General Techniques for Constructing Variational Integrators

Melvin Leok

Mathematics, University of California, San Diego

Joint work with James Hall, Cuicui Liao, Tatiana Shingel, and Joris Vankerschaver

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Jerry Marsden's Legacy in Discrete Geometry & Mechanics

Ph.D. Theses Directed

- **Sergey Pekarsky**, *Discrete Reduction of Mechanical Systems and Multisymplectic Geometry of Continuum Mechanics*, 2000.
- **Matthew West**, *Variational Integrators*, 2002 (defended 2004).
- **Razvan Fetecau**, *Variational Methods for Nonsmooth Mechanics*, 2003.
- **Anil Hirani**, *Discrete Exterior Calculus*, 2003.
- **Melvin Leok**, *Foundations of Computational Geometric Mechanics*, 2004.
- **Nawaf Bou-Rabee**, *Hamilton–Pontryagin Integrators on Lie Groups*, 2007.
- **Ari Stern**, *Geometric Discretizations of Lagrangian Mechanics and Field Theories*, 2009.
- **Ashley Moore**, *Discrete mechanics and optimal control for space trajectory design*, 2011.
- **Molei Tao**, *Multiscale geometric integration of deterministic and stochastic systems*, 2011.

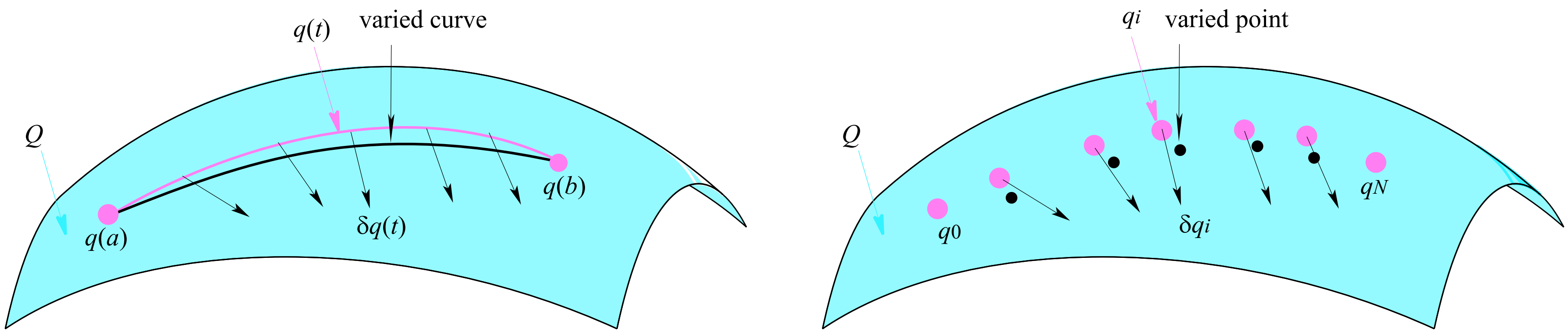
9 out of the 21 Ph.D. students since 2000.

Jerry Marsden's Legacy in Discrete Geometry & Mechanics

- **A blast from the past: some newly minted Ph.D.s**

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** $J_d : Q \times Q \to \mathfrak{g}^*$,

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

  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

- Given 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**,

$$L_d(q_0, q_1; h) = h\sum_{i=0}^n b_i L(q^i, v^i), \qquad (1)$$

where

$$(q^{i+1}, v^{i+1}) = \Psi_{(c_{i+1}-c_i)h}(q^i, v^i), \qquad q^0 = q_0, \qquad q^n = q_1. \quad (2)$$

- Note that while we formally require that the endpoints are included as quadrature points, i.e., $c_0 = 0$, and $c_n = 1$, the associated weights b_0, b_n can be zero, so this is does not constrain the type of quadrature formula we can consider.

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:

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

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

Shooting-Based Variational Integrators: Generalizations

Type I Variational Integrator for Hamiltonian Systems

- The **shooting-based discrete Lagrangian** is given by

$$L_d(q_0, q_1; h) = h \sum_{i=0}^{n} b_i \left[p^i v^i - H(q^i, p^i) \right]_{v^i = \partial H / \partial p(q^i, p^i)},$$

where

$$(q^{i+1}, p^{i+1}) = \Psi_{(c_{i+1} - c_i)h}(q^i, p^i), \qquad q^0 = q_0, \qquad q^n = q_1.$$

Type II Variational Integrator for Hamiltonian Systems

- The **shooting-based discrete Hamiltonian** is given by

$$H_d^+(q_0, p_1; h) = p^n q^n - h \sum_{i=0}^{n} b_i [p^i v^i - H(q^i, p^i)]_{v^i = \partial H / \partial p(q^i, p^i)},$$

where

$$(q^{i+1}, p^{i+1}) = \Psi_{(c_{i+1} - c_i)h}(q^i, p^i), \qquad q^0 = q_0, \qquad p^n = p_1.$$

Shooting-Based Variational Integrators

Optimality for Shooting-Based Variational Integrators

- While shooting-based variational integrators rely on a choice of a one-step method and a numerical quadrature formula, it is still possible to formulate the question of optimal rates of convergence if we consider **collocation one-step methods**.
- In particular, **collocation methods** pick out a unique element of a finite-dimensional function space by requiring that it satisfies the differential equation at a number of **collocation points**.
- Optimality of the shooting-based variational integrator then reduces to the optimality of the corresponding collocation method, which has been established for a large class of approximation spaces.

