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NOTETAKER CHECKLIST FORM

(Complete one for each talk.)

Name: ORI KATZ Email/Phone: ORIKATZ.OK@gmail.com

Speaker's Name: Melvin Leok

Talk Title: Variational discretizations of Gauge field theories using group-equivariant interpolation

Date: 10/9/18 Time: 3:30 am / pm (circle one)

Please summarize the lecture in 5 or fewer sentences: A systematic approach for constructing variational integrators by approximating the exact discrete Lagrangian is obtained, with good convergence rates. Many gauge field theories can be formulated using a multisymplectic Lagrangian formulation; a characterization of exact generating functionals that generate this formulation is presented. Eventually, the goal is to construct variational discretizations of GR, which is a 2nd order gauge-field theory.

CHECK LIST

(This is **NOT** optional, we will **not pay** for **incomplete** forms)

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Variational Discretizations of Gauge Field Theories using Group-equivariant Interpolation

Melvin Leok

Mathematics, University of California, San Diego

Joint work with Evan Gawlik, James Hall, and Joris Vankerschaver

Hamiltonian Systems, from Topology to Applications through Analysis I
MSRI, Berkeley, CA, October 9, 2018

NSF DMS-0726263 • DMS-100152 • DMS-1010687 (CAREER)
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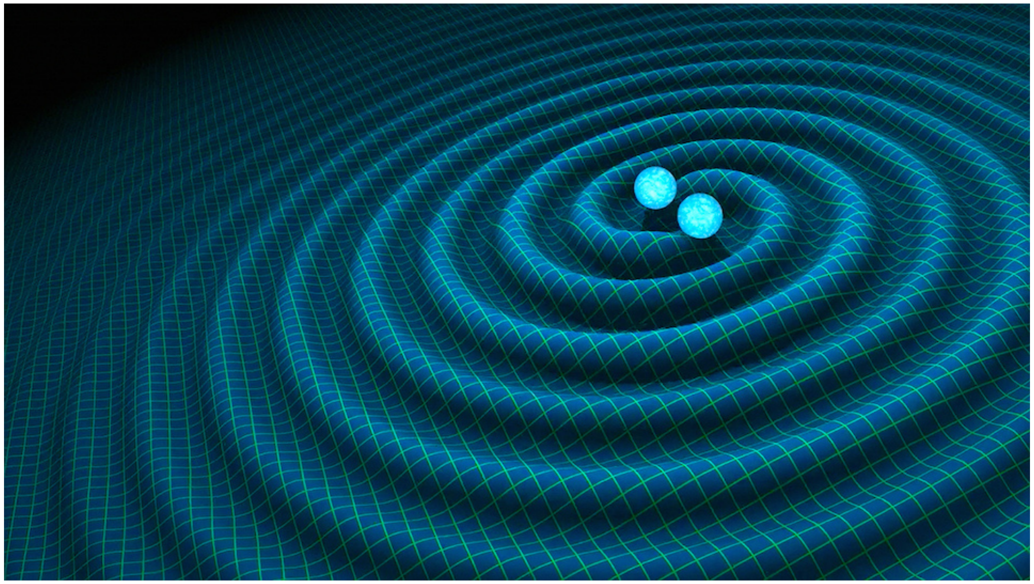
Gravitational Waves, LIGO, and Numerical Relativity



- **Gravitational waves** are ripples in the fabric of spacetime that were predicted by Einstein in 1916.
- Gravitational waves were directly observed on September 14, 2015 by the **Advanced LIGO project**.
- **Numerical relativity** is necessary to compute the black hole mergers that generate gravitational waves.

General Relativity and Gauge Field Theories

- The Einstein equations arise from the **Einstein–Hilbert action** defined on **Lorentzian metrics**,

$$S_G(g_{\mu\nu}) = \int \left[\frac{1}{16\pi G} g^{\mu\nu} R_{\mu\nu} + \mathcal{L}_M \right] \sqrt{-g} d^4x,$$

where $g = \det g_{\mu\nu}$ and $R_{\mu\nu} = R^{\alpha}_{\mu\alpha\nu}$ is the Ricci tensor.

- This yields the **Einstein field equations**,

$$G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} g^{\alpha\beta} R_{\alpha\beta} = 8\pi G T_{\mu\nu},$$

where $T_{\mu\nu} = -2\frac{\delta \mathcal{L}_M}{\delta g^{\mu\nu}} + g_{\mu\nu}\mathcal{L}_M$ is the stress-energy tensor.

- This is a **second-order gauge field theory**, with the spacetime diffeomorphisms as the gauge symmetry group.

Gauge Field Theories

- A **gauge symmetry** is a continuous local transformation on the field variables that leaves the system physically indistinguishable.
- A consequence of this is that the Euler–Lagrange equations are **underdetermined**, i.e., the evolution equations are insufficient to propagate all the fields.
- The **kinematic fields** have no physical significance, but the **dynamic fields** and their conjugate momenta have physical significance.
- The Euler–Lagrange equations are **overdetermined**, and the initial data on a Cauchy surface satisfies a constraint (usually elliptic).
- These degenerate systems are naturally described using **multi-Dirac** mechanics and geometry.

