

Generalized Galerkin Variational Integrators: Lie Group, Multiscale and Spectral Methods

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IMA Tutorial/Workshop: New Paradigms in Computation

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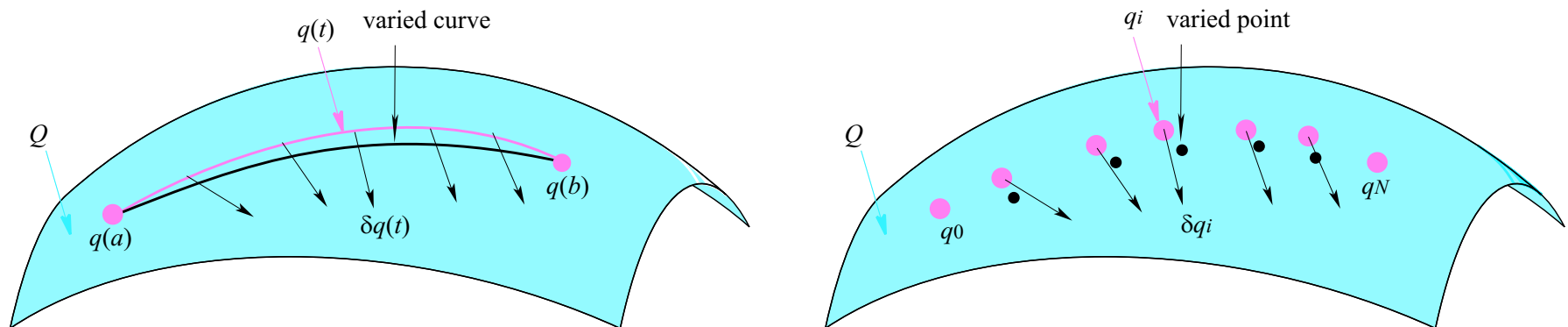
Motivation: Geometric Integration

■ 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.

Background Material

■ Discrete Variational Principle



● Discrete Lagrangian

$$L_d \approx \int_0^h L(q(t), \dot{q}(t)) dt$$

● Discrete Euler-Lagrange equation

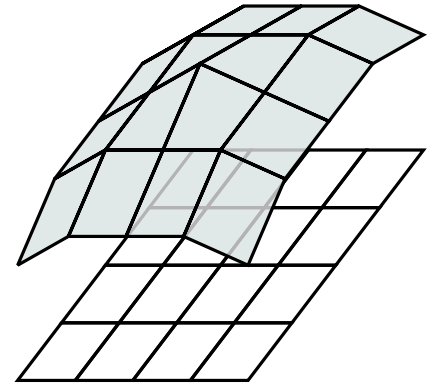
$$D_2 L_d(q_0, q_1) + D_1 L_d(q_1, q_2) = 0$$

- The discrete flows are **symplectic** and **momentum** preserving.

Multisymplectic Geometry

■ Geometry and Variational Mechanics

- **Base space** \mathcal{X} . The independent variables, typically $(n + 1)$ -spacetime, denoted by (x^0, \dots, x^n) .
- **Configuration bundle** $\pi : Y \rightarrow \mathcal{X}$.
- **Configuration** $q : \mathcal{X} \rightarrow Y$. Gives the field variables over each spacetime point.
- **First jet extension** J^1Y . Consists of the first partials of the field variables with respect to the independent variables.
- **Lagrangian density** $L : J^1Y \rightarrow \Omega^{n+1}(\mathcal{X})$.
- **Action integral** $\mathcal{S}(q) = \int_{\mathcal{X}} L(j^1q)$.
- **Hamilton's principle** $\delta\mathcal{S} = 0$.



Generalized Galerkin Variational Integrators

■ Key choices in discretizing a variational problem

- **Finite dimensional function space** to represent sections of the configuration bundle.
- **Numerical quadrature method** to accurately evaluate the action integral.

■ Contrast with standard discrete mechanics

- Not constrained to polynomial interpolation parametrized by field values at nodal points.