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 $N=1$,

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

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

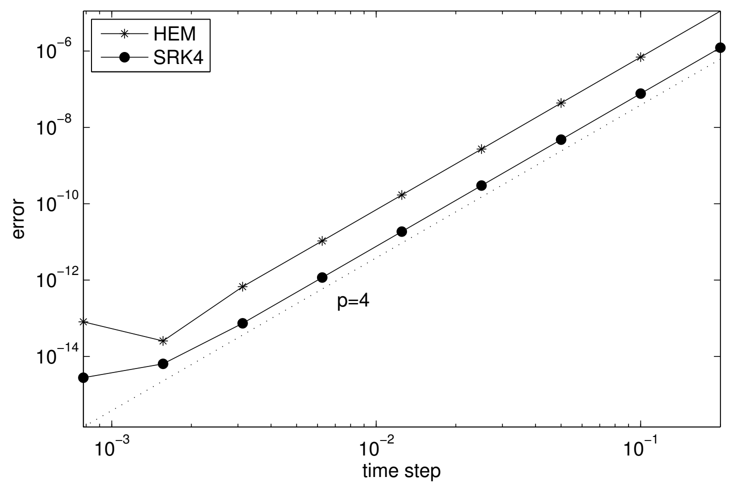
$$
\begin{aligned}
L_d(q_0, q_1, h) &= \frac{h}{2}\left(L(q_d(0), \dot{q}_d(0)) + L(q_d(h), \dot{q}_d(h))\right) \\
&\quad - \sum_{l=1}^{\lfloor n/2 \rfloor} \frac{B_{2l}}{(2l)!} h^{2l} \left(\frac{d^{2l-1}}{dt^{2l-1}} L(q_d(t), \dot{q}_d(t)) \bigg|_{t=h} - \frac{d^{2l-1}}{dt^{2l-1}} L(q_d(t), \dot{q}_d(t))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

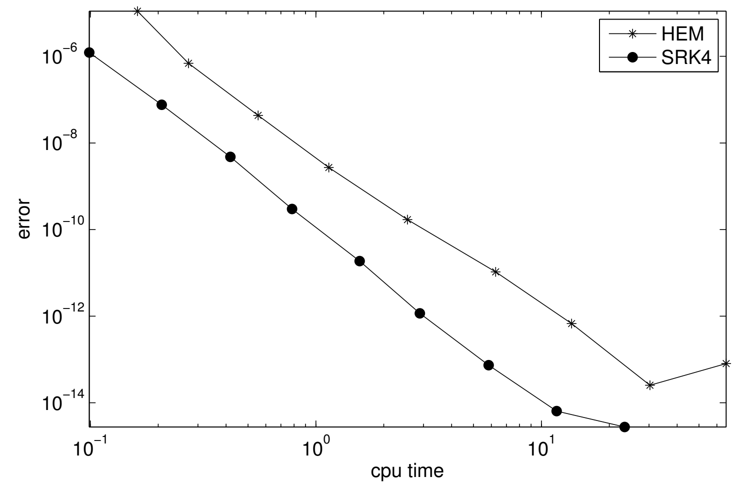
where $q_d(t) \in \mathcal{C}^s(Q)$ is determined by the boundary and prolongation-collocation conditions,

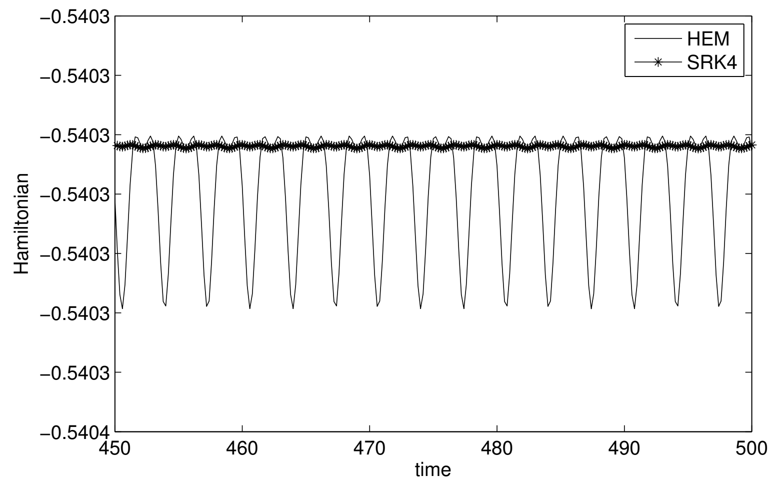
$$
\begin{aligned}
q_d(0) &= q_0 & q_d(h) &= q_1, \\
\ddot{q}_d(0) &= f(q_0) & \ddot{q}_d(h) &= f(q_1), \\
q_d^{(3)}(0) &= f'(q_0)\dot{q}_d(0) & q_d^{(3)}(h) &= f'(q_1)\dot{q}_d(h), \\
&\vdots & &\vdots \\
q_d^{(n)}(0) &= \frac{d^n}{dt^n} f(q_d(t)) \bigg|_{t=0} & q_d^{(n)}(h) &= \frac{d^n}{dt^n} f(q_d(t))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