Example: Electromagnetism

- Let $\mathbf{E}$ and $\mathbf{B}$ be the electric and magnetic vector fields respectively.
- We can write Maxwell's equations in terms of the scalar and vector potentials ϕ and $\mathbf{A}$ by,

$$\mathbf{E} = -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t}, \qquad \nabla^2\phi + \frac{\partial}{\partial t}(\nabla\cdot\mathbf{A}) = 0,$$

$$\mathbf{B} = \nabla\times\mathbf{A}, \qquad \Box\mathbf{A} + \nabla\left(\nabla\cdot\mathbf{A} + \frac{\partial\phi}{\partial t}\right) = 0.$$

- The following transformation leaves the equations invariant,

$$\phi \to \phi - \frac{\partial f}{\partial t}, \qquad \mathbf{A} \to \mathbf{A} + \nabla f.$$

- The associated Cauchy initial data constraints are,

$$\nabla\cdot\mathbf{B}^{(0)} = 0, \qquad \nabla\cdot\mathbf{E}^{(0)} = 0.$$

Example: Gauge conditions in EM

- One often addresses the indeterminacy due to gauge freedom in a field theory through the choice of a **gauge condition**.
- The **Lorenz gauge** is $\nabla \cdot \mathbf{A} = -\frac{\partial \phi}{\partial t}$, which yields,

$$\Box \phi = 0, \qquad \Box \mathbf{A} = 0.$$

- The **Coulomb gauge** is $\nabla \cdot \mathbf{A} = 0$, which yields,

$$\nabla^2 \phi = 0, \qquad \Box \mathbf{A} + \nabla \frac{\partial \phi}{\partial t} = 0.$$

- Given different initial and boundary conditions, some problems may be easier to solve in certain gauges than others. There is no systematic way of deciding which gauge to use for a given problem.

Noether's Theorem

Theorem (Noether's Theorem)

- For every continuous symmetry of an action, there exists a quantity that is conserved in time.

Example

- The simplest illustration of the principle comes from classical mechanics: a time-invariant action implies a conservation of the Hamiltonian, which is usually identified with energy.
- More precisely, if $S = \int_{t_a}^{t_b} L(q, \dot{q}) dt$ is invariant under the transformation $t \to t + \epsilon$, then

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

Noether's Theorem

Theorem (Noether's Theorem for Gauge Field Theories)

- For every differentiable, local symmetry of an action, there exists a **Noether current** obeying a continuity equation. Integrating this current over a spacelike surface yields a conserved quantity called a **Noether charge**.

Examples

- The Noether currents for electromagnetism are,

$$j_0 = \mathbf{E} \cdot \nabla f \qquad \qquad \mathbf{j} = -\mathbf{E}\frac{\partial f}{\partial t} + (\mathbf{B} \times \nabla) f$$

- The Einstein–Hilbert action for GR yields the stress-energy tensor,

$$T_{\mu\nu} = -2\frac{\delta \mathcal{L}_M}{\delta g^{\mu\nu}} + g_{\mu\nu}\mathcal{L}_M$$

as the Noether charge for spacetime diffeomorphism symmetry.

Consequences of Gauge Invariance in GR

- By **Noether's second theorem**, the spacetime diffeomorphism symmetry implies that only 6 of the 10 components of the Einstein equations are independent.
- Typically, this is addressed by imposing **gauge conditions**, such as the maximal slicing gauge, or de Donder (or harmonic) gauge. The de Donder gauge is Lorentz invariant and useful for gravitational waves.
- When formulated as an initial-value problem, the **Cauchy data is constrained**, and must satisfy the Gauss–Codazzi equations.
- The gauge symmetry implies that we obtain a **degenerate variational principle**.

Implications for Numerics

- We wish to study discretizations of general relativity that respect the **general covariance** of the system. This leads us to avoid using a tensor product discretization that presupposes a slicing of spacetime, rather we will consider **simplicial spacetime meshes**.
- We will consider **multi-Dirac mechanics** based on a Hamilton–Pontryagin variational principle for field theories that is well adapted to degenerate field theories.
- We will study **gauge-invariant discretizations** based on variational discretizations using gauge-equivariant approximation spaces.
- This is important because gauge-equivariant spacetime finite element spaces lead to gauge-invariant variational discretizations that satisfy a **multimomentum conservation law**.

Continuous Hamilton–Pontryagin principle

Pontryagin bundle and Hamilton–Pontryagin principle

- Consider the **Pontryagin bundle** $TQ \oplus T^*Q$, which has local coordinates (q, v, p).
- The **Hamilton–Pontryagin principle** is given by

$$\delta \int [L(q, v) - p(v - \dot{q})] = 0,$$

where we impose the second-order curve condition, $v = \dot{q}$ using Lagrange multipliers p.

