springer, 2006.

Lagrangian Variational Integrators

Discrete Variational Principle





- **Discrete Lagrangian**

$$L_d(q_0, q_1) \approx L_d^{\text{exact}}(q_0, q_1) \equiv \int_0^h L\left(q_{0,1}(t), \dot{q}_{0,1}(t)\right) dt,$$

  where $q_{0,1}(t)$ satisfies the Euler–Lagrange equations for L and the boundary conditions $q_{0,1}(0) = q_0$, $q_{0,1}(h) = q_1$.

- This is related to **Jacobi's solution** of the **Hamilton–Jacobi equation**.

Lagrangian Variational Integrators

Discrete Variational Principle

- **Discrete Hamilton's principle**

$$\delta \mathbb{S}_d = \delta \sum L_d(q_k, q_{k+1}) = 0,$$

where q_0, q_N are fixed.

Discrete Euler–Lagrange Equations

- **Discrete Euler-Lagrange equation**

$$D_2 L_d(q_{k-1}, q_k) + D_1 L_d(q_k, q_{k+1}) = 0.$$

- The associated discrete flow $(q_{k-1}, q_k) \mapsto (q_k, q_{k+1})$ is automatically symplectic, since it is equivalent to,

$$p_k = -D_1 L_d(q_k, q_{k+1}), \quad p_{k+1} = D_2 L_d(q_k, q_{k+1}),$$

which is the **Type I generating function** characterization of a symplectic map.

Lagrangian Variational Integrators

Main Advantages of Variational Integrators

- **Discrete Noether's Theorem**

  If the discrete Lagrangian L_d is (infinitesimally) G-invariant under the diagonal group action on $Q \times Q$,

  $$L_d(gq_0, gq_1) = L_d(q_0, q_1)$$

  then the **discrete momentum map** $J_d : Q \times Q \to \mathfrak{g}^*$,

  $$\langle J_d\left(q_k, q_{k+1}\right), \xi\rangle \equiv \left\langle D_1 L_d\left(q_k, q_{k+1}\right), \xi_Q\left(q_k\right)\right\rangle$$

  is preserved by the discrete flow.

Lagrangian Variational Integrators

Main Advantages of Variational Integrators

- **Variational Error Analysis**
  Since the exact discrete Lagrangian generates the exact solution of the Euler–Lagrange equation, the exact discrete flow map is *formally* expressible in the setting of variational integrators.
- This is analogous to the situation for B-series methods, where the exact flow can be expressed formally as a B-series.
- If a computable discrete Lagrangian L_d is of order r, i.e.,

$$L_d(q_0, q_1) = L_d^{\text{exact}}(q_0, q_1) + \mathcal{O}(h^{r+1})$$

  then the discrete Euler–Lagrange equations yield an order r accurate symplectic integrator.

Constructing Discrete Lagrangians

Systematic Approaches

- The theory of variational error analysis suggests that one should aim to construct computable approximations of the exact discrete Lagrangian.
- There are two equivalent characterizations of the exact discrete Lagrangian:
    - Euler–Lagrange boundary-value problem characterization,
    - Variational characterization,

  which lead to two general classes of computable discrete Lagrangians:
    - Shooting-based discrete Lagrangians.
    - Galerkin discrete Lagrangians,

Shooting-Based Variational Integrators

Boundary-Value Problem Characterization of L_d^{exact}

- The classical characterization of the exact discrete Lagrangian is Jacobi's solution of the Hamilton–Jacobi equation, and is given by,

$$L_d^{\text{exact}}(q_0, q_1) \equiv \int_0^h L\left(q_{0,1}(t), \dot{q}_{0,1}(t)\right) dt,$$

where $q_{0,1}(t)$ satisfies the Euler–Lagrange boundary-value problem.

Shooting-Based Discrete Lagrangians

- Replaces the solution of the Euler–Lagrange boundary-value problem with the shooting-based solution from a **one-step method**.
- Replace the integral with a **numerical quadrature formula**.

Shooting-Based Variational Integrators

Shooting-Based Discrete Lagrangian

- Consider a one-step method $\Psi_h : TQ \to TQ$, and a numerical quadrature formula
$$\int_0^h f(x)dx \approx h\sum_{i=0}^{n} b_i f(x(c_i h)),$$
with quadrature weights b_i and quadrature nodes $0 = c_0 < c_1 < \ldots < c_{n-1} < c_n = 1$.
- We construct the **shooting-based discrete Lagrangian**,
$$L_d(q_0, q_1; h) = h\textstyle\sum_{i=0}^{n} b_i L(q^i, v^i),$$
where
$$(q^{i+1}, v^{i+1}) = \Psi_{(c_{i+1}-c_i)h}(q^i, v^i), \qquad q^0 = q_0, \qquad q^n = q_1.$$

Shooting-Based Variational Integrators

Implementation Issues

- While one can view the implicit definition of the discrete Lagrangian separately from the implicit discrete Euler–Lagrange equations,

$$p_0 = -D_1 L_d(q_0, q_1; h), \qquad p_1 = D_2 L_d(q_0, q_1; h),$$

in practice, one typically considers the two sets of equations together to implicitly define a one-step method:

$$\begin{aligned}
L_d(q_0, q_1; h) &= h \sum\nolimits_{i=0}^{n} b_i L(q^i, v^i), \\
(q^{i+1}, v^{i+1}) &= \Psi_{(c_{i+1}-c_i)h}(q^i, v^i), \qquad i = 0, \dots n-1, \\
q^0 &= q_0, \\
q^n &= q_1, \\
p_0 &= -D_1 L_d(q_0, q_1; h), \\
p_1 &= D_2 L_d(q_0, q_1; h).
\end{aligned}$$

Shooting-Based Variational Integrators

■ Shooting-Based Implementation

- Given (q_0, p_0), we let $q^0 = q_0$, and guess an initial velocity v^0.
- We obtain $(q^i, v^i)_{i=1}^n$ by setting $(q^{i+1}, v^{i+1}) = \Psi_{(c_{i+1}-c_i)h}(q^i, v^i)$.
- We let $q_1 = q^n$, and compute $p_1 = D_2 L_d(q_0, q_1; h)$.
- Unless the initial velocity v^0 is chosen correctly, the equation $p_0 = -D_1 L_d(q_0, q_1; h)$ will not be satisfied, and one needs to compute the sensitivity of $-D_1 L_d(q_0, q_1; h)$ on v^0, and iterate on v^0 so that $p_0 = -D_1 L_d(q_0, q_1; h)$ is satisfied.
- This gives a one-step method $(q_0, p_0) \mapsto (q_1, p_1)$.
- In practice, a good initial guess for v^0 can be obtained by inverting the continuous Legendre transformation $p = \partial L / \partial v$.

Shooting-Based Variational Integrators: Inheritance

Theorem: Order of accuracy

- Given a p-th order one-step method Ψ_h, a q-th order quadrature formula, and a Lipschitz continuous Lagrangian L, the shooting-based discrete Lagrangian has order of accuracy $\min(p, q)$.

Theorem: Symmetric discrete Lagrangians

- Given a self-adjoint one-step method Ψ_h, and a symmetric quadrature formula ($c_i + c_{n-i} = 1$, $b_i = b_{n-i}$), the associated shooting-based discrete Lagrangian is self-adjoint.

Theorem: Group-invariant discrete Lagrangians

- Given a G-equivariant one-step method $\Psi_h : TQ \rightarrow TQ$, and a G-invariant Lagrangian $L : TQ \rightarrow \mathbb{R}$, the associated shooting-based discrete Lagrangian is G-invariant, and hence *preserves a discrete momentum map*.

Some related approaches

Prolongation–Collocation variational integrators

- Intended to minimize the number of internal stages, while allowing for high-order approximation.
- Allows for the efficient use of automatic differentiation coupled with adaptive force evaluation techniques to increase efficiency.

