Computational Geometric Uncertainty Propagation for Hamiltonian Systems on a Lie Group

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Hamiltonian Uncertainty Propagation on Lie Groups

Nonlinear Uncertainty Propagation on Lie Groups

- Many mechanical systems of contemporary engineering interest have configuration manifolds that are products of Lie groups and homogeneous spaces.
- Efficient characterization of uncertainty in simulations is important in order to quantify the reliability of the simulation results in the face of uncertainty in initial conditions and model parameters.
- The advection of a probability density by a dynamical flow is fundamental to problems of data assimilation, machine learning, system identification, and state estimation.
- Moments of a distribution do not make sense on a manifold, therefore we need to consider alternative representations of probability densities on manifolds.

Uncertainty Propagation

Symplectic Uncertainty Propagation

- **Liouvile equation**: describes the propagation of a probability density p along a vector field X without diffusion.
- If the vector field is Hamiltonian, it reduces to $\frac{dp}{dt} = 0$.
- The probability density is preserved along a Hamiltonian flow.

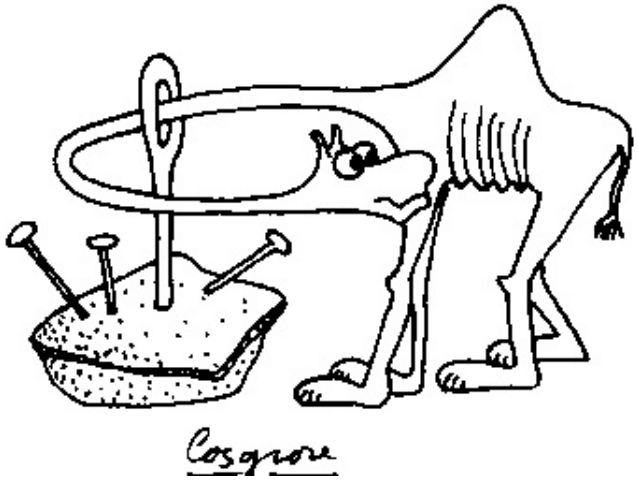
The essential ideas

- Augment the base space of spacetime with additional directions corresponding to parameters with uncertainty in them.
- Instead of using trajectories of sample points to compute statistics, as in Monte Carlo, use it to **reconstruct the distribution**.
- The uncertainty distribution is **advected** by the flow, and the flows at different parametric values are uncoupled.

Uncertainty Propagation

The role of symplecticity

- Consider an initial uniform probability density on an ellipsoid. Since the flow is symplectic, it is volume-preserving.
- But can we arbitrarily compress the probability distribution in one direction at the expense of the other directions?



Gromov's nonsqueezing theorem in symplectic geometry

- The nonsqueezing theorem states that the initial projected volume of a subdomain onto position-momentum planes is a lower bound to the projected volume of the symplectic image of the subdomain.
- It is therefore essential that the uncertainty in a Hamiltonian system be propagated using a symplectic method.

Uncertainty Propagation

Extensions to Lie Groups

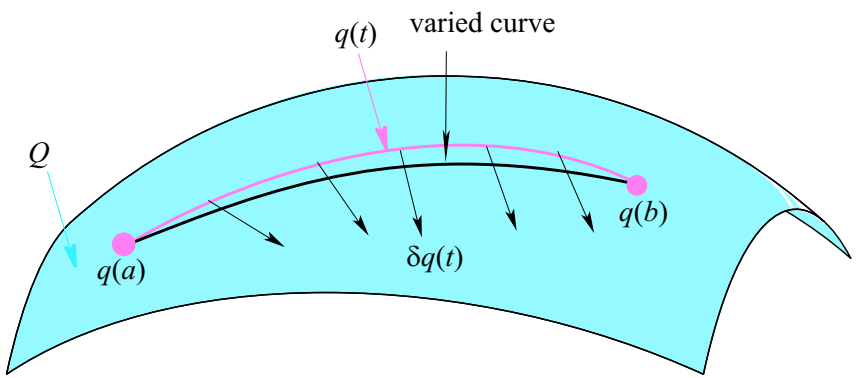
- Use Lie group variational integrators for the individual flows.
- Use **noncommutative harmonic analysis**. Complete basis for $L^2(G)$ using irreducible unitary group representations.
- More explicitly, a **group representation** $\varphi : G \to GL(\mathbb{C}^n)$ is a group homomorphism, i.e., $\varphi(g \cdot h) = \varphi(g) \cdot \varphi(h)$.
- The **Peter-Weyl theorem** states,