■ Relevant numerical analysis considerations

- Adaptivity
- Approximability
- Accuracy

Multiscale Variational Integrators

■ Finite Dimensional Function Spaces

- Motivated by the approach of Multiscale Finite Elements, instead of looking for solutions to the discrete Hamilton's principle in polynomial spaces, consider instead solutions of the form,

$$q(t; \{p_j\}, \omega, a_0, a_1) = \left(\sum_{j=0}^n p_j t^j \right) (1 + a_0 \sin(\omega t) + a_1 \cos(\omega t))$$

- These function spaces approximate the **highly oscillatory** nature of the solution well, in contrast to polynomial function spaces, thereby **avoiding approximation-theoretic errors**.
- In general, the function space has to be augmented with solutions of the **cell problem**, which describes the behavior of the fast scales when the slow scales are frozen.

Multiscale Variational Integrators

■ Constrained Discrete Variational Principle

- To couple the variational problem between time steps, we require that the interpolating function is continuous across the knot points.
- This results in a constrained variational principle, where **Lagrange multipliers** are used to enforce the continuity conditions.
- When the finite dimensional function space includes the endpoint values of q in its parametrization, the Lagrange multipliers can be eliminated from the equations to obtain the **Discrete Euler–Lagrange** equations, and stationarity conditions for the remaining parameters.

Multiscale Variational Integrators

■ Integrating Highly Oscillatory Functions

- Filon-Christoffel numerical quadrature schemes, recently analyzed by Arieh Iserles, are designed to evaluate integrals of the form,

$$I_h[f] = \int_0^h f(x)e^{i\omega x} dx.$$

- If $c_1 < c_2 < \dots < c_\nu$ are nodes in $[0, 1]$ which correspond to Gauss-Christoffel quadrature of order $p \in \nu, \nu + 1, \dots, 2\nu$, then the quadrature error of the **Filon-type method** is,

$$\begin{aligned} & \mathcal{O}(h^{p+1}), & \text{if } h\omega \ll 1 \\ & \mathcal{O}(h^\nu), & \text{if } h\omega = \mathcal{O}(1) \\ & \mathcal{O}(h^{\nu+1}/(h\omega)), & \text{if } h\omega \gg 1 \\ & \mathcal{O}(h^{\nu+1}/(h\omega)^2), & \text{if } h\omega \gg 1, c_1 = 0, c_\nu = 1. \end{aligned}$$

Multiscale Variational Integrators

■ Advantages

- The contribution of the fast dynamics are directly accounted for in the multiscale method, allowing for significantly larger time-steps.
- It becomes easier to construct numerical schemes that are robust to resonant instabilities.
- There is no need to identify fast/slow forces, or fast/slow variables in the construction of these multiscale variational integrators.

■ Disadvantages

- The initial fast frequency has to be estimated numerically.
- Both the function space and the quadrature weights depend on the fast frequency ω , resulting in a highly implicit scheme that may be expensive for large systems.

Variational Lie Group Techniques

■ Basic Idea

- To stay on the Lie group, we parametrize the curve by the initial point g_0 , and elements of the Lie algebra ξ_i , such that,

$$g_d(t) = \exp \left(\sum \xi_i t^i \right) g_0$$

- This involves standard interpolatory methods on the Lie algebra that are lifted to the group using the exponential map.
- Allows the construction of higher-order G -invariant discrete Lagrangians on Lie groups, and their corresponding discrete Euler–Poincaré equations.

Higher-Order Lie Group Variational Integrators

Equations

$$L_d(g_0, g_1) = h \sum_{i=1}^s b_i L \left(L_{g_0} \exp(\xi(c_i h)), \right. \\ \left. T_{\exp(\xi(c_i h))} L_{g_0} \cdot T_e L_{\exp(\xi(c_i h))} \cdot \text{dexp}_{\text{ad}_{\xi(c_i h)}}(\dot{\xi}(c_i h)) \right)$$

with $\xi^0 = 0$, $\xi^s = \psi_{g_0}(g_1)$, and the other Lie algebra elements implicitly defined by