Taylor variational integrators

- Taylor variational integrators allow one to reuse the prolongation of the Euler–Lagrange vector field at the initial time to compute the approximation at the quadrature points.
- As such, these methods scale better when using higher-order quadrature formulas, since the cost of evaluating the integrand is reduced dramatically.

Prolongation–Collocation Variational Integrators

Euler–Maclaurin quadrature formula

- If f is sufficiently differentiable on (a, b), then for any $m > 0$,

$$\int_a^b f(x)dx = \frac{\theta}{2}\left[f(a) + 2\sum_{k=1}^{N-1} f(a+k\theta) + f(b)\right] - \sum_{l=1}^{m} \frac{B_{2l}}{(2l)!}\theta^{2l}\left(f^{(2l-1)}(b) - f^{(2l-1)}(a)\right) - \frac{B_{2m+2}}{(2m+2)!}N\theta^{2m+3}f^{(2m+2)}(\xi)$$

  where B_k are the Bernoulli numbers, $\theta = (b-a)/N$ and $\xi \in (a, b)$.

- When $N = 1$,

$$K(f) = \frac{h}{2}[f(0) + f(h)] - \sum_{l=1}^{m} \frac{B_{2l}}{(2l)!}h^{2l}\left(f^{(2l-1)}(h) - f^{(2l-1)}(0)\right),$$

  and the error of approximation is $\mathcal{O}(h^{2m+3})$.

Prolongation–Collocation Variational Integrators

Two-point Hermite Interpolant

- A **two-point Hermite interpolant** $q_d(t)$ of degree $d = 2n - 1$ can be used to approximate the curve. It has the form

$$q_d(t) = \sum_{j=0}^{n-1} \left(q^{(j)}(0) H_{n,j}(t) + (-1)^j q^{(j)}(h) H_{n,j}(h-t) \right),$$

where

$$H_{n,j}(t) = \frac{t^j}{j!}(1 - t/h)^n \sum_{s=0}^{n-j-1} \binom{n+s-1}{s} (t/h)^s$$

are the Hermite basis functions.

- By construction,

$$q_d^{(r)}(0) = q^{(r)}(0), \qquad q_d^{(r)}(h) = q^{(r)}(h), \qquad r = 0, 1, \ldots n-1.$$

Prolongation–Collocation Variational Integrators

Prolongation–Collocation Discrete Lagrangian

- The **prolongation–collocation discrete Lagrangian** is

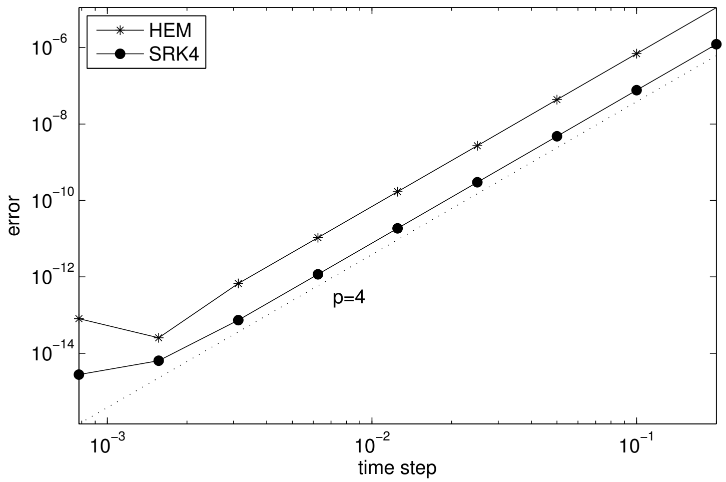
$$L_d(q_0, q_1, h) = \frac{h}{2}(L(q_d(0), \dot{q}_d(0)) + L(q_d(h), \dot{q}_d(h)))$$
$$- \sum_{l=1}^{\lfloor n/2 \rfloor} \frac{B_{2l}}{(2l)!} h^{2l} \left(\frac{d^{2l-1}}{dt^{2l-1}} L(q_d(t), \dot{q}_d(t)) \bigg|_{t=h} - \frac{d^{2l-1}}{dt^{2l-1}} L(q_d(t), \dot{q}_d(t)) \bigg|_{t=0} \right),$$

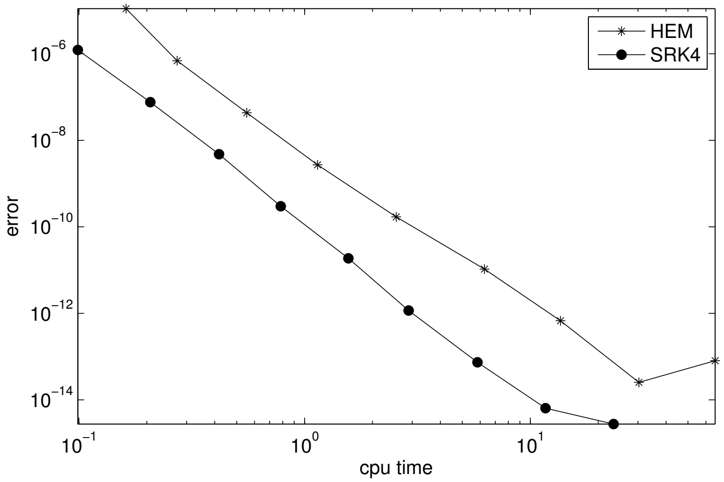
where $q_d(t) \in \mathcal{C}^s(Q)$ is determined by the boundary and prolongation-collocation conditions,

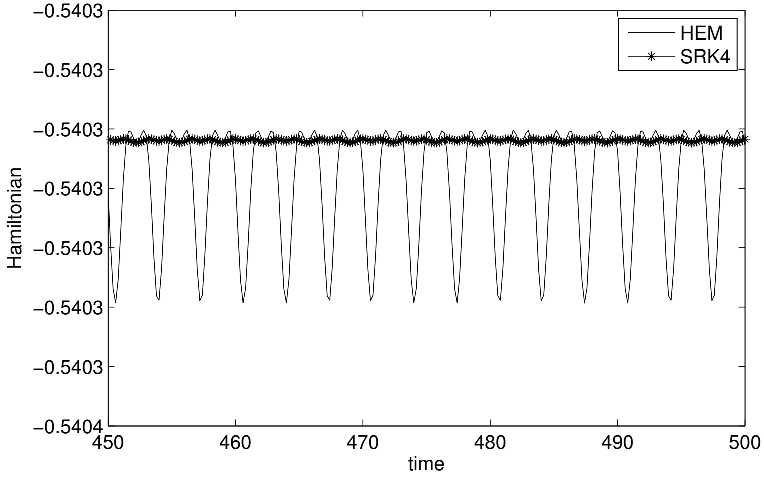
$$\begin{aligned}
q_d(0) &= q_0 & q_d(h) &= q_1, \\
\ddot{q}_d(0) &= f(q_0) & \ddot{q}_d(h) &= f(q_1), \\
q_d^{(3)}(0) &= f'(q_0)\dot{q}_d(0) & q_d^{(3)}(h) &= f'(q_1)\dot{q}_d(h), \\
&\vdots & &\vdots \\
q_d^{(n)}(0) &= \frac{d^n}{dt^n} f(q_d(t)) \bigg|_{t=0} & q_d^{(n)}(h) &= \frac{d^n}{dt^n} f(q_d(t)) \bigg|_{t=h}
\end{aligned}$$