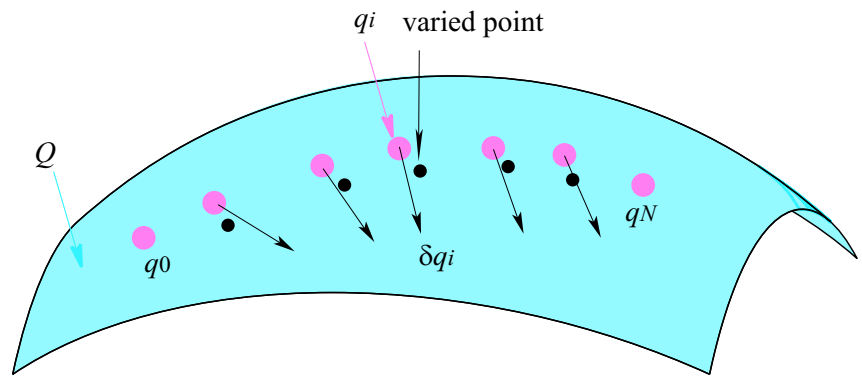
$$L^2(G) = \bigoplus_{\varphi \in \hat{G}} V_\varphi,$$

  and $g \mapsto \langle e^j, \varphi(g) \cdot e_i \rangle$ form a basis for the vector space V_φ.
- For compact Lie groups and Lie groups with bi-invariant Haar measures, techniques from computational harmonic analysis generalize, including Fast Fourier Transforms, Plancherel theorem.

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 $q_{0,1}(0) = q_0$, $q_{0,1}(h) = q_1$.

- **Discrete Euler-Lagrange equation**

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

Galerkin Variational Integrators

Variational Characterization of L_d^{exact}

- An alternative characterization of the exact discrete Lagrangian,

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

  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**.

Galerkin Variational Integrators

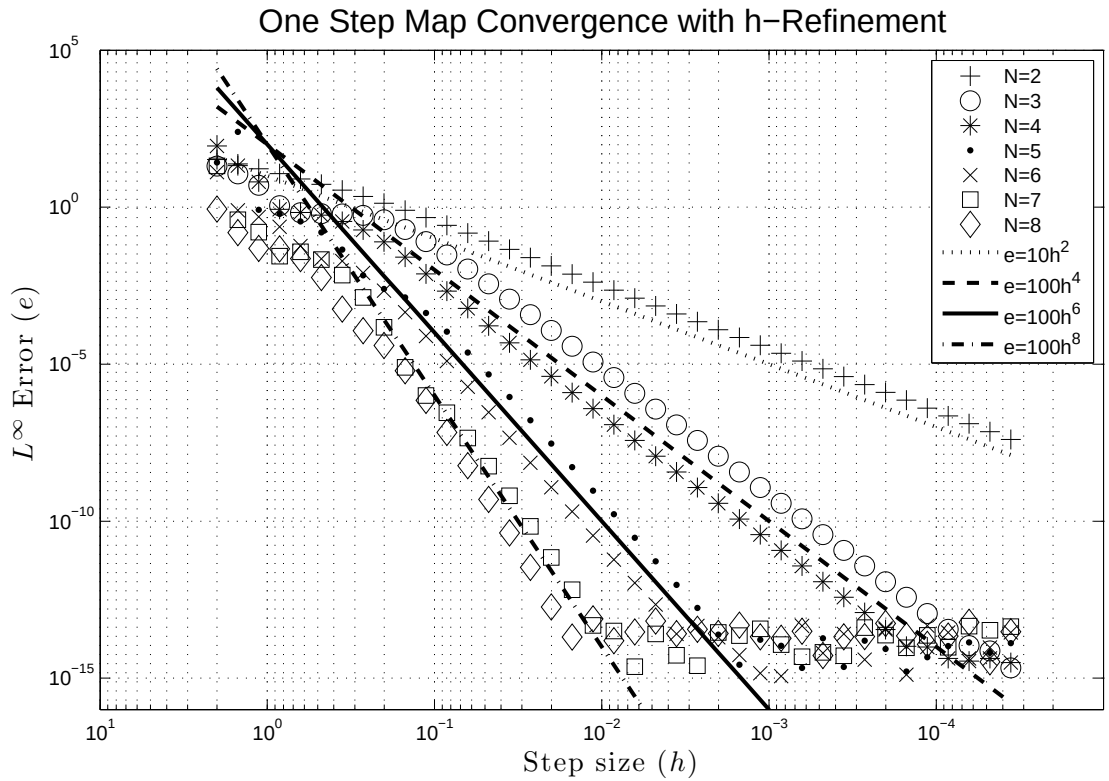
Theorem: Optimality of Galerkin Variational Integrators

- 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.
- Spectral variational integrators are **geometrically convergent**.
- The Galerkin curves converge at the square root of the rate of convergence of the solution at discrete times.