Prolongation–Collocation Variational Integrators

Numerical Experiments: Pendulum

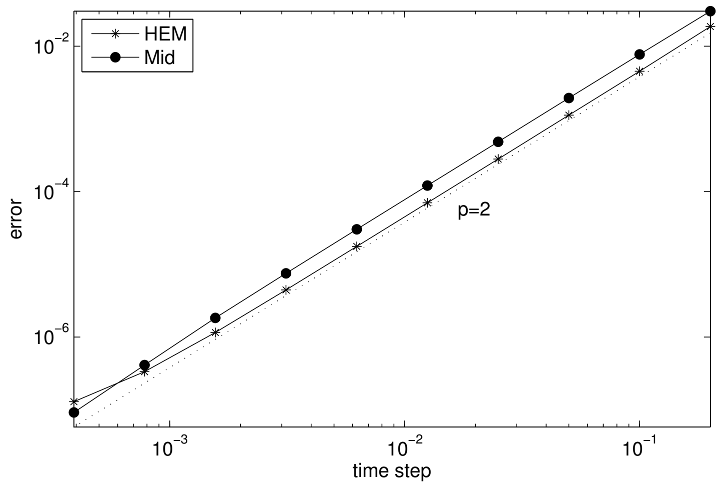


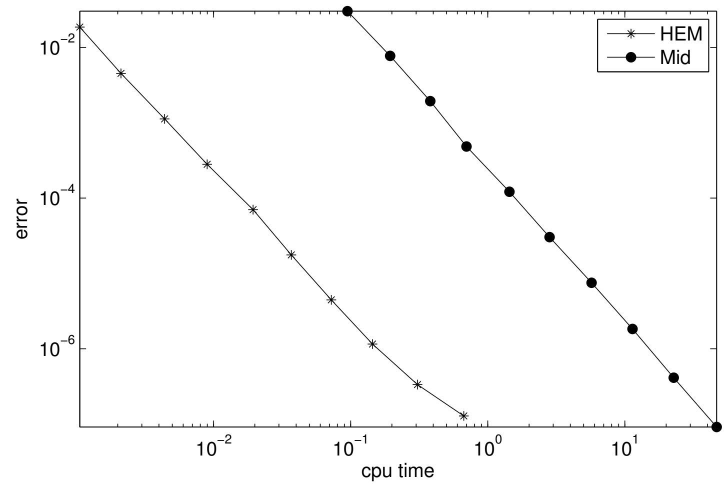


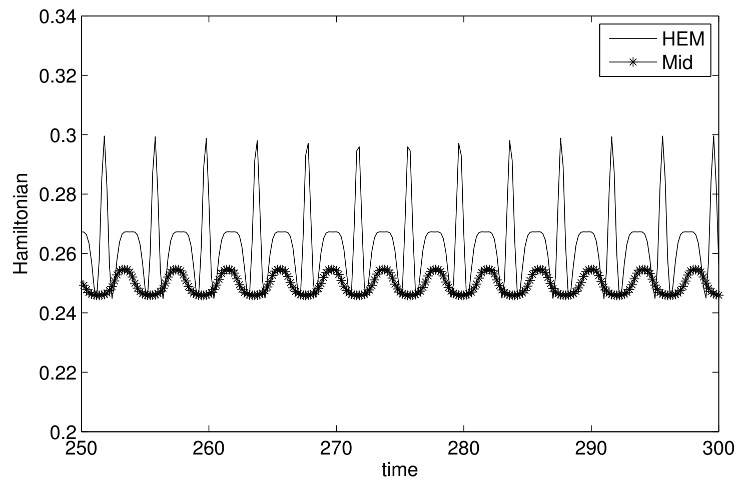


Prolongation–Collocation Variational Integrators

Numerical Experiments: Duffing oscillator







Taylor Variational Integrators

Taylor Discrete Lagrangian

- Consider a p-th order accurate Taylor method,

$$\Psi_h(q_0, \tilde{v}_0) = \left(\sum\nolimits_{k=0}^{p} \frac{h^k}{k!} q^{(k)}(0), \sum\nolimits_{k=1}^{p} \frac{h^{k-1}}{(k-1)!} q^{(k)}(0) \right)$$

  where one computes $q^{(k)}(0)$ by considering the prolongation of the Euler–Lagrange vector field, and evaluating it at $(q_0, \tilde{v}_0)$.

- The **Taylor Discrete Lagrangian** is given by

$$L_d(q_0, q_1; h) = h \sum\nolimits_{i=0}^{n} b_i L(\Psi_{c_i h}(q_0, \tilde{v}_0))$$

  where $\pi_Q \circ \Psi_h(q_0, \tilde{v}_0) = q_1$.

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

Galerkin Lagrangian Variational Integrator

- 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 $B_i = \int_0^1 \psi_i(\tau)d\tau$, $A_{ij} = \int_0^{c_i} \psi_j(\tau)d\tau$.

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

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

  is G-invariant.

Galerkin Variational Integrators

Optimal Rates of Convergence

- A desirable property of a Galerkin numerical method based on a finite-dimensional space $F_d \subset F$, is that it should exhibit **optimal rates of convergence**, which is to say that the numerical solution $q_d \in F_d$ and the exact solution $q \in F$ satisfies,

$$\|q - q_d\| \leq c \inf_{\tilde{q} \in F_d} \|q - \tilde{q}\|.$$

- This means that the rate of convergence depends on the best approximation error of the finite-dimensional function space.