Prolongation–Collocation Variational Integrators

Numerical Experiments: Pendulum

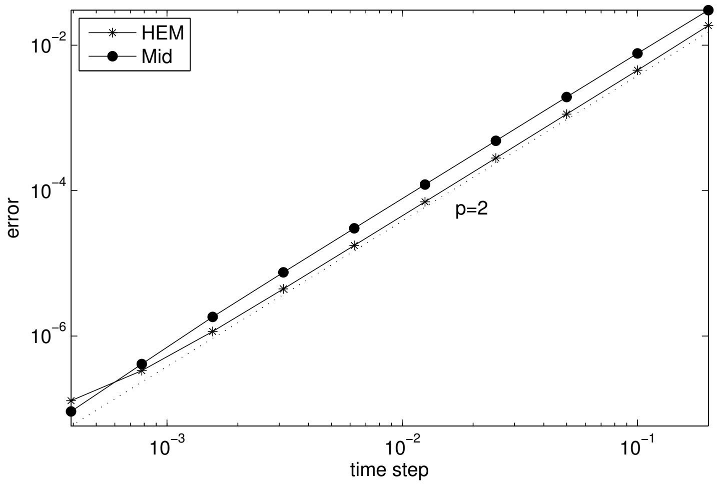


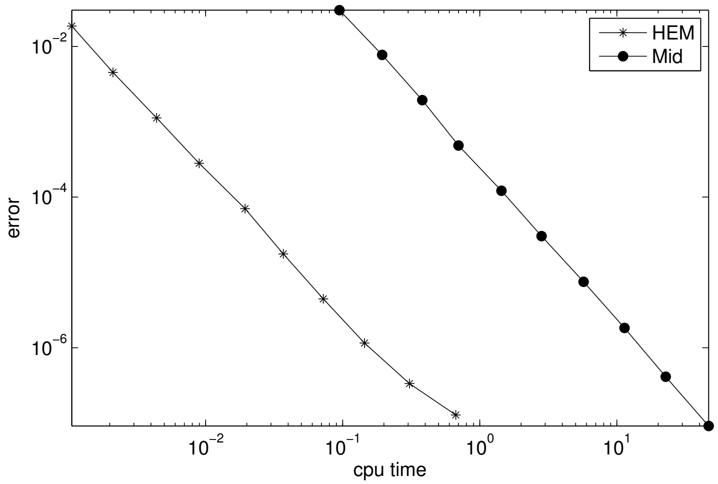


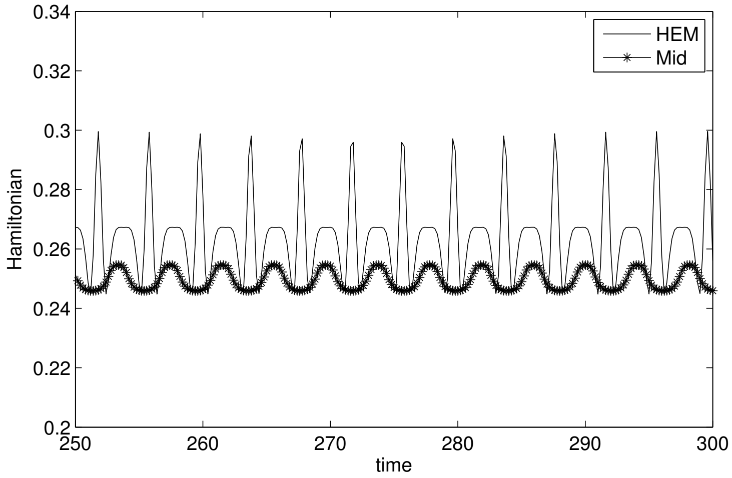


Prolongation–Collocation Variational Integrators

Numerical Experiments: Duffing oscillator







Galerkin Variational Integrators

Variational Characterization of L_d^{exact}

- An alternative characterization of the exact discrete Lagrangian,

$$L_d^{\text{exact}}(q_0, q_1) \equiv \underset{\substack{q \in C^2([0,h],Q) \\ q(0)=q_0, q(h)=q_1}}{\text{ext}} \int_0^h L(q(t), \dot{q}(t))dt,$$

  which naturally leads to Galerkin discrete Lagrangians.

Galerkin Discrete Lagrangians

- Replace the infinite-dimensional function space $C^2([0, h], Q)$ with a **finite-dimensional function space**.
- Replace the integral with a **numerical quadrature formula**.
- The element of the finite-dimensional function space that is chosen depends on the choice of the quadrature formula.

Galerkin Variational Integrators: Inheritence

Theorem: Group-invariant discrete Lagrangians

- If the interpolatory function $\varphi(g^\nu; t)$ is G-equivariant, and the Lagrangian, $L : TG \to \mathbb{R}$, is G-invariant, then the Galerkin discrete Lagrangian, $L_d : G \times G \to \mathbb{R}$, given by

$$L_d(g_0, g_1) = \underset{\substack{g^\nu \in G; \\ g^0 = g_0; g^s = g_1}}{\operatorname{ext}} h \sum_{i=1}^{s} b_i L(T\varphi(g^\nu; c_i h)),$$

is G-invariant.

Galerkin Variational Integrators

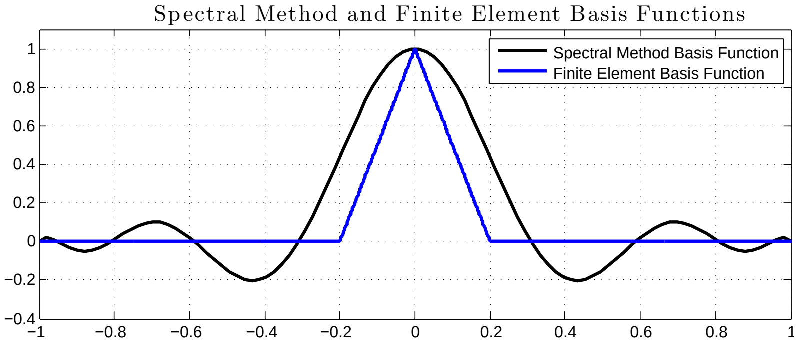
Optimal Rates of Convergence

- Ideally, a Galerkin numerical method based on a finite-dimensional space $F_d \subset F$ should be **optimally convergent**, i.e., the numerical solution $q_d \in F_d$ and the exact solution $q \in F$ satisfies,
$$\|q - q_d\| \leq c \inf_{\tilde{q} \in F_d} \|q - \tilde{q}\|.$$
- For Galerkin variational integrators, this involves showing that the extremizers of an approximating sequence of functionals,
$$L_d^i(q_0, q_1) \equiv \operatorname{ext}_{q \in \mathcal{C}_i} h \sum_{j=1}^{s_i} b_j^i L(q(c_j^i h), \dot{q}(c_j^i h)),$$
converges to the extremizer of the limiting functional at a rate determined by the best approximation error,
$$|L_d^i(q_0, q_1) - L_d^{\text{exact}}(q_0, q_1)| \leq c \inf_{\tilde{q} \in \mathcal{C}_i} \|q - \tilde{q}\|,$$
which is a refinement of Γ-convergence,