Galerkin Variational Integrators

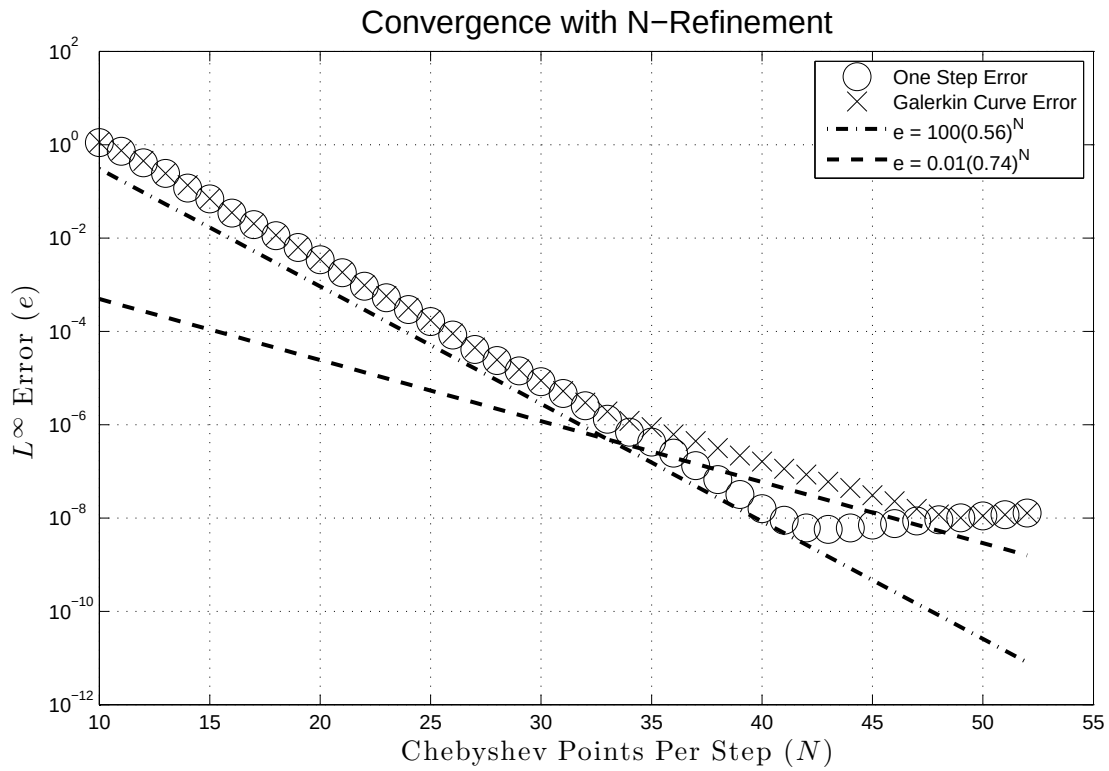
Numerical Results: Order Optimal Convergence



- Order optimal convergence of the Kepler 2-body problem with eccentricity 0.6 over 100 steps of $h = 2.0$.

Spectral Galerkin Variational Integrators

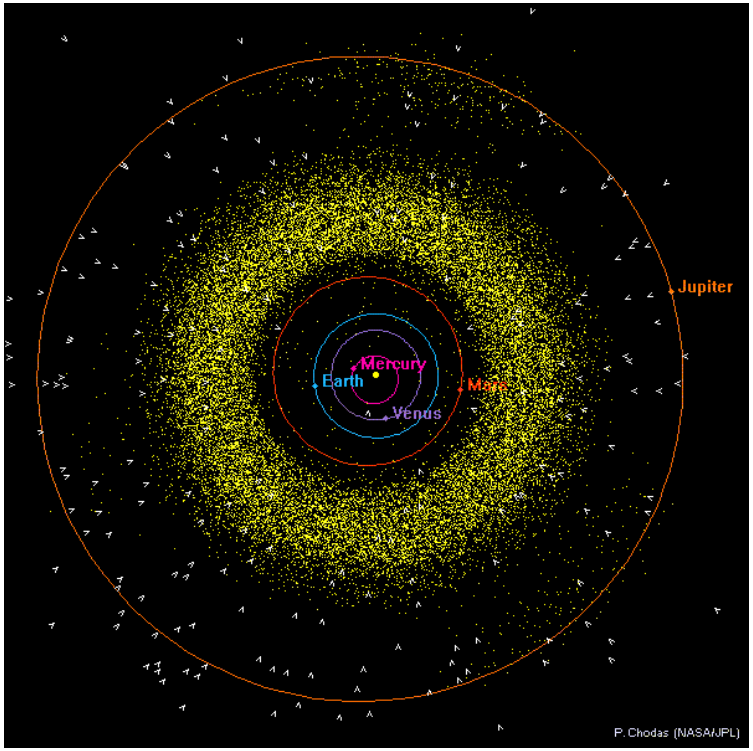
Numerical Results: Geometric Convergence