Continuous Hamilton–Pontryagin principle

Implicit Lagrangian systems

- Taking variations in q, v, and p yield

$$\delta \int [L(q,v) - p(v - \dot{q})] dt$$
$$= \int \left[\frac{\partial L}{\partial q} \delta q + \left(\frac{\partial L}{\partial v} - p \right) \delta v - (v - \dot{q}) \delta p + p \delta \dot{q} \right] dt$$
$$= \int \left[\left(\frac{\partial L}{\partial q} - \dot{p} \right) \delta q + \left(\frac{\partial L}{\partial v} - p \right) \delta v - (v - \dot{q}) \delta p \right] dt,$$

  where we used integration by parts, and the fact that the variation δq vanishes at the endpoints.

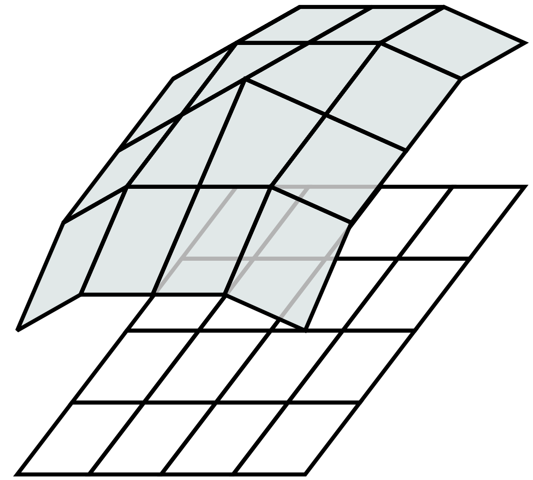
- This recovers the **implicit Euler–Lagrange equations**,

$$\dot{p} = \frac{\partial L}{\partial q}, \qquad p = \frac{\partial L}{\partial v}, \qquad v = \dot{q}.$$

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, $\mathcal{S}(q) = \int_{\mathcal{X}} L(j^1 q)$.
- **Hamilton's principle** states, $\delta\mathcal{S} = 0$.

Continuous Multi-Dirac Mechanics

Hamilton–Pontryagin for Fields[1]

- In coordinates, the Hamilton–Pontryagin principle for fields is

$$S(y^A, y^A_\mu, p^\mu_A) = \int_U \left[p^\mu_A \left(\frac{\partial y^A}{\partial x^\mu} - v^A_\mu \right) + L(x^\mu, y^A, v^A_\mu) \right] d^{n+1}x,$$

which yields the implicit Euler–Lagrange equations,

$$\frac{\partial p^\mu_A}{\partial x^\mu} = \frac{\partial L}{\partial y^A}, \quad p^\mu_A = \frac{\partial L}{\partial v^A_\mu}, \quad \text{and} \quad \frac{\partial y^A}{\partial x^\mu} = v^A_\mu.$$

- The Legendre transform involves both the energy and momentum,

$$p^\mu_A = \frac{\partial L}{\partial v^A_\mu}, \qquad p = L - \frac{\partial L}{\partial v^A_\mu} v^A_\mu.$$

[1] J. Vankerschaver, H. Yoshimura, ML, *The Hamilton-Pontryagin Principle and Multi-Dirac Structures for Classical Field Theories*, J. Math. Phys., 53(7), 072903, 2012.

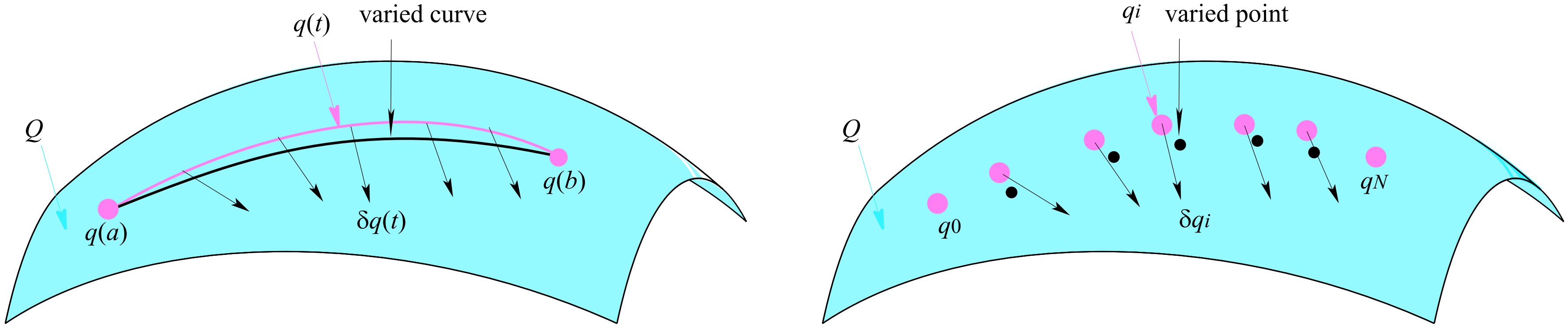
Geometric Discretizations

Geometric Integrators

- Given the fundamental role of gauge symmetry and their associated conservation laws in gauge field theories, it is natural to consider discretizations that preserve these properties.
- **Geometric Integrators** are a class of numerical methods that preserve geometric properties, such as symplecticity, momentum maps, and Lie group or homogeneous space structure of the dynamical system to be simulated.
- This tends to result in numerical simulations with better long-time numerical stability, and qualitative agreement with the exact flow.