Galerkin Variational Integrators

Spectral Variational Integrators

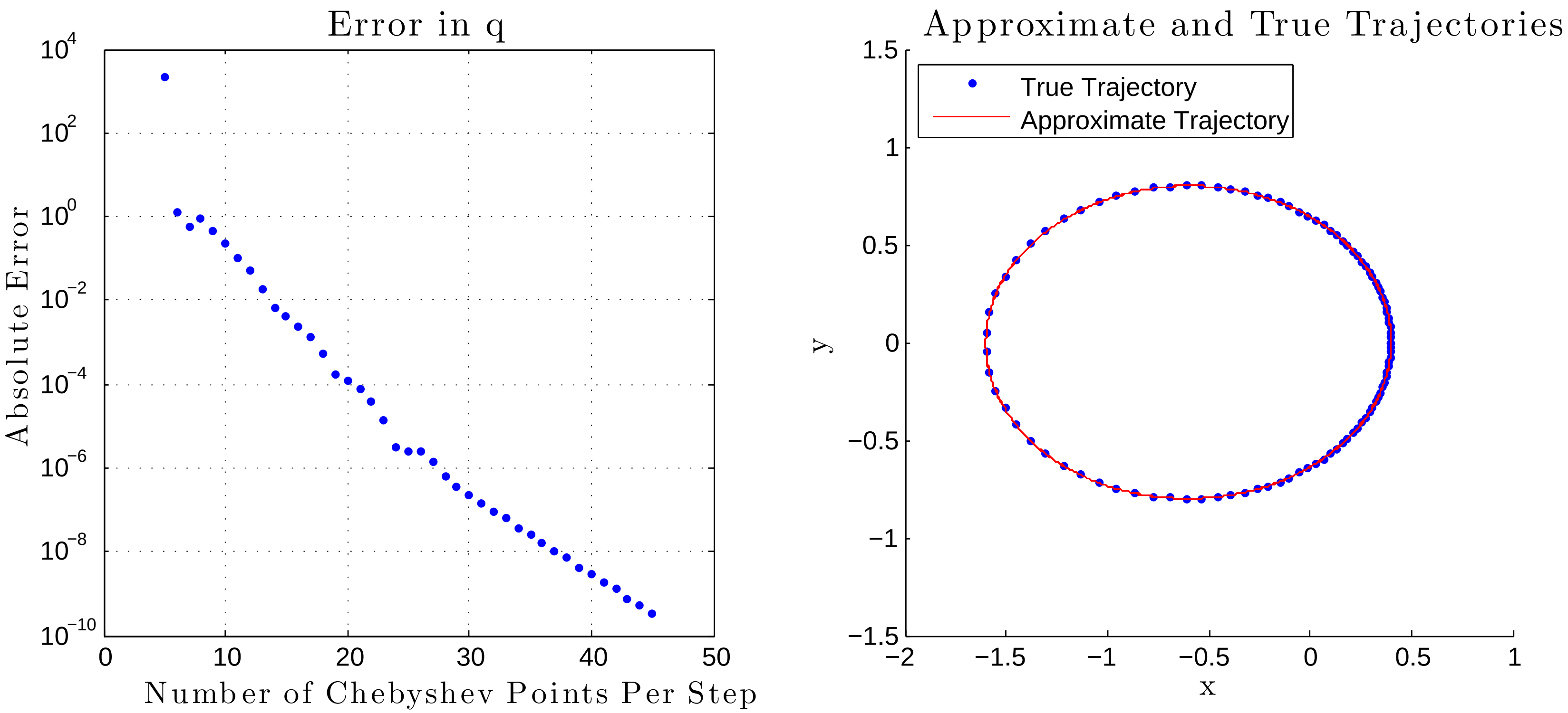
- Spectral variational integrators are a class of Galerkin variational integrators based on **spectral basis functions**, for example, the **Chebyshev polynomials**.



- This leads to variational integrators that increase accuracy by p-refinement as opposed to h-refinement.
- By refining the proof of Γ-convergence by Müller and Ortiz, it can be shown that they are **geometrically convergent**.

Spectral Variational Integrators

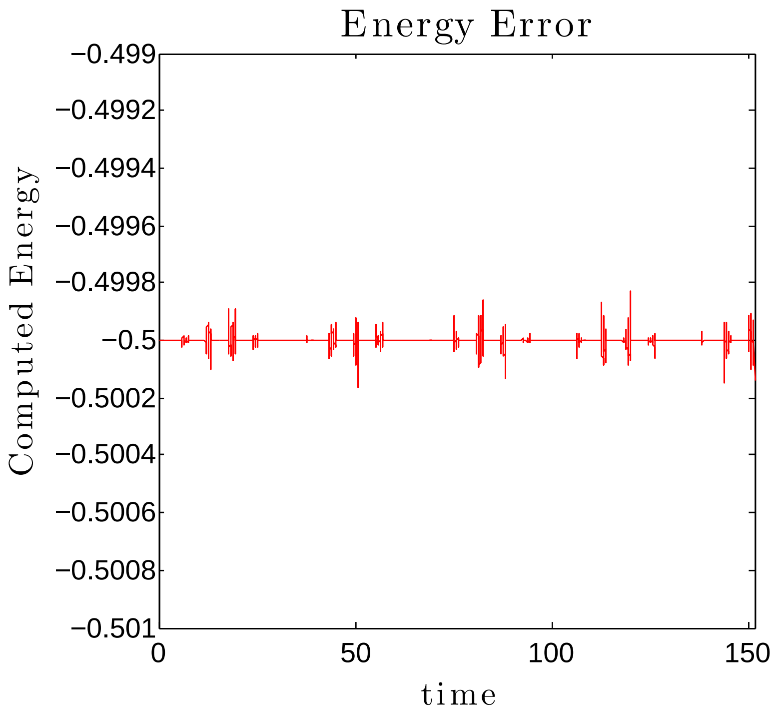
Numerical Experiments: Kepler 2-Body Problem

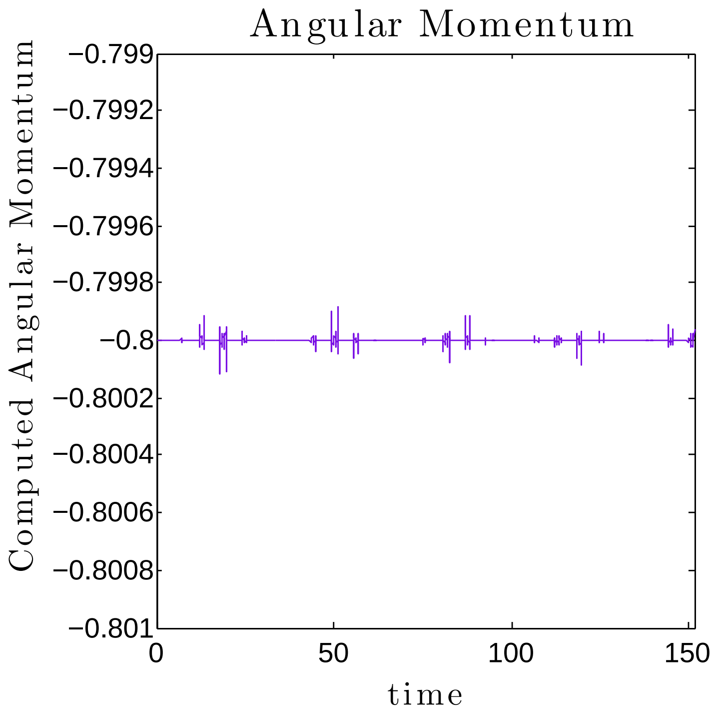


- $h = 1.5$, $T = 150$, and 20 Chebyshev points per step.