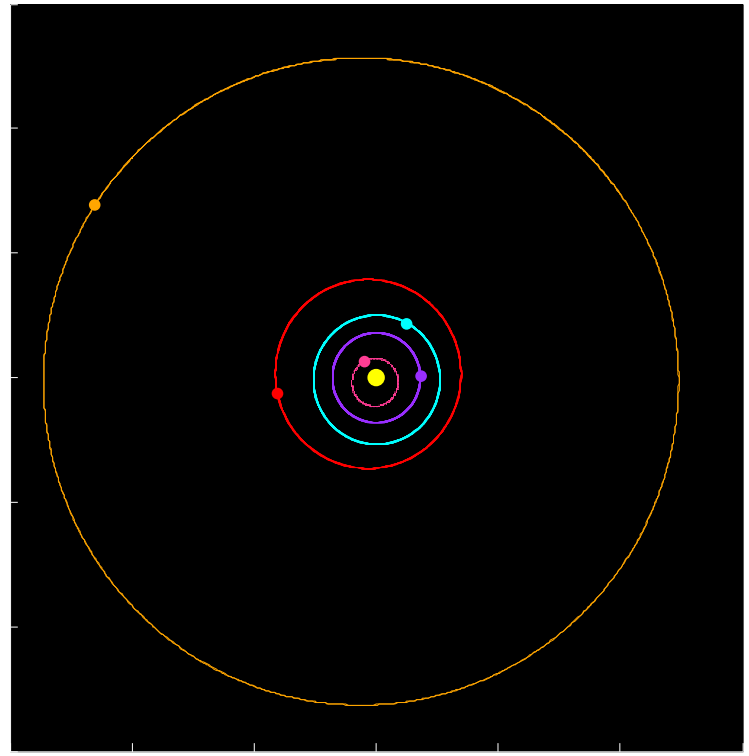


- Geometric convergence of the Kepler 2-body problem with eccentricity 0.6 over 100 steps of $h = 2.0$.