$$h \sum_{i=1}^s b_i \left[\frac{\partial L}{\partial g}(c_i h) T_{\exp(\xi(c_i h))} L_{g_0} \cdot T_e L_{\exp(\xi(c_i h))} \cdot \text{dexp}_{\text{ad}_{\xi(c_i h)}} \tilde{l}_{\nu, s}(c_i) \right. \\ \left. + \frac{1}{h} \frac{\partial L}{\partial \dot{g}}(c_i h) T_{\exp(\xi(c_i h))}^2 L_{\exp(\xi(c_i h))} \cdot T_e^2 L_{\exp(\xi(c_i h))} \right. \\ \left. \cdot \text{ddexp}_{\text{ad}_{\xi(c_i h)}} \dot{\tilde{l}}_{\nu, s}(c_i) \right] = 0.$$

Higher-Order Discrete Euler–Poincaré Equations

■ Discrete Euler–Poincaré Equations

$$l'_d(f_{k-1k})TR_{f_{k-1k}} \text{Ad}_{f_{k-1k}}^{-1} l'_d(f_{kk+1})TR_{f_{kk+1}} = 0.$$

■ Higher-Order Reduced Discrete Lagrangian

$$l_d(f_{kk+1}) = h \sum_{i=1}^s b_i l \left(\text{dexp}_{\text{ad}_{\xi(c_i h)}}(\dot{\xi}(c_i h)) \right),$$

where

$$\xi(\xi^\nu; \tau h) = \sum_{\kappa=0}^s \xi^\kappa \tilde{l}_{\kappa,s}(\tau), \quad \xi^0 = 0, \quad \xi^s = \log(f_{kk+1}),$$

and $\{\xi^\nu\}_{\nu=1}^{s-1}$, are defined implicitly by

$$0 = h \sum_{i=1}^s b_i \left[\frac{\partial l}{\partial \eta}(c_i h) \text{dexp}_{\text{ad}_{\xi(c_i h)}} \dot{\tilde{l}}_{\nu,s}(c_i) \right].$$

Example of a Lie Group Variational Integrator

■ 3D Pendulum

● Lagrangian

$$L(R, \omega) = \frac{1}{2} \int_{Body} \|S(\tilde{\rho})\omega\|^2 dm - V(R),$$

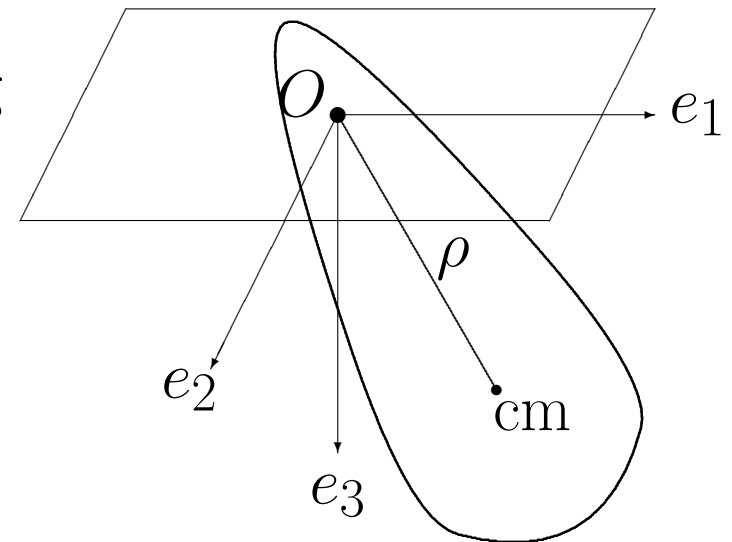
where $S(\cdot) : \mathbb{R}^3 \mapsto \mathbb{R}^{3 \times 3}$ is a skew mapping such that $S(x)y = x \times y$.