Spectral Variational Integrators

Numerical Experiments: Kepler 2-Body Problem

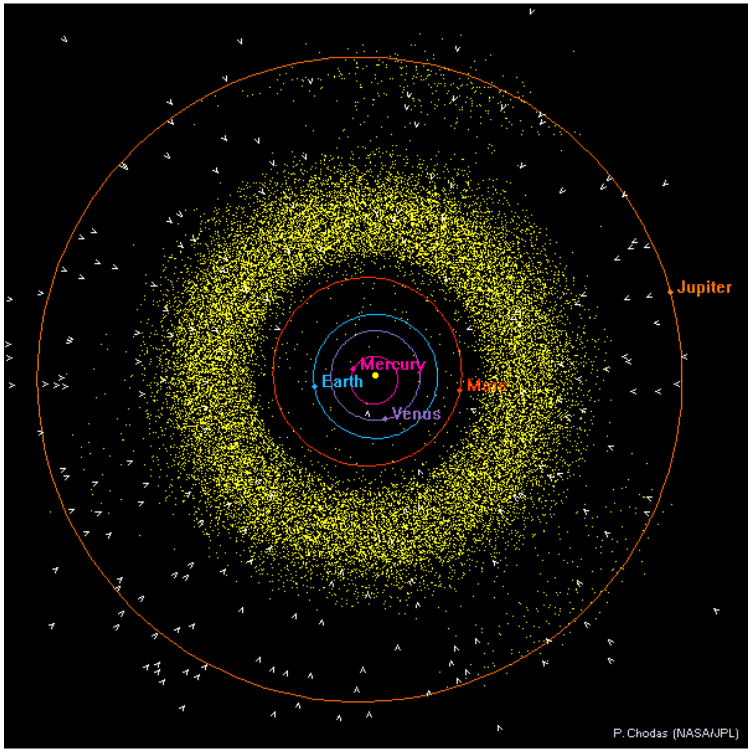




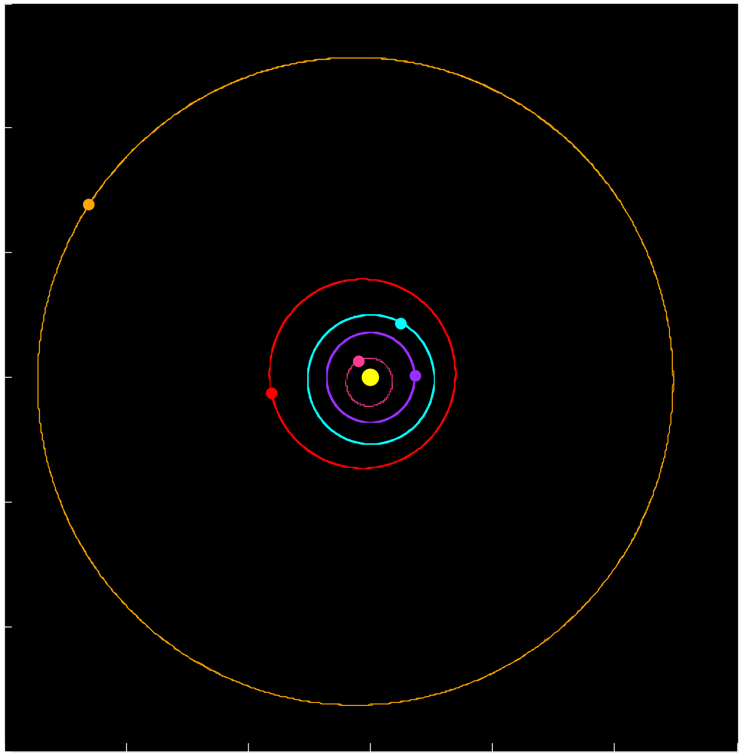
- $h = 1.5$, $T = 150$, and 20 Chebyshev points per step.

Spectral Variational Integrators

Numerical Experiments: Solar System Simulation



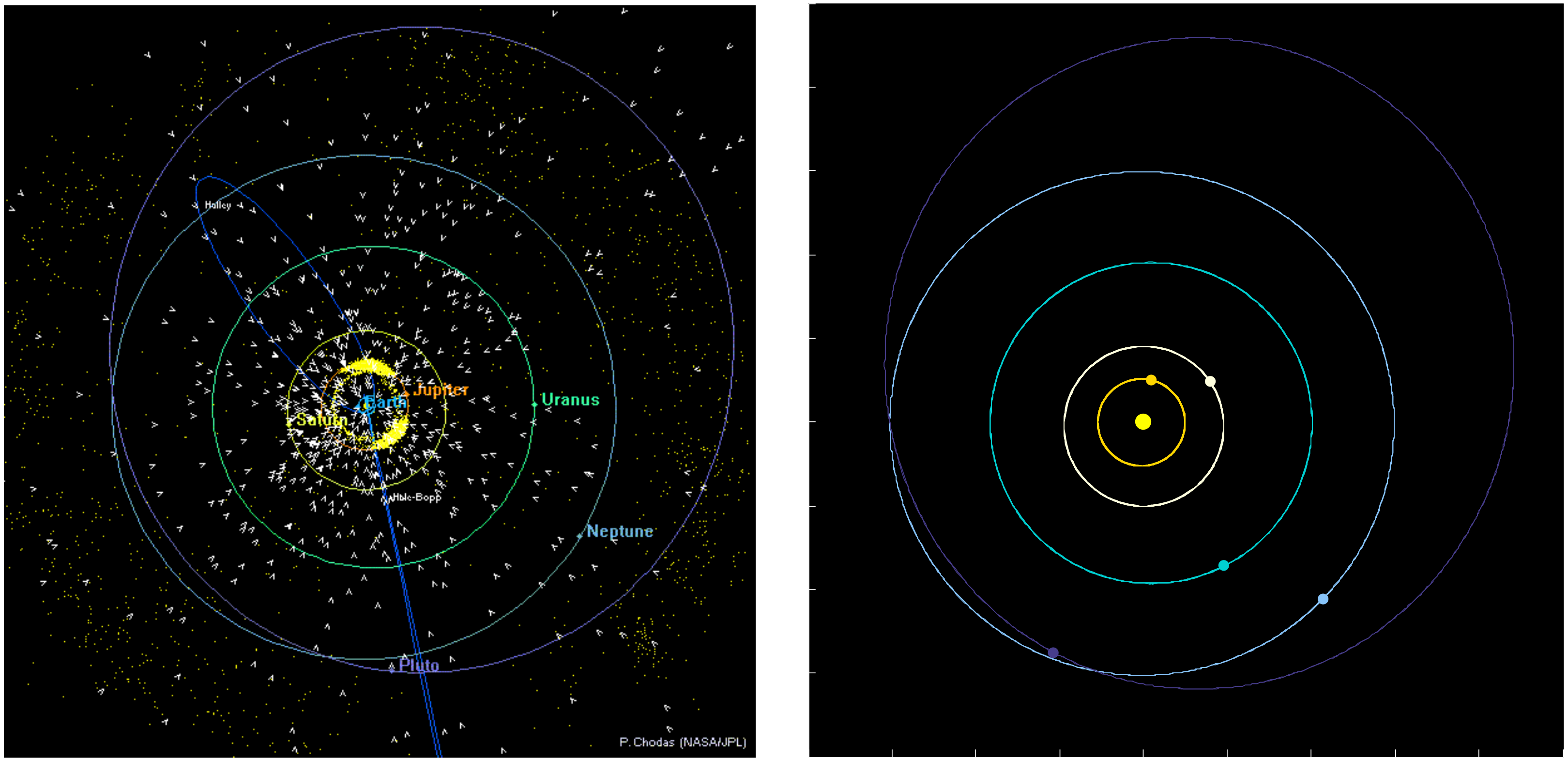
P. Chodas (NASA/JPL)



- Comparison of inner solar system orbital diagrams from a spectral variational integrator and the JPL Solar System Dynamics Group.
- $h = 100$ days, $T = 27$ years, 25 Chebyshev points per step.

Spectral Variational Integrators

Numerical Experiments: Solar System Simulation



P. Chodas (NASA/JPL)

- Comparison of outer solar system orbital diagrams from a spectral variational integrator and the JPL Solar System Dynamics Group. Inner solar system was aggregated, and $h = 1825$ days.

Generalization to Discrete Hamiltonian Systems

Generating Functions for Symplectic Transformations

Type I

$$\begin{bmatrix} p_k \\ p_{k+1} \end{bmatrix} = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} DL_d(q_k, q_{k+1})$$

Type II

$$\begin{bmatrix} p_k \\ q_{k+1} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} DH_d^+(q_k, p_{k+1})$$

Type III

$$\begin{bmatrix} q_k \\ p_{k+1} \end{bmatrix} = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} DH_d^-(p_k, q_{k+1})$$

Type IV

$$\begin{bmatrix} q_k \\ q_{k+1} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} DR_d(p_k, p_{k+1})$$

Degenerate Hamiltonian Systems

Degenerate Hamiltonians

- A Hamiltonian $H : T^*Q \to \mathbb{R}$ is **degenerate** if the **Legendre transformation** $\mathbb{F}H : T^*Q \to TQ$, $(q,p) \mapsto (q, \partial H/\partial p)$, is non-invertible.