Spectral Variational Integrators

Numerical Experiments: Solar System Simulation

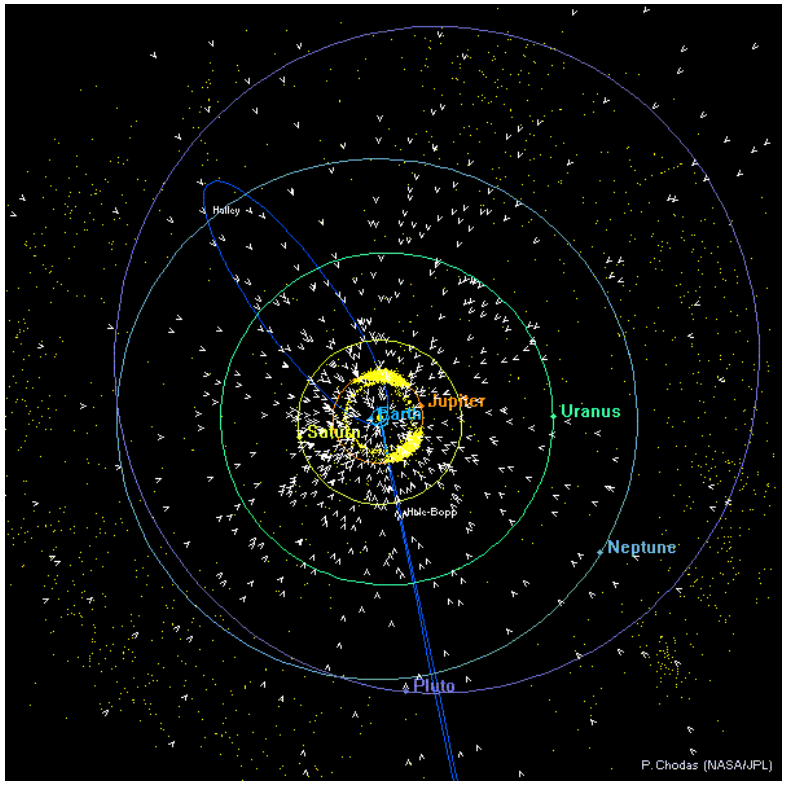


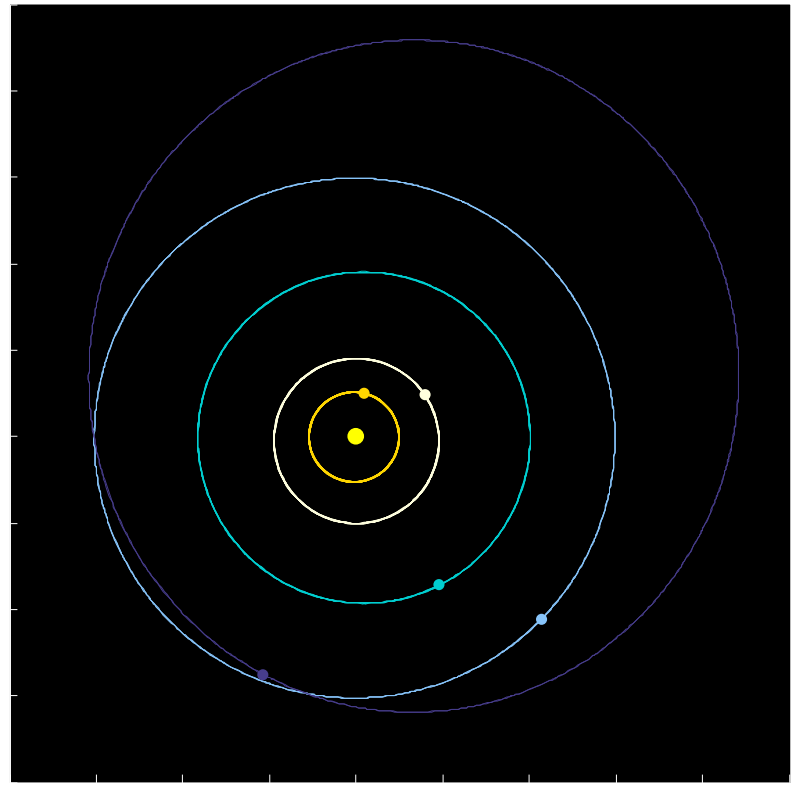


- Comparison of inner solar system orbital diagrams from a spectral variational integrator and the JPL Solar System Dynamics Group.
- $h = 100$ days, $T = 27$ years, 25 Chebyshev points per step.

Spectral Variational Integrators

Numerical Experiments: Solar System Simulation

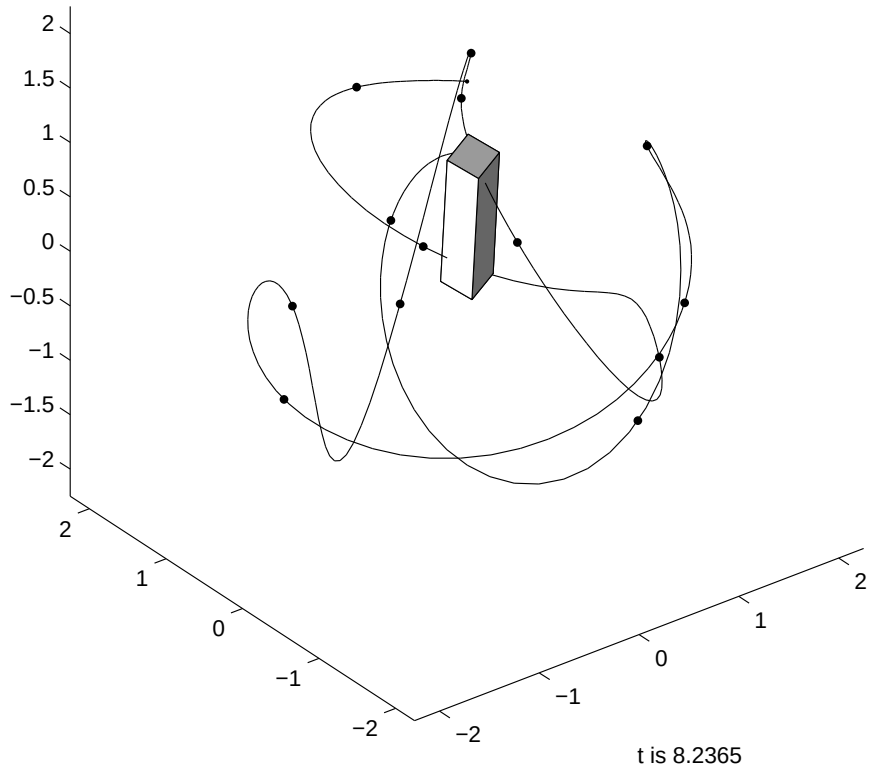




- Comparison of outer solar system orbital diagrams from a spectral variational integrator and the JPL Solar System Dynamics Group. Inner solar system was aggregated, and $h = 1825$ days.