The Classical Lagrangian View of 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**.

The Classical Lagrangian View of 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**

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

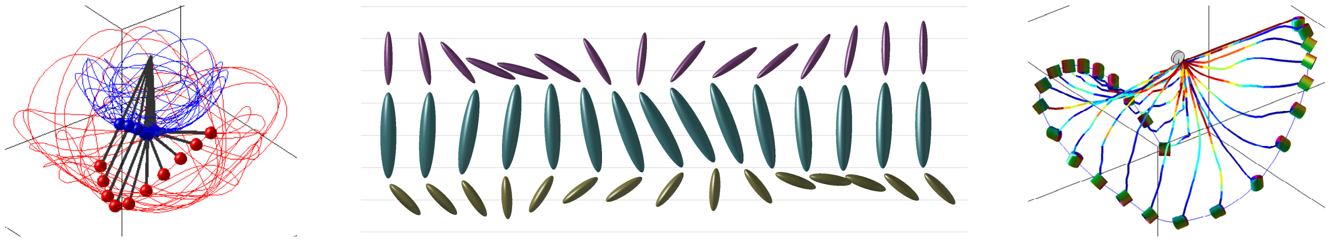
- The associated discrete flow $(q_{k-1}, q_k) \mapsto (q_k, q_{k+1})$ is automatically symplectic, since it is equivalent to,

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

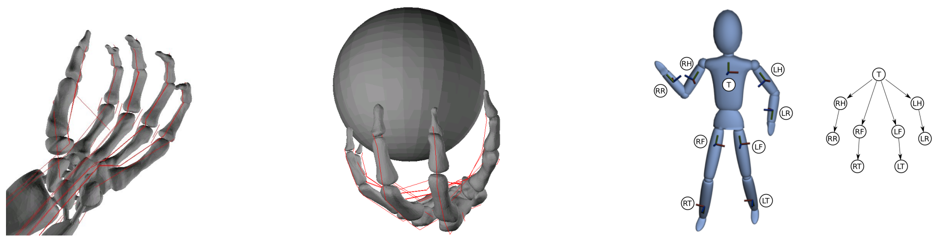
which is the characterization of a symplectic map in terms of a **Type I generating function** (discrete Lagrangian).

Examples of Variational Integrators

• Multibody Systems

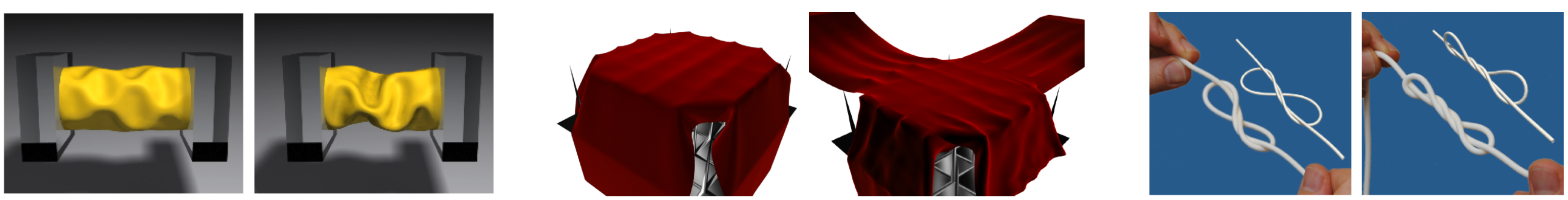


Simulations courtesy of Taeyoung Lee, George Washington University.



Simulations courtesy of Todd Murphey, Northwestern University.

• Continuum Mechanics



Simulations courtesy of Eitan Grinspun, Columbia University.

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**[2]
  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.

[2] J. E. Marsden and M. West, *Discrete mechanics and variational integrators*, Acta Numerica 10, 357-514, 2001.

Constructing Discrete Lagrangians

Revisiting the Exact Discrete Lagrangian

- Consider an alternative expression for 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 is more amenable to discretization.

Ritz 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**.
- **Group-equivariant** function spaces yield G-invariant discrete Lagrangians, which induce **momentum-preserving** integrators.

Ritz Variational Integrators

Optimal Rates of Convergence

- A desirable property of a Ritz 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.

Ritz Variational Integrators

Optimality of Ritz 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,

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

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.
- 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.