● Equations of motion

$$J\dot{\omega} + \omega \times J\omega = M,$$

where $S(M) = \frac{\partial V^T}{\partial R} R - R^T \frac{\partial V}{\partial R}$.

$$\dot{R} = RS(\omega).$$



Example of a Lie Group Variational Integrator

■ 3D Pendulum

- Discrete Lagrangian

$$L_d(R_k, F_k) = \frac{1}{h} \operatorname{tr} [(I_{3 \times 3} - F_k) J_d] - \frac{h}{2} V(R_k) - \frac{h}{2} V(R_{k+1}).$$

- Discrete Equations of Motion

$$\begin{aligned} J\omega_{k+1} &= F_k^T J\omega_k + hM_{k+1}, \\ S(J\omega_k) &= \frac{1}{h} \left(F_k J_d - J_d F_k^T \right), \\ R_{k+1} &= R_k F_k. \end{aligned}$$

Example of a Lie Group Variational Integrator

■ Automatically staying on the rotation group

- The magic begins with the ansatz,

$$F_k = e^{S(f_k)},$$

and the Rodrigues' formula, which converts the equation,

$$S(J\omega_k) = \frac{1}{h} \left(F_k J_d - J_d F_k^T \right),$$

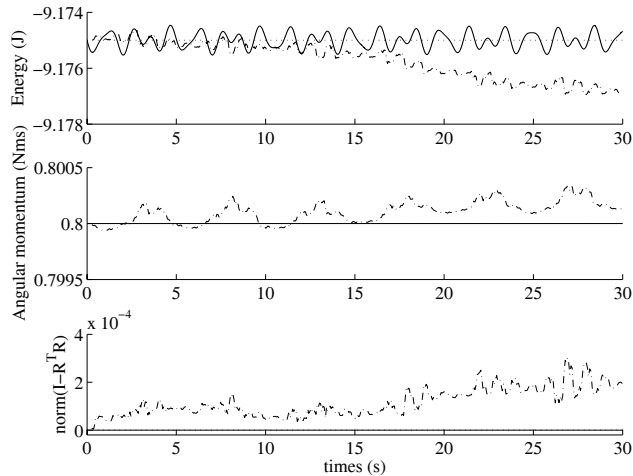
into

$$hJ\omega_k = \frac{\sin \|f_k\|}{\|f_k\|} Jf_k + \frac{1 - \cos \|f_k\|}{\|f_k\|^2} f_k \times Jf_k.$$

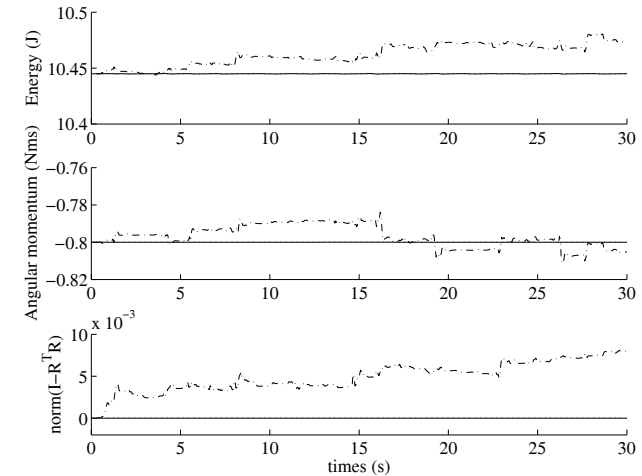
- Since F_k is now the exponential of a skew matrix, it is automatically a rotation matrix, which means that $R_{k+1} = R_k F_k$ is automatically a rotation matrix.

Example of a Lie Group Variational Integrator

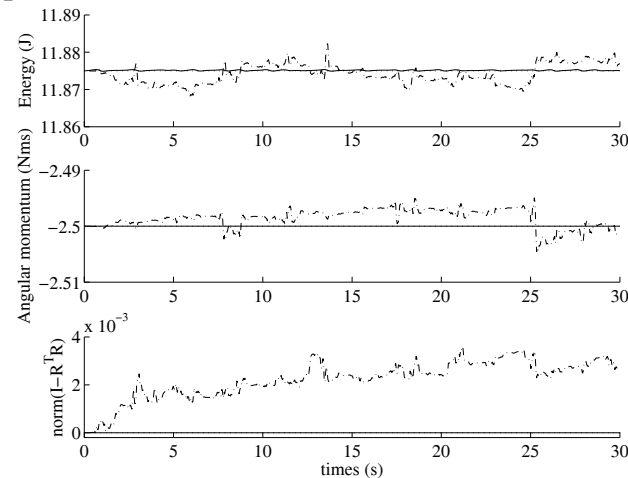
Numerical Preservation of Conserved Quantities