Spectral Lie Group Variational Integrators

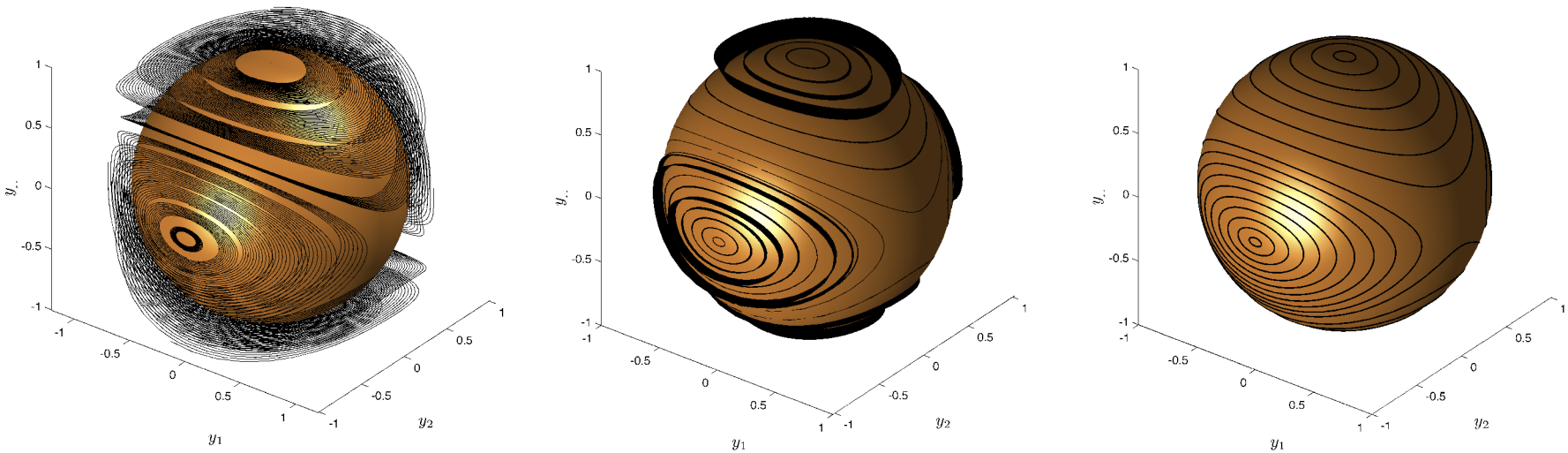
Numerical Experiments: 3D Pendulum



- $n = 20$, $h = 0.6$. The black dots represent the discrete solution, and the solid lines are the Galerkin curves. Some steps involve a rotation angle of almost π, which is close to the chart singularity.

Spectral Lie Group Variational Integrators

Numerical Experiments: Free Rigid Body



Explicit Euler MATLAB ode45 Lie Group Variational Integrator

- The conserved quantities are the norm of body angular momentum, and the energy. Trajectories lie on the intersection of the angular momentum sphere and the energy ellipsoid.
- These figures illustrate the extent to the numerical methods preserve the quadratic invariants.

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,

$$g_d(t) = \exp\left(\sum \xi^s \tilde{l}_{\kappa,s}(t)\right) g_0$$

- This involves standard interpolatory methods on the Lie algebra that are lifted to the group using the exponential map.
- Automatically stays on the Lie group without the need for reprojection, constraints, or local coordinates.
- Cayley transform based methods perform 5-6 times faster, without loss of geometric conservation properties.

Example of a Lie Group Variational Integrator

3D Pendulum

- **Lagrangian**

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

where $\widehat{\cdot}: \mathbb{R}^3 \to \mathbb{R}^{3\times 3}$ is a skew mapping such that $\widehat{x}y = x \times y$.