Ritz Variational Integrators

Theorem: Optimality of Ritz Variational Integrators[3] [4]

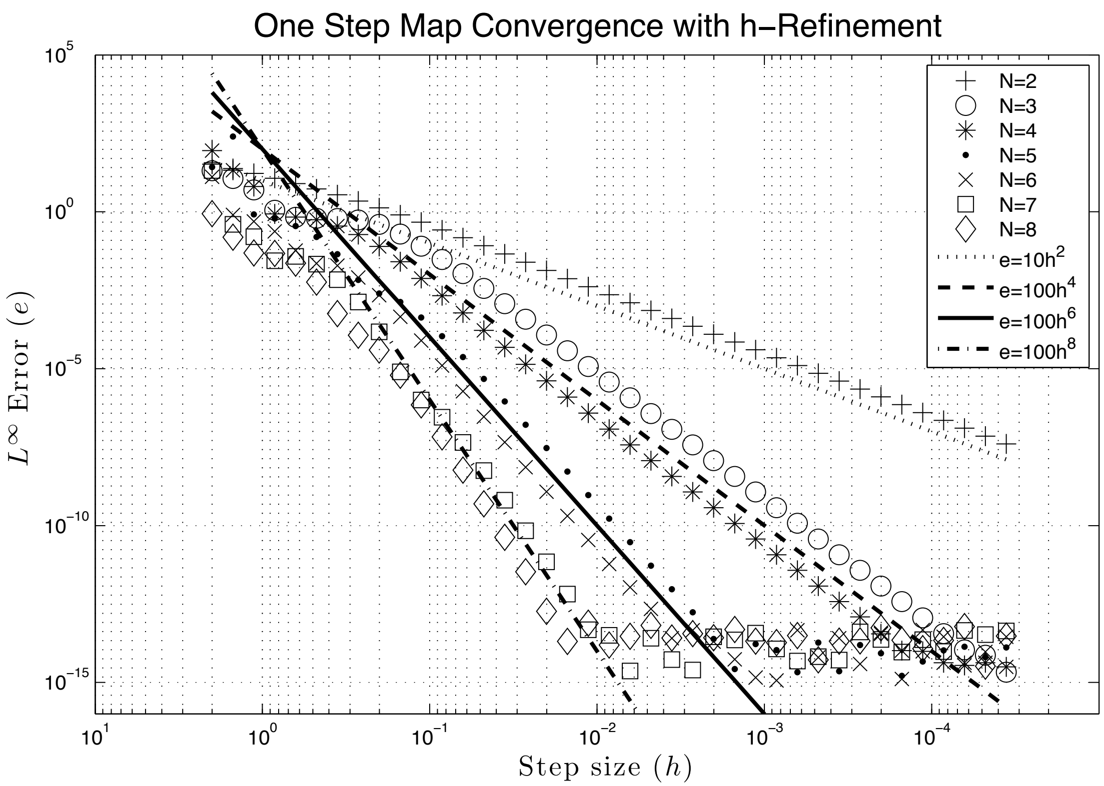
- Under suitable technical hypotheses:
  - Regularity of L in a closed and bounded neighboorhood;
  - The quadrature rule is sufficiently accurate;
  - The discrete and continuous trajectories *minimize* their actions;

  the Ritz 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.
- Shows that Ritz variational integrators are **order optimal**; spectral variational integrators are **geometrically convergent**.

[3] J. Hall, ML, *Spectral Variational Integrators*, Numerische Mathematik, 130(4), 681-740, 2015.
[4] J. Hall, ML, *Lie Group Spectral Variational Integrators*, Found. Comput. Math., 17(1), 199-257, 2017.

Ritz Variational Integrators

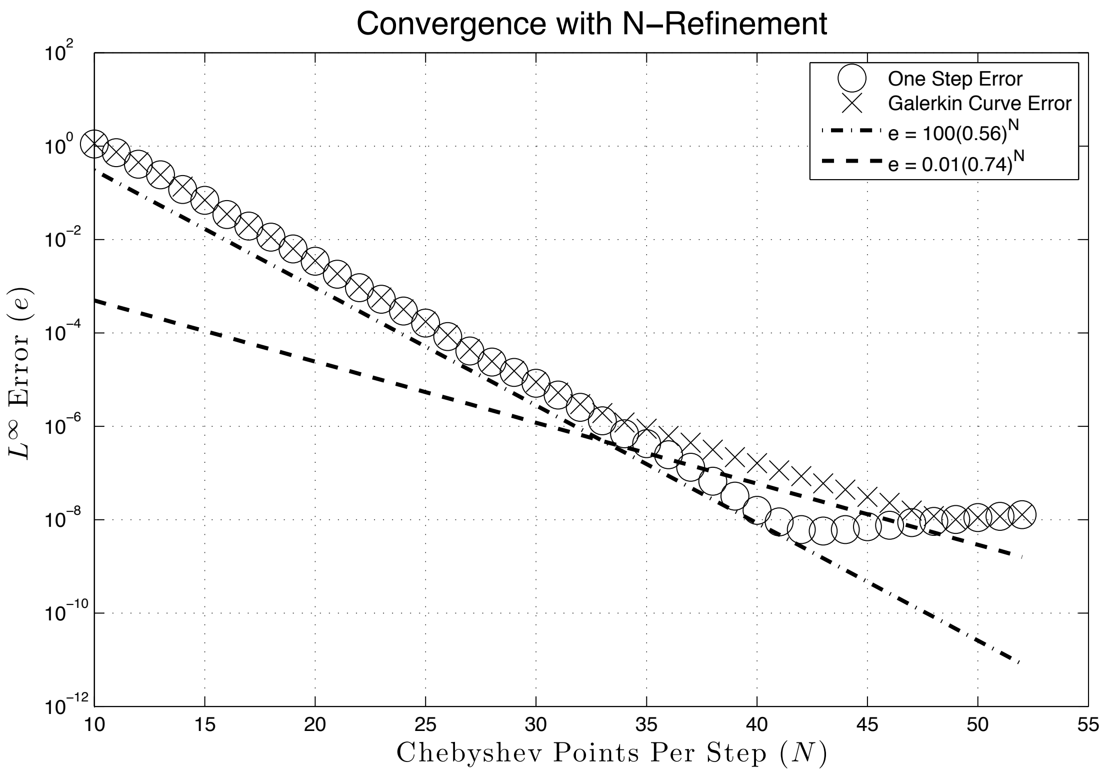
Numerical Results: Order Optimal Convergence