Perturbation of hanging equilibrium



Perturbation of inverted equilibrium



Perturbation of horizontal position

Schrödinger Equation

■ Variational derivation

- Let \mathcal{H} be the space of complex-valued functions ψ on \mathbb{R}^3 , and

$$\langle \psi_1, \psi_2 \rangle = \int \psi_1(x) \bar{\psi}_2(x) d^3x .$$

- The Lagrangian density is given by

$$\mathcal{L}(j^1\psi) = \frac{i\hbar}{2} \{ \dot{\psi} \bar{\psi} - \psi \dot{\bar{\psi}} \} - \hat{H} \psi \bar{\psi},$$

$$\hat{H}\psi = -\frac{\hbar^2}{2m} \nabla^2 \psi + V \psi.$$

- Schrödinger Equation (Linear, time-dependent)

$$i\hbar \dot{\psi} = \left\{ -\frac{\hbar^2}{2m} \nabla^2 + V \right\} \psi .$$

Schrödinger Equation

■ Pseudospectral Variational Integrator

- Shape functions using a tensor product of a spectral expansion in space, and a polynomial expansion in time.
- For example, in (1+1)-spacetime, with periodic boundary conditions, the interpolatory function is given by

$$\psi(x, (\tau + l)\Delta t) = \frac{1}{2\pi} \sum'_{k=-N/2}^{N/2} e^{ikx} \left((1 - \tau)\hat{v}_k^l + \tau\hat{v}_k^{l+1} \right),$$

which is a Fourier series in space, and linear interpolation in time.

- The interesting thing is that the action integral restricted to this function space can be exactly evaluated, without the need for numerical quadrature, so that we can analyze the approximation theoretic effects in isolation.

Schrödinger Equation

■ Pseudospectral Variational Integrator

- Discrete action sum given by

$$\begin{aligned}
 \mathbb{S}_d = & \frac{i\hbar}{4\pi} \sum''_{k=-N/2}^{N/2} \left[\hat{v}_k^{l+1} \bar{v}_k^l - \hat{v}_k^l \bar{v}_k^{l+1} \right] - \frac{\hbar^2 k^2 \Delta t}{24\pi^2} \sum''_{k=-N/2}^{N/2} \left[\hat{v}_k^l (2\bar{v}_k^l + \bar{v}_k^{l+1}) + \hat{v}_k^{l+1} (\bar{v}_k^l + 2\bar{v}_k^{l+1}) \right] \\
 & - \frac{\Delta t}{24\pi^2} \left(\sum'_{n=-N/2}^{-1} \sum'_{m=-N/2}^{N/2+n} + \sum'_{n=0}^{N/2} \sum'_{m=n-N/2}^{N/2} \right) \hat{V}_{n-m} \left[\hat{v}_m^l (2\bar{v}_n^l + \bar{v}_n^{l+1}) + \hat{v}_m^{l+1} (\bar{v}_n^l + 2\bar{v}_n^{l+1}) \right] \\
 & + \lambda_l \left(1 - \frac{1}{2\pi} \sum''_{k=-N/2}^{N/2} \hat{v}_k^l \bar{v}_k^l \right)
 \end{aligned}$$

- Could also consider fully spectral variational integrators.
- Would be interesting to compare spectral codes with spectral variational integrators to see if variational methods have advantages that persist even when compared to codes with spectral accuracy.

Conclusion

■ Current Work and Future Directions

- Using the knowledge of fast/slow forces/variables to construct more efficient multiscale variational integrators.
- Relating multiscale variational integrators to averaging methods, WKB analysis, homogenization techniques, multiscale finite element methods, and heterogeneous multiscale methods.
- Relating Lie group variational integrators and Lie group techniques based on Magnus and Fer expansions.
- Extend construction of G -invariant discrete Lagrangians to homogeneous spaces using G -equivariant interpolation.

Slides available at,

http://www.math.lsa.umich.edu/~mleok/ima_npc2005.pdf