- This obstructs the construction of variational integrators for degenerate Hamiltonian systems by traversing via the Lagrangian side.

$$\begin{tikzcd}
H(q,p) \arrow[r, "\mathbb{F}H"] \arrow[d, dashed] & L(q,\dot{q}) \arrow[d] \\
H_d^+(q_0,p_1) & L_d(q_0,q_1) \arrow[l, "\mathbb{F}L_d"']
\end{tikzcd}$$

- The goal is to **construct discrete Hamiltonians directly**, so that the diagram commutes for hyperregular Hamiltonians.

Degenerate Hamiltonian Systems

Toy Motivating Example

- Consider the Hamiltonian,

$$H(q,p) = qp.$$

- The Legendre transformation is,

$$(q,p) \mapsto (q, \partial H/\partial p) = (q,q),$$

which is clearly non-invertible.

- Furthermore, the associated Lagrangian is identically zero,

$$L(q,\dot{q}) = \operatorname*{ext}_{p} \left[p\dot{q} - H(q,p) \right] = p\dot{q} - qp \big|_{\dot{q}=\partial H/\partial p = q} \equiv 0.$$

Degenerate Hamiltonian Systems

Toy Motivating Example (Boundary Data)

- The Hamilton's equations are,

$$\begin{aligned} \dot{q} &= \partial H / \partial p = q, \\ \dot{p} &= -\partial H / \partial q = -p. \end{aligned}$$

- The exact solutions are,

$$\begin{aligned} q(t) &= q(0) \exp(t), \\ p(t) &= p(0) \exp(-t), \end{aligned}$$

which are generally incompatible with the (q_0, q_1) boundary conditions for discrete Lagrangians, but it is compatible with the (q_0, p_1) boundary conditions for discrete Hamiltonians.

Exact Discrete Hamiltonian

Sketch of Approach

- The exact discrete Lagrangian is a Type I generating function,

$$L_d^{\text{exact}}(q_0, q_1) \equiv \underset{\substack{q\in C^2([0,h],Q) \\ q(0)=q_0, q(h)=q_1}}{\text{ext}} \int_0^h L(q(t), \dot{q}(t))dt,$$

  expressed in terms of a continuous Lagrangian.

- Use the continuous Legendre transformation to obtain,

$$L(q, \dot{q}) = p\dot{q} - H(q, p).$$

Exact Discrete Hamiltonian

Sketch of Approach

- Use the discrete Legendre transformation,

$$\begin{tikzcd} L_d(q_k, q_{k+1}) \arrow[r] \arrow[d] & H_d^+(q_k, p_{k+1}) \arrow[d] \\ H_d^-(p_k, q_{k+1}) \arrow[r] & R_d(p_k, p_{k+1}) \end{tikzcd}$$

to obtain a Type II generating function,

$$H^+_{d,\text{exact}}(q_k, p_{k+1}) = \underset{\substack{(q,p)\in C^2([t_k,t_{k+1}],T^*Q) \\ q(t_k)=q_k, p(t_{k+1})=p_{k+1}}}{\text{ext}} p(t_{k+1})q(t_{k+1}) - \int_{t_k}^{t_{k+1}} [p\dot{q} - H(q,p)]\, dt.$$

Type II Hamilton–Jacobi Equation and Jacobi's Solution

Proposition

- Consider the function,

$$S_2(q_0, p, t) = \underset{\substack{(q,p)\in C^2([0,t],T^*Q) \\ q(0)=q_0, p(t)=p}}{\operatorname{ext}} \left(p(t)q(t) - \int_0^t \left[p(s)\dot{q}(s) - H(q(s), p(s)) \right] ds \right).$$

- This satisfies the **Type II Hamilton–Jacobi equation**,

$$\frac{\partial S_2(q_0, p, t)}{\partial t} = H\left(\frac{\partial S_2}{\partial p}, p \right).$$

Discrete Type II Hamilton–Jacobi Equation

Theorem

- Consider the **discrete extremum function**,

$$\mathcal{S}_d^k(p_k) = p_k q_k - \sum\nolimits_{l=0}^{k-1} \left[p_{l+1} q_{l+1} - H_d^+(q_l, p_{l+1}) \right],$$

  which is the discrete action sum up to time t_k evaluated along a solution of the discrete Hamilton's equations, viewed as a function of the momentum p_k.

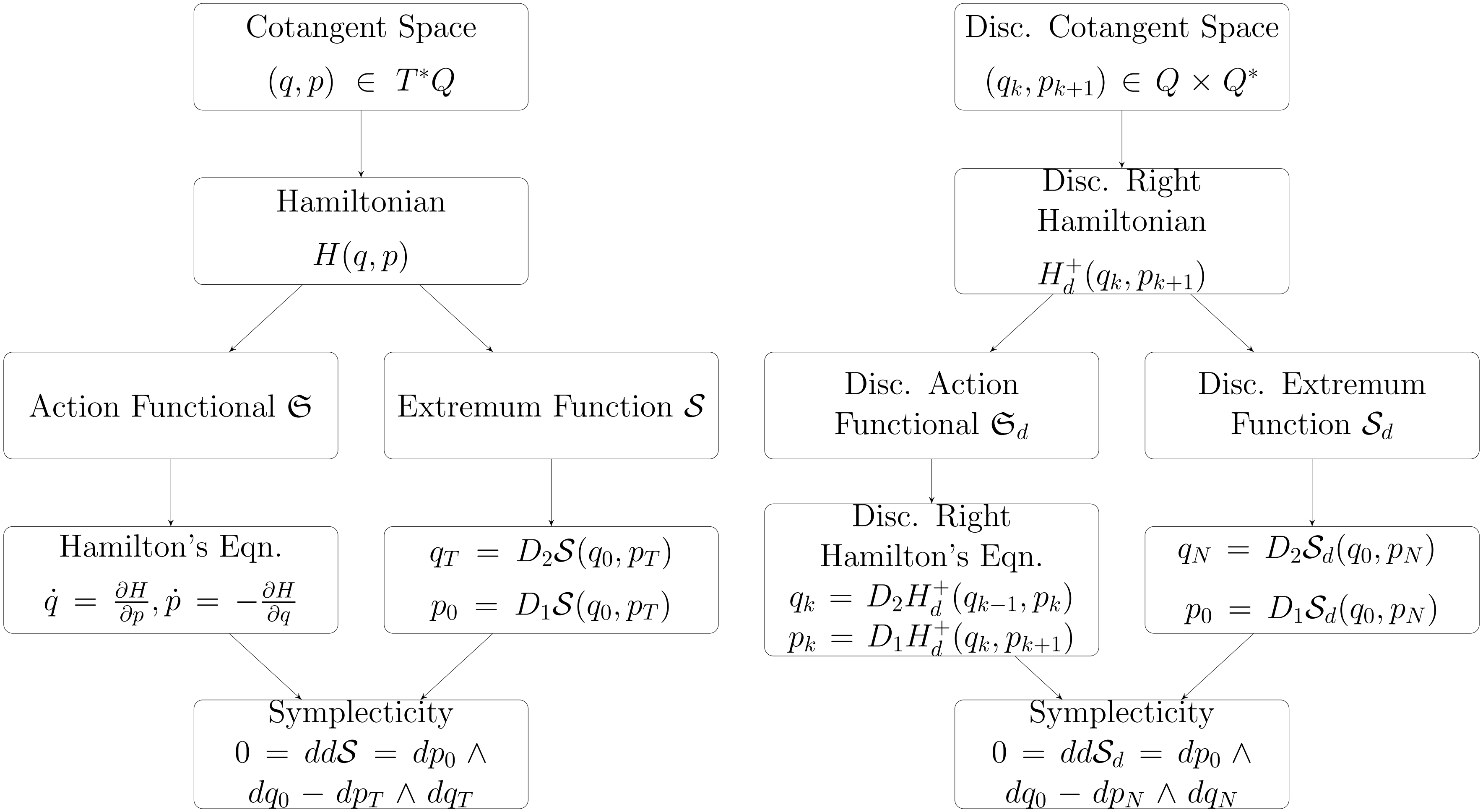
- This is essentially a **discrete Type II Jacobi's solution**.