- **Equations of motion**

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

where $\widehat{M} = \frac{\partial V}{\partial R}^T R - R^T \frac{\partial V}{\partial R}$.

$$\dot{R} = R\widehat{\omega}.$$

Example of a Lie Group Variational Integrator

3D Pendulum

- **Discrete Lagrangian**

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

- **Discrete Equations of Motion**

$$\begin{aligned} J\omega_{k+1} &= F_k^T J\omega_k + \frac{h}{2}M_k + \frac{h}{2}M_{k+1}, \\ S(J\omega_k) &= \frac{1}{h}\left(F_k J_d - J_d F_k^T\right), \\ R_{k+1} &= R_k F_k. \end{aligned}$$

Example of a Lie Group Variational Integrator

Automatically staying on the rotation group

- The magic begins with the ansatz,

$$F_k = e^{\widehat{f_k}},$$

and the Rodrigues' formula, which converts the equation,

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

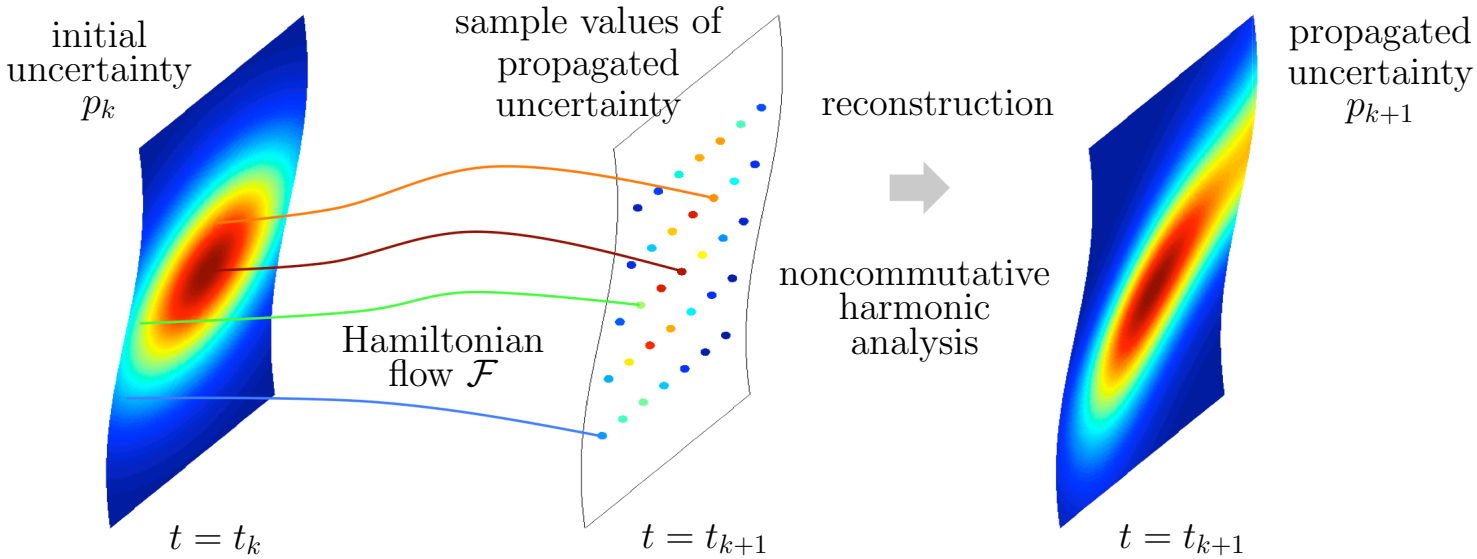
into

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

- Since F_k is the exponential of a skew matrix, it is a rotation matrix, and by matrix multiplication $R_{k+1} = R_k F_k$ is a rotation matrix.