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

Spectral Ritz Variational Integrators

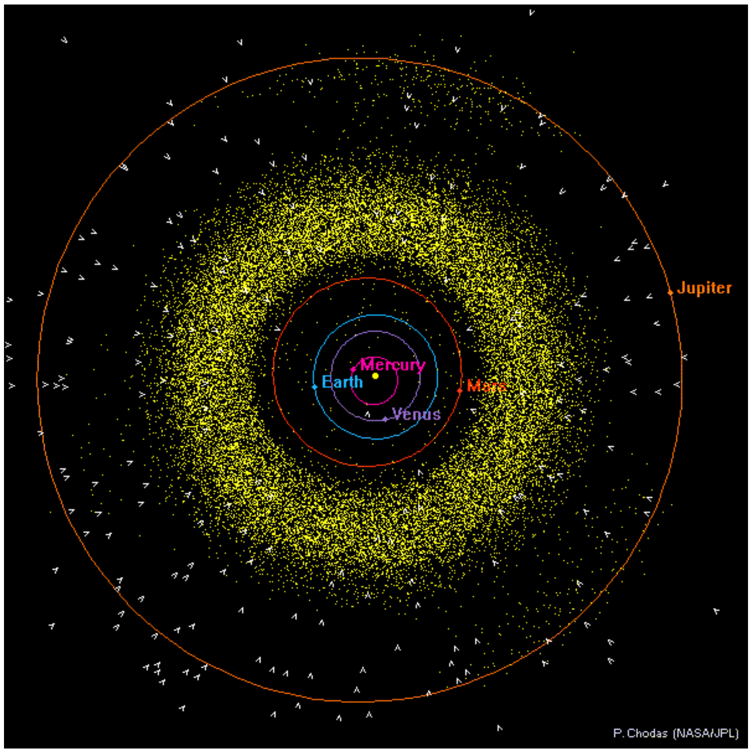
Numerical Results: Geometric Convergence

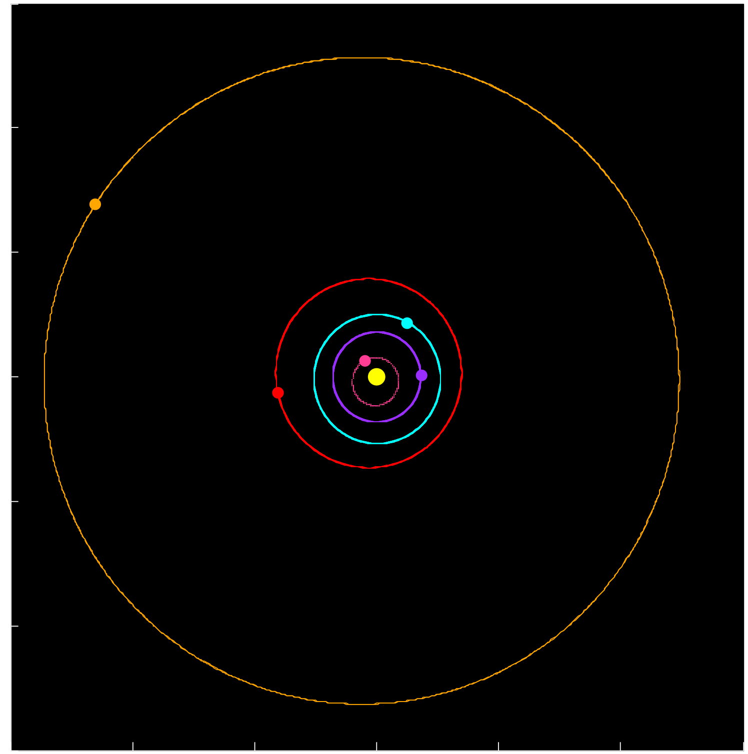


- Geometric convergence of the Kepler 2-body problem with eccentricity 0.6 over 100 steps of $h = 2.0$.