- Then, these satisfy the **discrete Type II Hamilton–Jacobi equation**,

$$\mathcal{S}_d^{k+1}(p_{k+1}) - \mathcal{S}_d^k(p_k) = H_d^+(D\mathcal{S}_d^k(p_k), p_{k+1}) - p_k \cdot D\mathcal{S}_d^k(p_k).$$

Hamiltonian Mechanics

Continuous and Discrete Time Correspondence



Cotangent Space

$(q, p) \in T^*Q$

Hamiltonian

$H(q, p)$

Action Functional $\mathfrak{S}$

Extremum Function $\mathcal{S}$

Hamilton's Eqn.

$\dot{q} = \frac{\partial H}{\partial p}, \dot{p} = -\frac{\partial H}{\partial q}$

$$q_T = D_2\mathcal{S}(q_0, p_T)$$
$$p_0 = D_1\mathcal{S}(q_0, p_T)$$

Symplecticity

$0 = dd\mathcal{S} = dp_0 \wedge dq_0 - dp_T \wedge dq_T$

Disc. Cotangent Space

$(q_k, p_{k+1}) \in Q \times Q^*$

Disc. Right Hamiltonian

$H_d^+(q_k, p_{k+1})$

Disc. Action Functional $\mathfrak{S}_d$

Disc. Extremum Function $\mathcal{S}_d$

Disc. Right Hamilton's Eqn.

$$q_k = D_2 H_d^+(q_{k-1}, p_k)$$
$$p_k = D_1 H_d^+(q_k, p_{k+1})$$

$$q_N = D_2\mathcal{S}_d(q_0, p_N)$$
$$p_0 = D_1\mathcal{S}_d(q_0, p_N)$$

Symplecticity

$0 = dd\mathcal{S}_d = dp_0 \wedge dq_0 - dp_N \wedge dq_N$

Galerkin Hamiltonian Variational Integrator

Generalized Representation

- The generalized Galerkin Hamiltonian variational integrator can be written in the following compact form,

$$\begin{aligned}
q_1 &= q_0 + h\sum\nolimits_{i=1}^{s} B_i V^i, \\
p_1 &= p_0 - h\sum\nolimits_{i=1}^{s} b_i \frac{\partial H}{\partial q}(Q^i, P^i), \\
Q^i &= q_0 + h\sum\nolimits_{j=1}^{s} A_{ij} V^j, && i = 1, \dots, s, \\
0 &= \sum\nolimits_{i=1}^{s} b_i P^i \psi_j(c_i) - p_0 B_j + h\sum\nolimits_{i=1}^{s} (b_i B_j - b_i A_{ij}) \frac{\partial H}{\partial q}(Q^i, P^i), && j = 1, \dots, s, \\
0 &= \sum\nolimits_{i=1}^{s} \psi_i(c_j) V^i - \frac{\partial H}{\partial p}(Q^j, P^j), && j = 1, \dots, s,
\end{aligned}$$

where (b_i, c_i) are the quadrature weights and quadrature points, and $B_i = \int_0^1 \psi_i(\tau)d\tau$, $A_{ij} = \int_0^{c_i} \psi_j(\tau)d\tau$.

Galerkin Lagrangian Variational Integrator

Generalized Representation

- The generalized Galerkin Lagrangian variational integrator can be written in the following compact form,

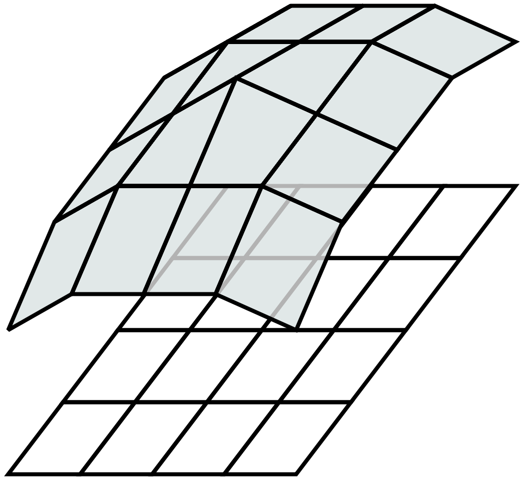
$$\begin{aligned}
q_1 &= q_0 + h\sum\nolimits_{i=1}^{s} B_i V^i, \\
p_1 &= p_0 + h\sum\nolimits_{i=1}^{s} b_i \frac{\partial L}{\partial q}(Q^i, \dot{Q}^i), \\
Q^i &= q_0 + h\sum\nolimits_{j=1}^{s} A_{ij} V^j, && i = 1, \ldots, s \\
0 &= \sum\nolimits_{i=1}^{s} b_i \frac{\partial L}{\partial \dot{q}}(Q^i, \dot{Q}^i)\psi_j(c_i) - p_0 B_j - h\sum\nolimits_{i=1}^{s}(b_i B_j - b_i A_{ij})\frac{\partial L}{\partial q}(Q^i, \dot{Q}^i), && j = 1, \ldots, s \\
0 &= \sum\nolimits_{i=1}^{s} \psi_i(c_j) V^i - \dot{Q}^j, && j = 1, \ldots, s
\end{aligned}$$

  where (b_i, c_i) are the quadrature weights and quadrature points, and $B_i = \int_0^1 \psi_i(\tau)d\tau$, $A_{ij} = \int_0^{c_i} \psi_j(\tau)d\tau$.

- When either the Hamiltonian or Lagrangian are hyperregular, these two methods are equivalent.

PDE Generalization: Multisymplectic Geometry

Ingredients



- **Base space** $\mathcal{X}$. $(n+1)$-spacetime.
- **Configuration bundle**. Given by $\pi : Y \to \mathcal{X}$, with the fields as the fiber.
- **Configuration** $q : \mathcal{X} \to Y$. Gives the field variables over each spacetime point.
- **First jet** J^1Y. The first partials of the fields with respect to spacetime.

Variational Mechanics

- **Lagrangian density** $L : J^1Y \to \Omega^{n+1}(\mathcal{X})$.
- **Action integral** given by, $\mathcal{S}(q) = \int_{\mathcal{X}} L(j^1q)$.
- **Hamilton's principle** states, $\delta\mathcal{S} = 0$.

Multisymplectic Exact Discrete Lagrangian

What is the PDE analogue of a generating function?

- Recall the implicit characterization of a symplectic map in terms of generating functions:

$$\begin{cases} p_k = -D_1 L_d(q_k, q_{k+1}) \\ p_{k+1} = D_2 L_d(q_k, q_{k+1}) \end{cases} \qquad \begin{cases} p_k = D_1 H_d^+(q_k, p_{k+1}) \\ q_{k+1} = D_2 H_d^+(q_k, p_{k+1}) \end{cases}$$

- Symplecticity follows as a trivial consequence of these equations, together with $\mathbf{d}^2 = 0$, as the following calculation shows:

$$\begin{aligned} \mathbf{d}^2 L_d(q_k, q_{k+1}) &= \mathbf{d}(D_1 L_d(q_k, q_{k+1}) dq_k + D_2 L_d(q_k, q_{k+1}) dq_{k+1}) \\ &= \mathbf{d}(-p_k dq_k + p_{k+1} dq_{k+1}) \\ &= -dp_k \wedge dq_k + dp_{k+1} \wedge dq_{k+1} \end{aligned}$$

Multisymplectic Exact Discrete Lagrangian

Analogy with the ODE case

- We consider a multisymplectic analogue of Jacobi's solution:

$$L_d^{\text{exact}}(q_0, q_1) \equiv \int_0^h L\left(q_{0,1}(t), \dot{q}_{0,1}(t)\right) dt,$$

  where $q_{0,1}(t)$ satisfies the Euler–Lagrange boundary-value problem.