Galerkin Variational Integrators

Optimality of Galerkin Variational Integrators

- Given a sequence of finite-dimensional function spaces $\mathcal{C}_1 \subset \mathcal{C}_2 \subset \ldots \subset C^2([0,h],Q) \equiv \mathcal{C}_\infty$.
- For a correspondingly accurate sequence of quadrature formulas,

$$L_d^i(q_0,q_1) \equiv \operatorname*{ext}_{q\in\mathcal{C}_i} h \sum_{j=1}^{s_i} b_j^i L(q(c_j^i h), \dot{q}(c_j^i h)),$$

where $L_d^\infty(q_0,q_1) = L_d^{\text{exact}}(q_0,q_1)$.

- Proving $L_d^i(q_0,q_1) \to L_d^\infty(q_0,q_1)$, corresponds to Γ-convergence.

Galerkin Variational Integrators

Optimality of Galerkin Variational Integrators

- For optimality, we require the bound,

$$L_d^i(q_0, q_1) = L_d^\infty(q_0, q_1) + c \inf_{\tilde{q} \in \mathcal{C}_i} \|q - \tilde{q}\|,$$

  where we need to relate the rate of Γ-convergence with the best approximation properties of the family of approximation spaces.

- The proof of optimality of Galerkin variational integrators will involve refining the proof of Γ-convergence by Müller and Ortiz.

Galerkin Variational Integrators

Theorem: Optimality of Galerkin Variational Integrators

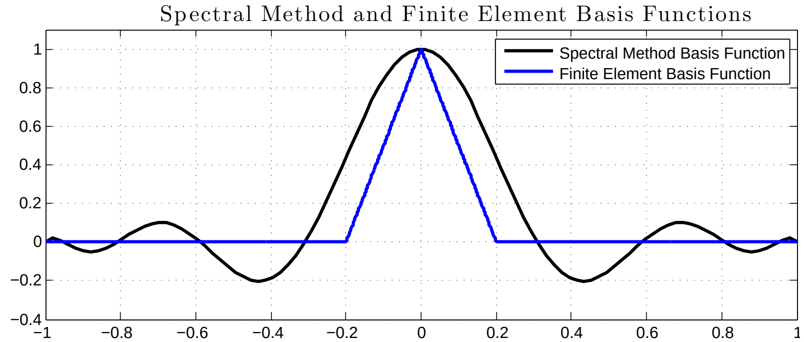
- Under suitable technical hypotheses:
  - Regularity of L in a closed and bounded neighboorhood;
  - The quadrature rule is sufficiently accurate;
  - The discrete and continuous trajectories *minimize* their actions;

  the Galerkin discrete Lagrangian has the same approximation properties as the best approximation error of the approximation space.
- The critical assumption is action minimization. For Lagrangians $L = \dot{q}^T M \dot{q} - V(q)$, and sufficiently small h, this assumption holds.
- In particular, this shows that Galerkin variational integrators based on polynomial spaces are **order optimal**, and spectral variational integrators are **geometrically convergent**.

Galerkin Variational Integrators

Spectral Variational Integrators

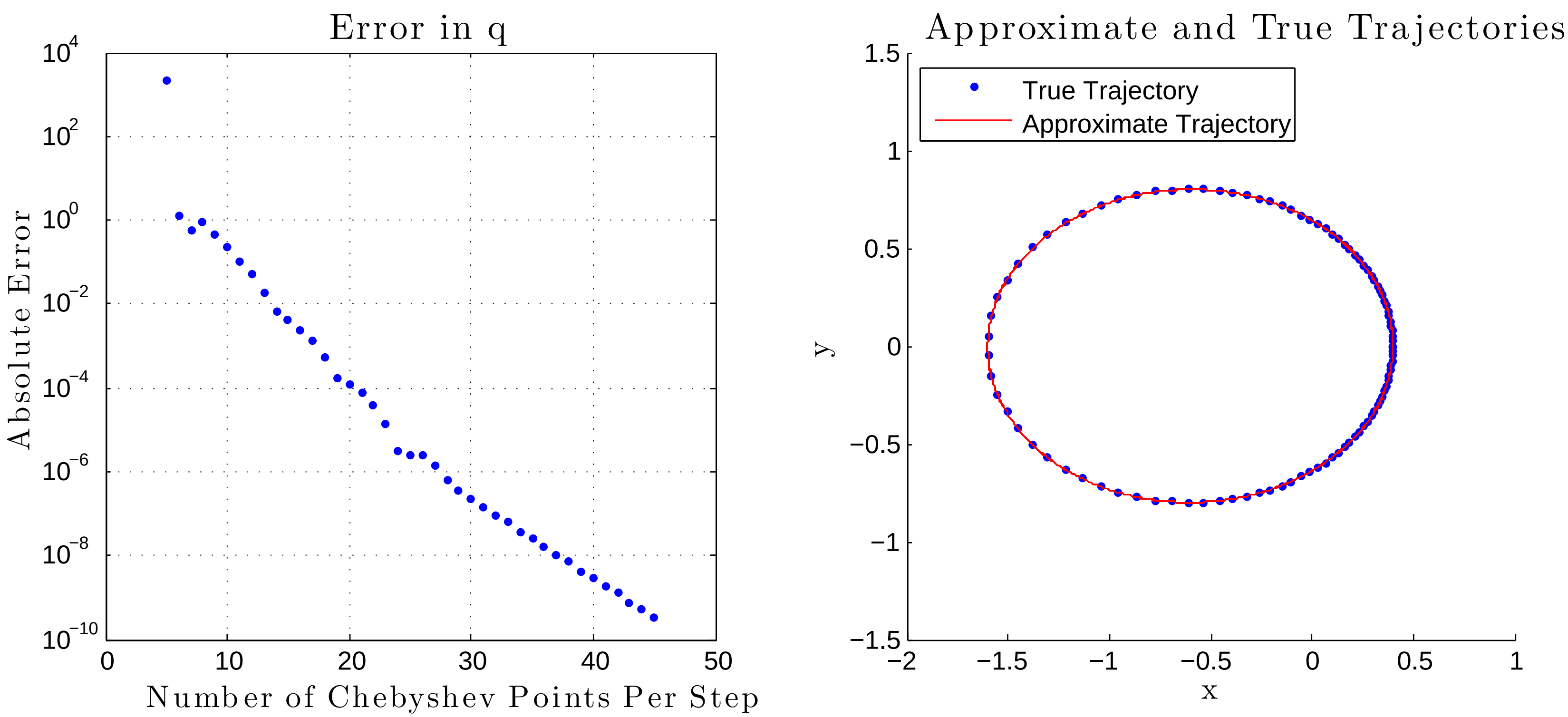
- Spectral variational integrators are a class of Galerkin variational integrators based on **spectral basis functions**, for example, the **Chebyshev polynomials**.