Spectral Ritz Variational Integrators

Numerical Experiments: Solar System Simulation

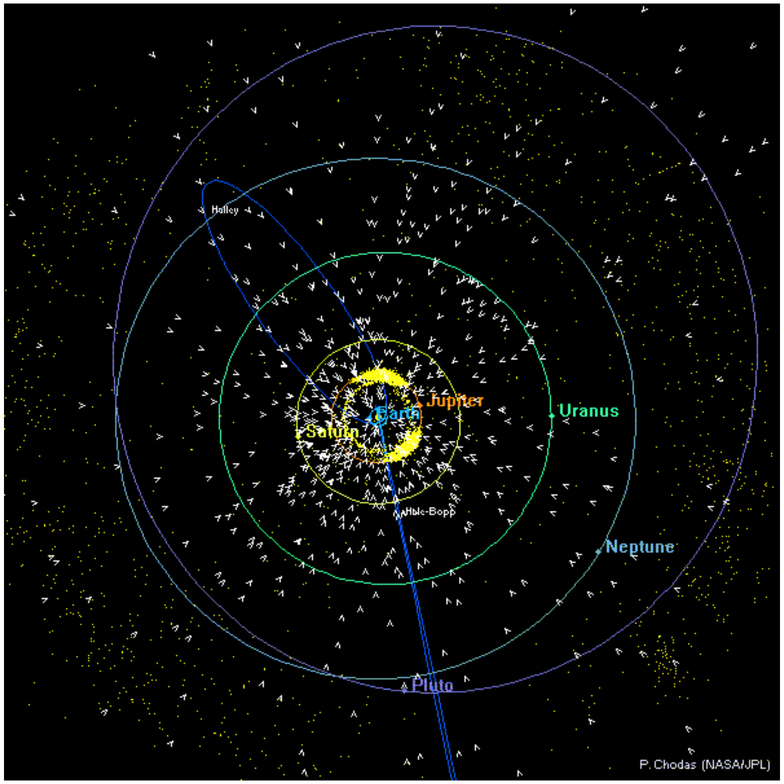


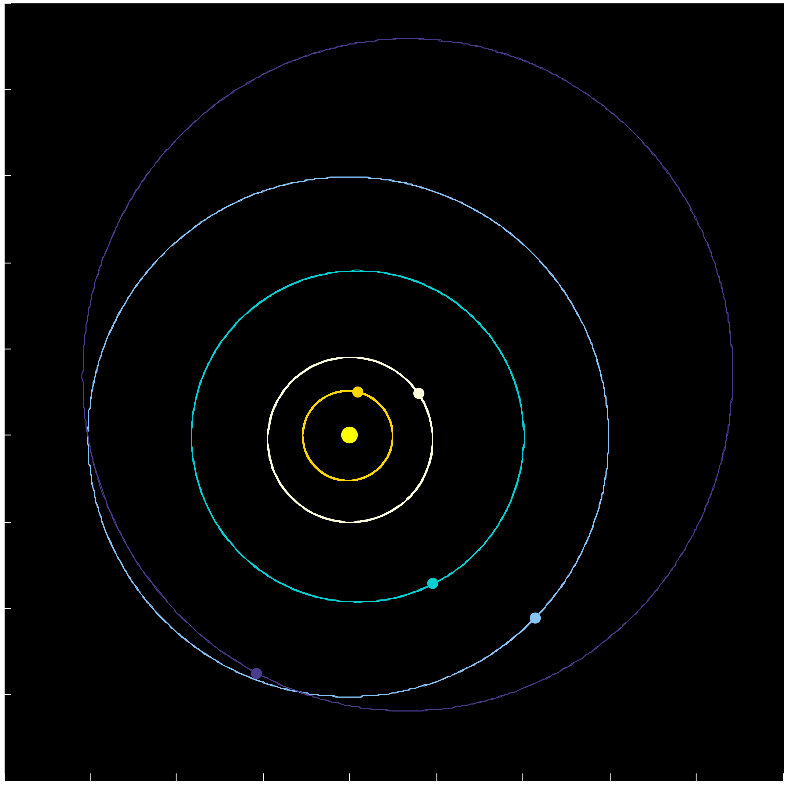


- Comparison of inner solar system orbital diagrams from a spectral variational integrator and the JPL Solar System Dynamics Group.
- $h = 100$ days, $T = 27$ years, 25 Chebyshev points per step.