- This is given by,

$$L_d^{\text{exact}}(\varphi|_{\partial\Omega}) \equiv \int_\Omega L(j^1\tilde{\varphi})$$

  where $\tilde{\varphi}$ satisfies the boundary conditions $\tilde{\varphi}|_{\partial\Omega} = \varphi|_{\partial\Omega}$, and $\tilde{\varphi}$ satisfies the Euler–Lagrange equation in the interior of Ω.

Multisymplectic Exact Discrete Lagrangian

Multisymplectic Relation

- If one takes variations of the **multisymplectic exact discrete Lagrangian** with respect to the boundary conditions, we obtain,
$$\partial_{\varphi(x,t)} L_d^{\text{exact}}(\varphi|_{\partial\Omega}) = p_\perp(x,t),$$
where $(x,t) \in \partial\Omega$, and $p_\perp$ is the component of the multimomentum that is normal to the boundary $\partial\Omega$ at the point (x,t).

- These equations, taken at every point on $\partial\Omega$ constitute a **multisymplectic relation**, which is the PDE analogue of,
$$\begin{cases} p_k = -D_1 L_d(q_k, q_{k+1}) \\ p_{k+1} = D_2 L_d(q_k, q_{k+1}) \end{cases}$$
where the sign in the equations come from the orientation of the boundary of the time interval.

Multisymplectic Exact Discrete Hamiltonian

Analogue of Type II and III generating functions

- Discrete Hamiltonian mechanics is described in terms of Type II and III generating functions.
- In the PDE setting, the analogue of specifying (q_k, p_{k+1}) or (p_k, q_{k+1}) is to specify:
  - fields φ on $A \subset \partial\Omega$;
  - normal component of the multimomentum $p_\perp$ on $B = \partial\Omega \backslash A$.
- Then, we have,

$$H_d^{\text{exact}}(\varphi|_A, p_\perp|_B) = \int_B \varphi p_\perp - \int_\Omega L(j^1\tilde{\varphi}),$$

where $\tilde{\varphi}$ satisfies the prescribed boundary conditions, and the Euler–Lagrange equations.

Exact Multisymplectic Generating Functions

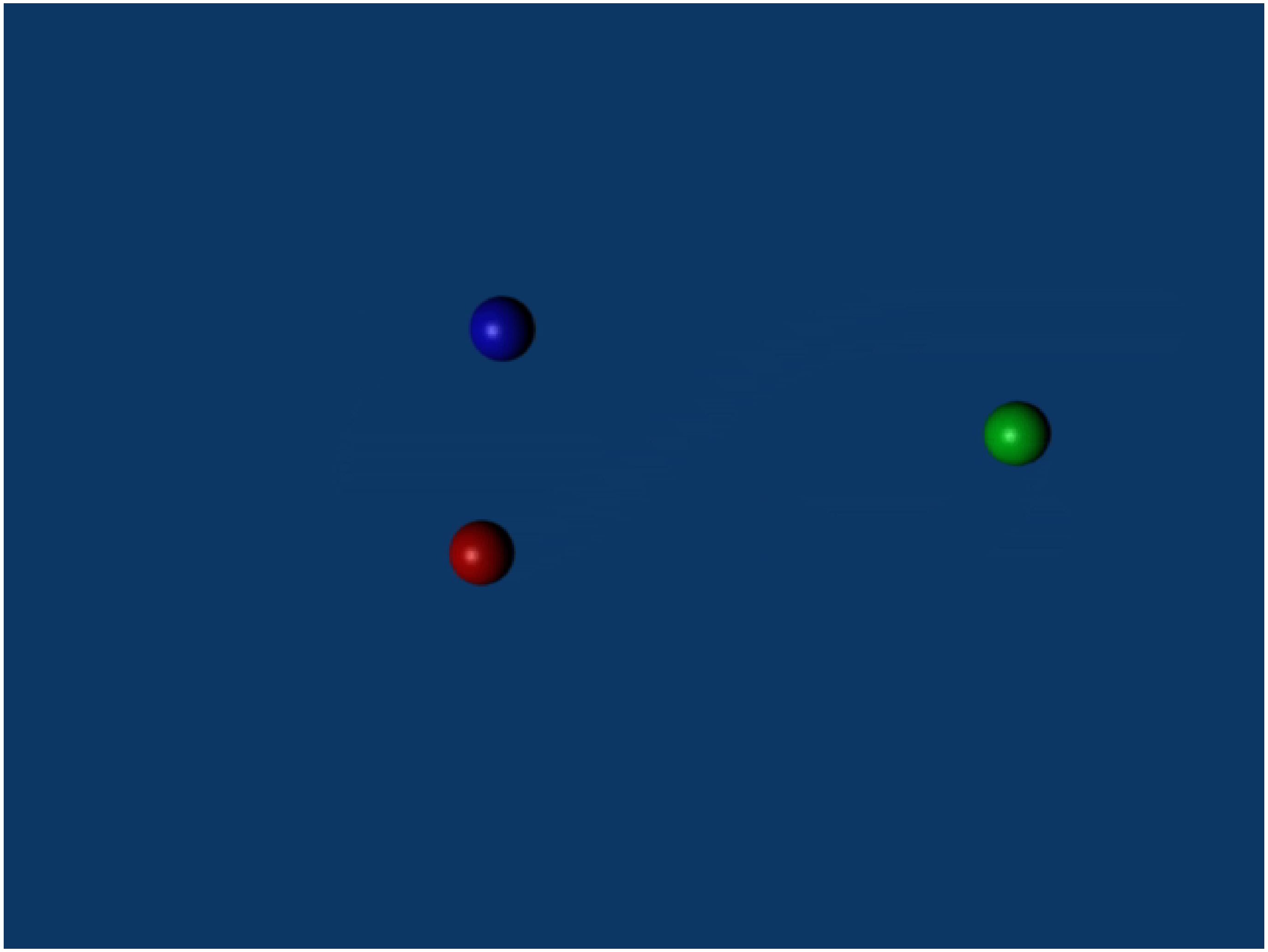
Implications for Geometric Integration

- The multisymplectic generating functions depend on boundary conditions on an infinite set, and one needs to consider a finite-dimensional subspace of allowable boundary conditions.
- Let π be a projection onto allowable boundary conditions.
- In the variational error order analysis, we need to compare:
  - $L_d^{\text{computable}}(\pi\varphi|_{\partial\Omega})$
  - $L_d^{\text{exact}}(\pi\varphi|_{\partial\Omega})$
  - $L_d^{\text{exact}}(\varphi|_{\partial\Omega})$
- The comparison between the last two objects involves establishing well-posedness of the boundary-value problem, and the approximation properties of the finite-dimensional boundary conditions.

Summary

- The **variational** and **boundary-value problem** characterization of the exact discrete Lagrangian naturally lead to **Galerkin variational integrators** and **shooting-based variational integrators**.
- These provide a systematic framework for constructing variational integrators based on a choice of:
  - one-step method;
  - finite-dimensional approximation space;
  - numerical quadrature formula.
- The resulting variational integrators can be shown to inherit properties like **order of accuracy**, and **momentum preservation** from the properties of the chosen one-step method, approximation space, or quadrature formula.

Questions?



arXiv:1001.1408 arXiv:1101.1995 arXiv:1102.2685