- This leads to variational integrators that increase accuracy by p-refinement as opposed to h-refinement.

Spectral Variational Integrators

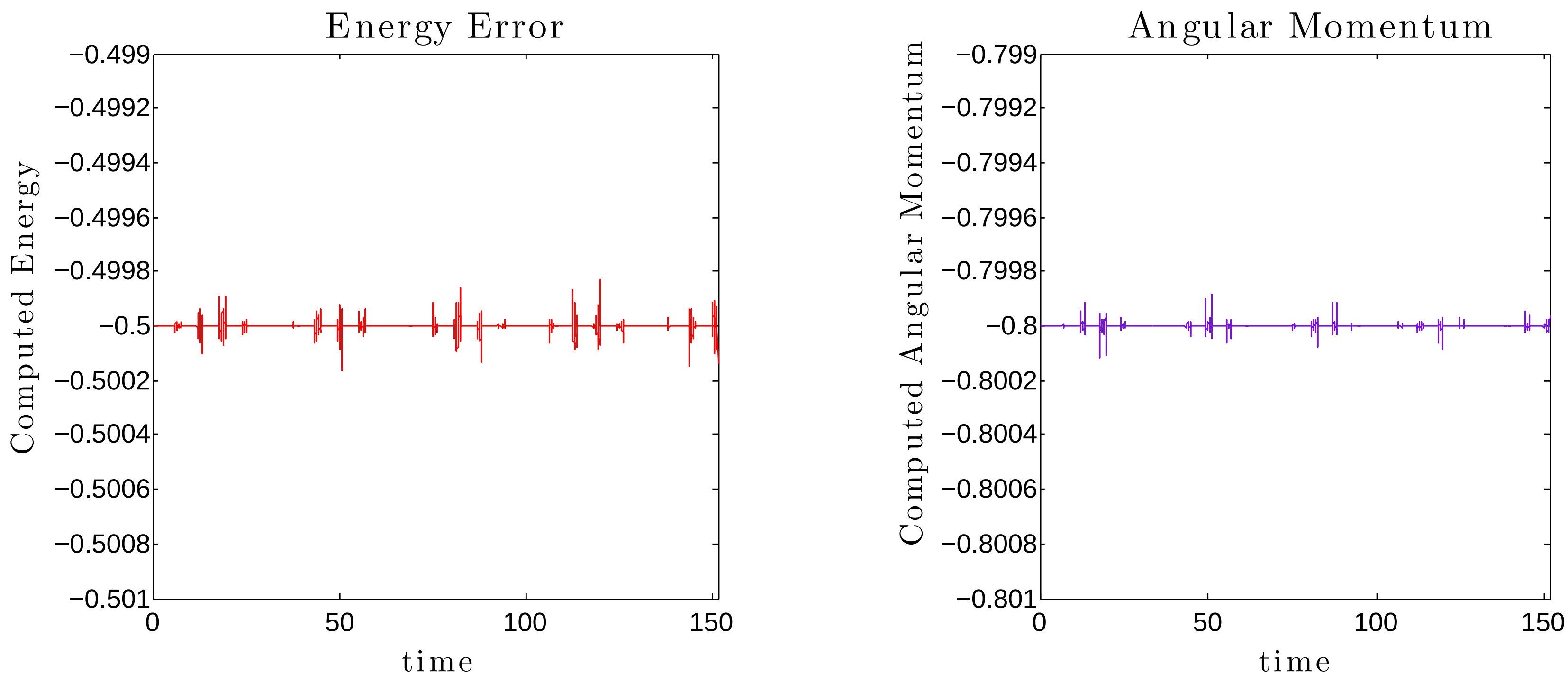
Numerical Experiments: Kepler 2-Body Problem