Uncertainty Propagation

Symplectic Uncertainty Propagation Algorithm

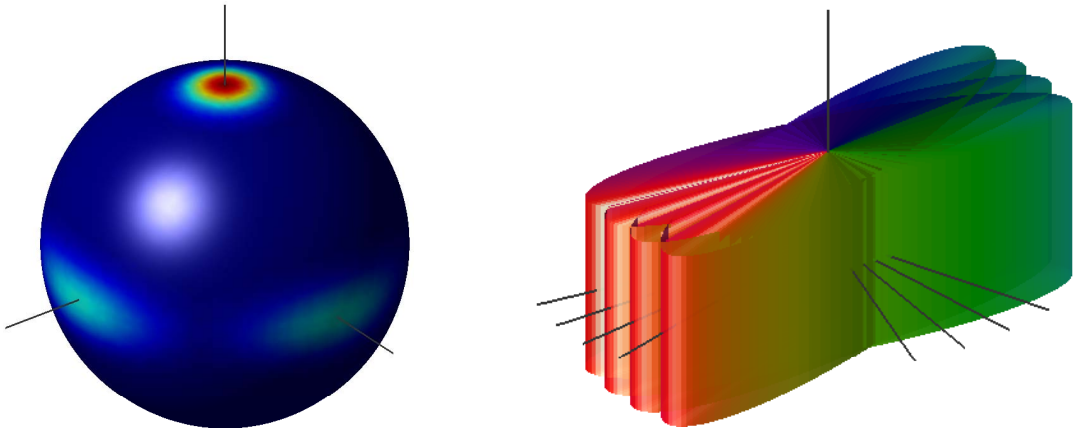


Incorporating Diffusion: Splitting Method

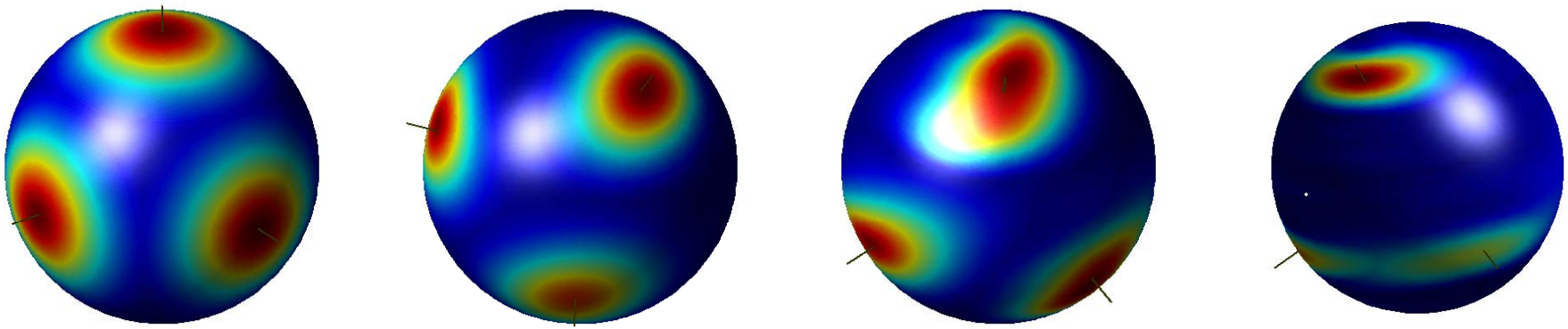
- A diffusion problem reduces to a type of the heat equation, which can be solved efficiently using computational harmonic analysis.
- General uncertainty propagation problems can be decomposed into advection and diffusion.

Uncertainty Propagation Example on $\mathrm{SO}(3)$

- **Visualization of Attitude Uncertainty on a Sphere**



- **Propagation of Attitude Uncertainty on $SO(3)$**



$t = 0.0$ $t = 0.2$ $t = 0.4$ $t = 1$

Information Geometry and Discrete Mechanics

Divergence functions

- Divergence functions are non-symmetric measures of proximity, such as the Kullback–Leibler, or Bergman divergences.
- Divergence functions encode a metric, and they are first-order accurate symplectic generating functions for the geodesic flow, and are second-order accurate when the information manifold is Hessian.

Applications to Machine Learning

- Given a sequence of estimates $\{x_i\}$ and samples of the actual distributin $\{y_i\}$, we can construct a discrete Lagrangian for generating the discrete dynamics for a machine learning application by using,

$$L_d(x_i, x_{i+1}) = \mathcal{D}(x_i, x_{i+1}) + \mathcal{D}(x_{i+1}, y_{i+1}),$$

where $\mathcal{D}(\cdot, \cdot)$ defines both the metric and the potential.

Summary

Lie group variational integrators

- A combination of Lie group ideas with variational integrators, with the properties:
  - global, and singularity-free.
  - symplectic, momentum preserving.
  - automatically stays on the Lie group without the need for constraints, reprojection, or local coordinates.

Uncertainty Propagation on Lie groups

- Allows the propagation of uncertainty on nonlinear spaces, without assuming that the density is localized to a single coordinate chart.
- A combination of noncommutative harmonic analysis, generalized polynomial chaos, and Lie group variational integrators.

References

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2. J. Hall, ML, *Lie Group Spectral Variational Integrators*, arXiv:1402.3327.
3. T. Lee, ML, N.H. McClamroch, *Global Symplectic Uncertainty Propagation on $SO(3)$*, Proc. IEEE Conf. on Decision and Control, 61-66, 2008.

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Happy 20th Anniversary Control and Dynamical Systems!

Dedicated to the memory of Jerrold E. Marsden, 1942–2010

Advisor, mentor, role model, collaborator, colleague, and friend.