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

Spectral Variational Integrators

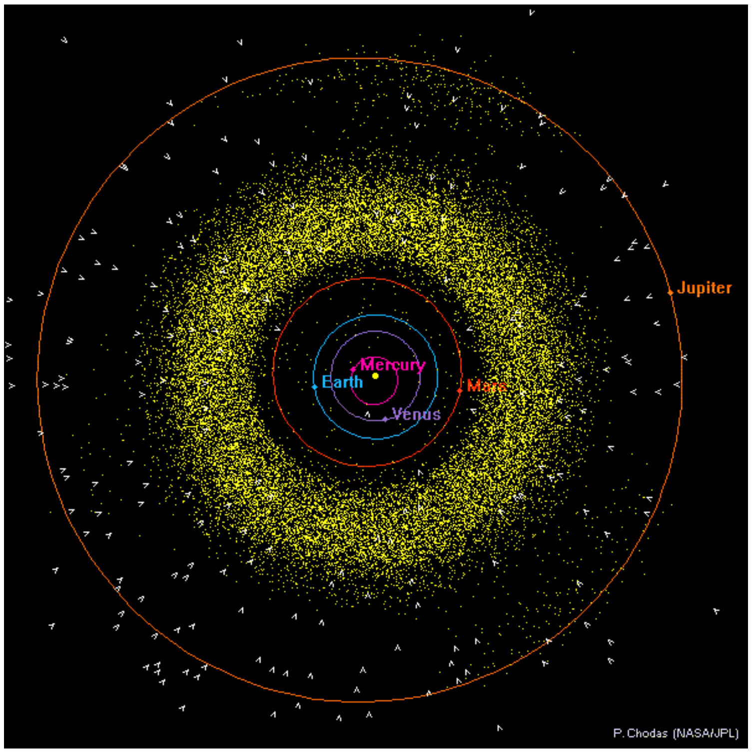
Numerical Experiments: Kepler 2-Body Problem

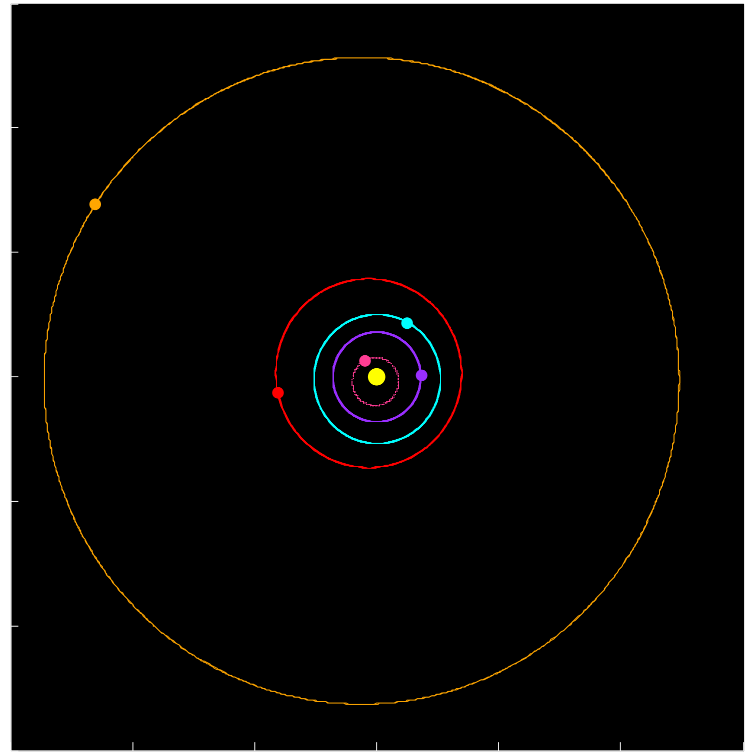


- $h = 1.5$, $T = 150$, and 20 Chebyshev points per step.

Spectral Variational Integrators

Numerical Experiments: Solar System Simulation

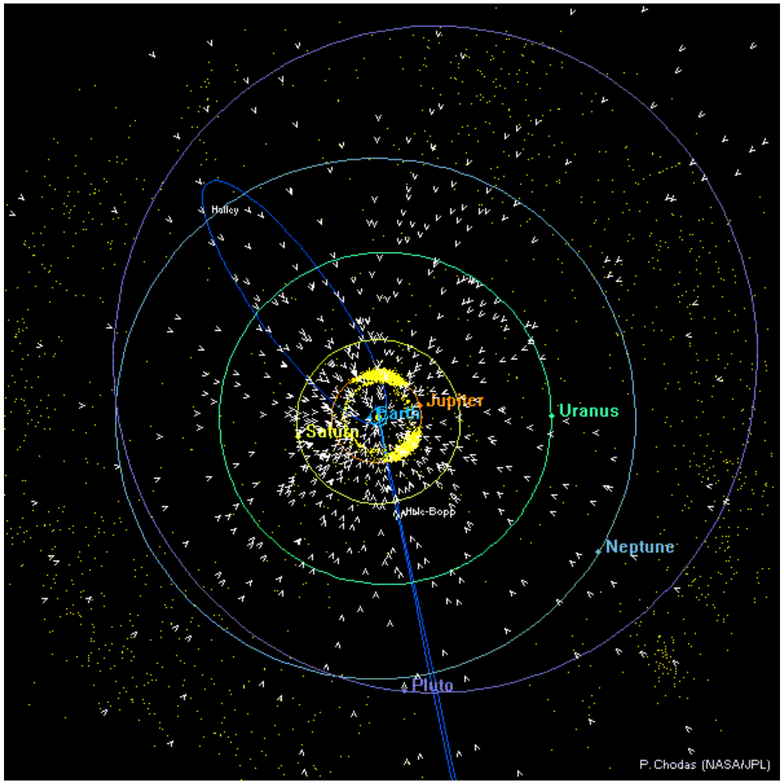


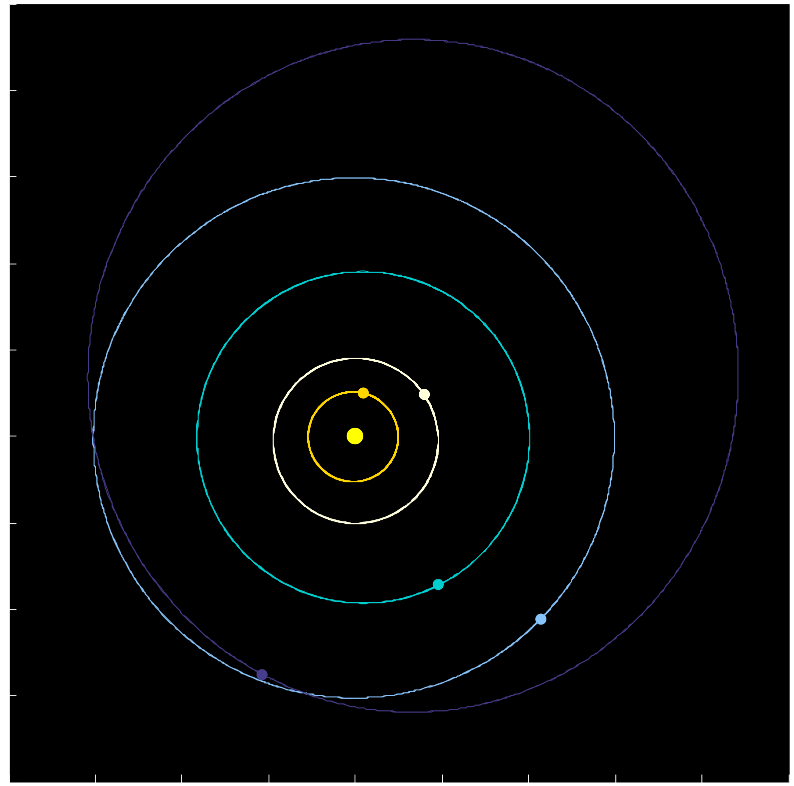


- Comparison of inner solar system orbital diagrams from a spectral variational integrator and the JPL Solar System Dynamics Group.
- $h = 100$ days, $T = 27$ years, 25 Chebyshev points per step.

Spectral Variational Integrators

Numerical Experiments: Solar System Simulation

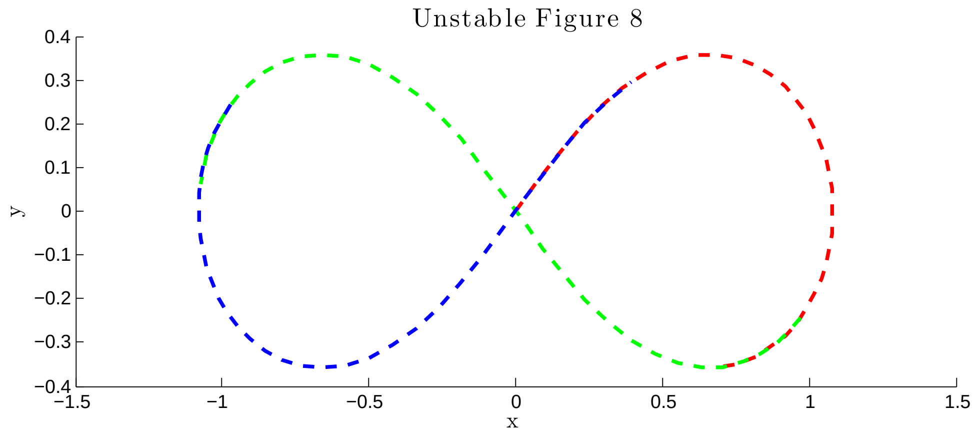


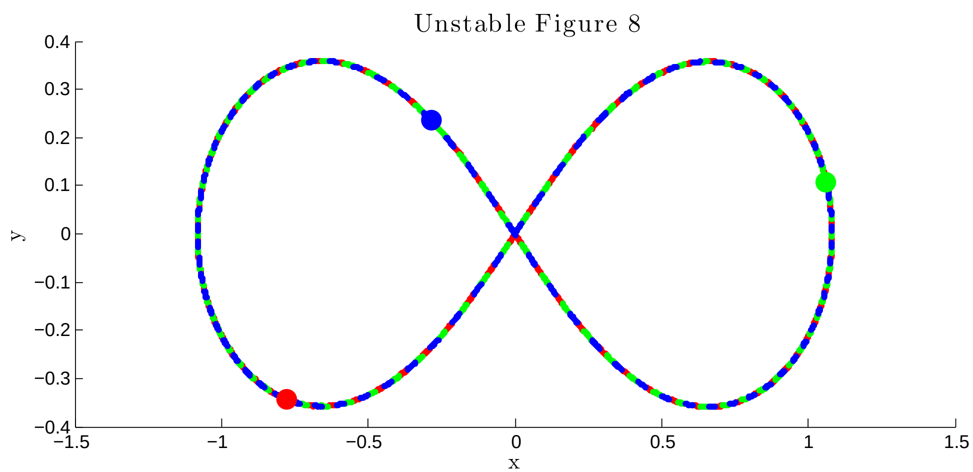


- Comparison of outer solar system orbital diagrams from a spectral variational integrator and the JPL Solar System Dynamics Group. Inner solar system was aggregated, and $h = 1825$ days.

Spectral Variational Integrators

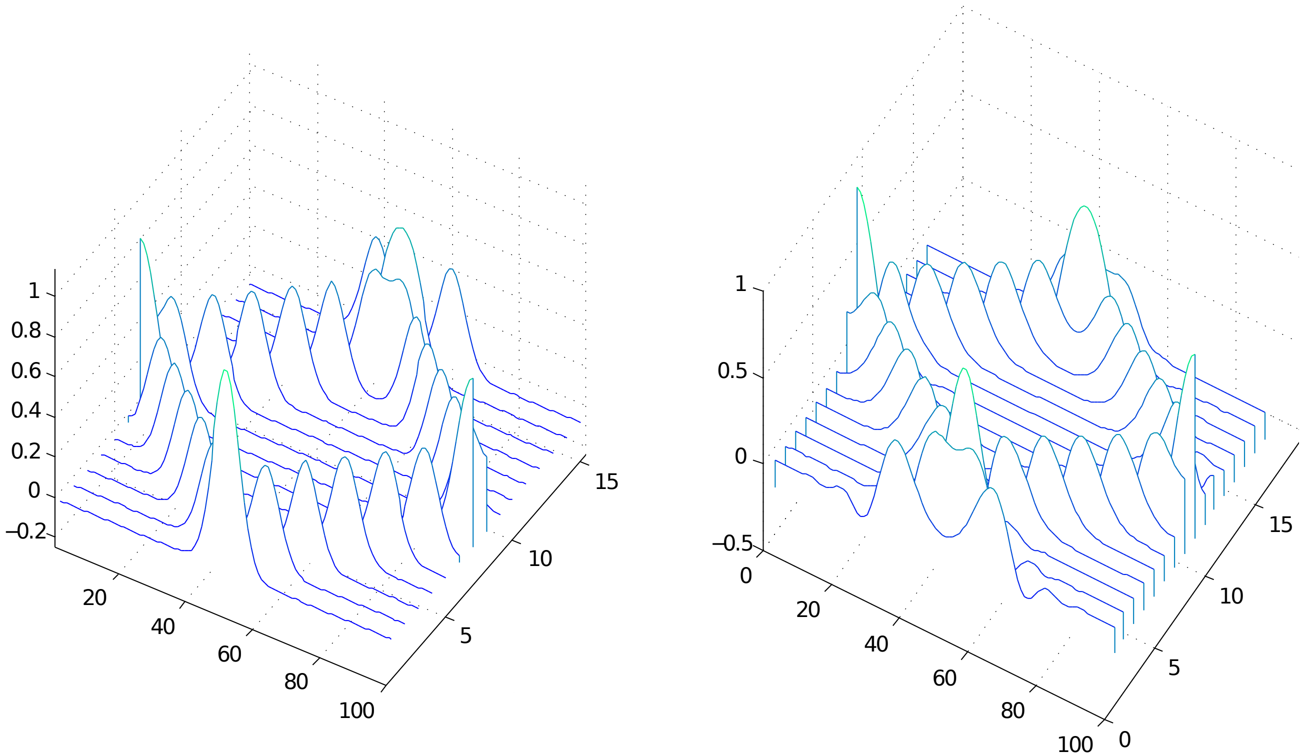
Numerical Experiments: Unstable Figure Eight





Spectral Variational Integrators

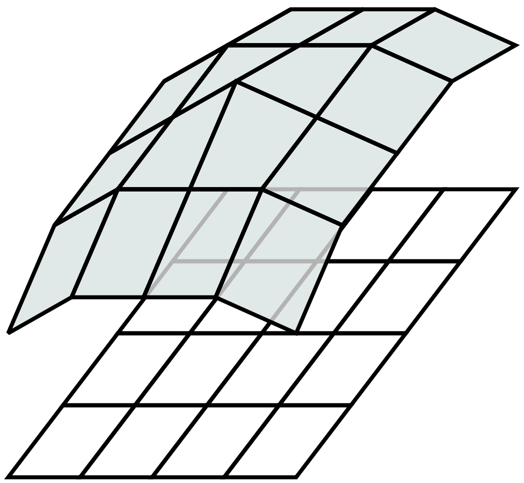
Numerical Experiments: Pseudospectral Wave Equation



- The wave equation $u_{tt} = u_{xx}$ on S^1 is described by the Lagrangian density function, $L(\varphi, \dot{\varphi}) = \frac{1}{2}|\dot{\varphi}(x,t)|^2 - \frac{1}{2}|\nabla\varphi(x,t)|^2$.
- Discretized using spectral in space, and linear in time.

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.

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.

References

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