Spectral Ritz Variational Integrators

Numerical Experiments: Solar System Simulation

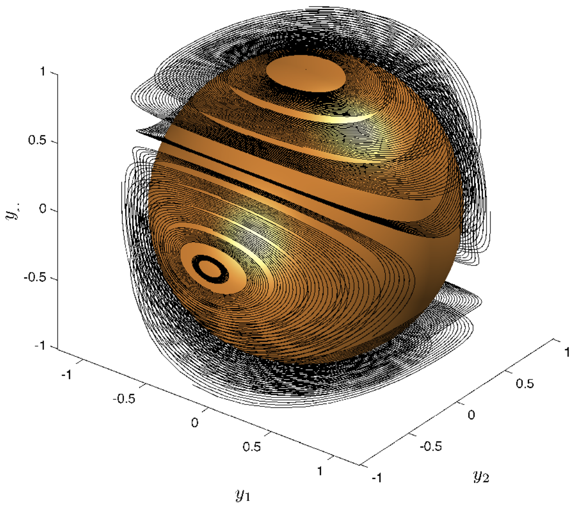




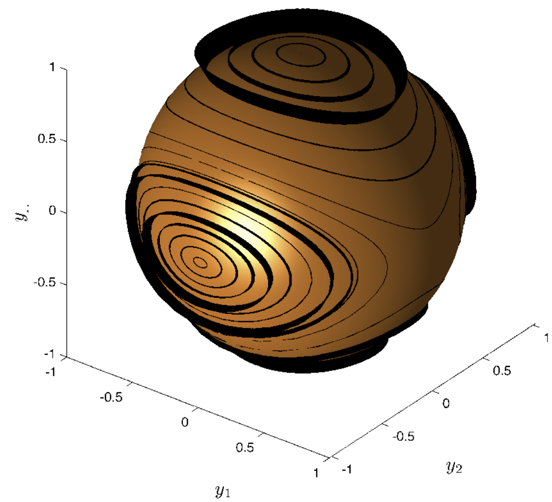
- Comparison of outer solar system orbital diagrams from a spectral variational integrator and the JPL Solar System Dynamics Group. Inner solar system was aggregated, and $h = 1825$ days.

Spectral Lie Group Variational Integrators

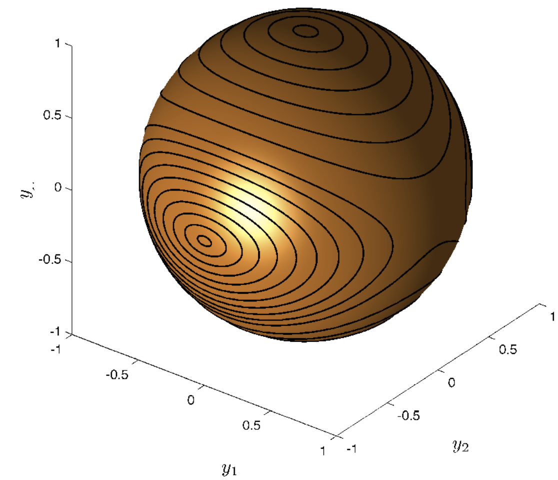
Numerical Experiments: Free Rigid Body



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.

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.

- The **boundary Lagrangian**[5] 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.

[5] C. Liao, J. Vankerschaver, ML, *Generating Functionals and Lagrangian PDEs*, J. Math. Phys., 54(8), 082901, 2013.

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 a codimension-1 differential form, that by Hodge duality can be viewed as the normal component (to the boundary $\partial\Omega$) of the multimomentum at the point (x,t).

- These equations, taken at every point on $\partial\Omega$ constitute a **multi-symplectic 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 comes from the orientation of the boundary.

Gauge Symmetries and Variational Discretizations

Theorem (Discrete Noether's Theorem)

- If the discrete boundary Lagrangian is invariant with respect to the lifted action of a gauge symmetry group on the space of boundary data, then it satisfies a discrete multimomentum conservation law.

Theorem (Group-Invariant Ritz Discrete Lagrangians)

- Given a group-equivariant approximation space, and a Lagrangian density that is invariant under the lifted group action, the associated Ritz discrete boundary Lagrangian is group-invariant.

Implications for Geometric Integration

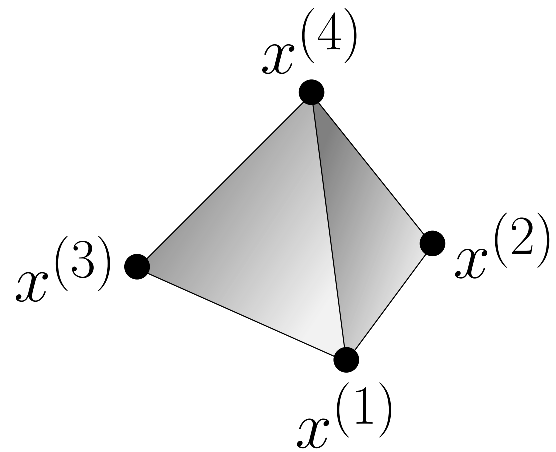
- We need finite elements that take values in the space of Lorentzian metrics that are group-equivariant.
- Two current approaches, **geodesic finite elements** and **group-equivariant interpolation on symmetric spaces**.

Interpolation of Lorentzian Metrics

- Let $\mathcal{L}$ denote the space of **Lorentzian metric tensors**:

$$\mathcal{L} = \{L \in \mathbb{R}^{4\times 4} \mid L = L^T,\ \det L \neq 0,\ \mathrm{signature}(L) = (3,1)\}.$$

- Given $L^{(i)} \in \mathcal{L}$ at the vertices $x^{(i)}$ of a simplex Ω, find a continuous function $\mathcal{I}L : \Omega \to \mathcal{L}$ such that:
  - $\mathcal{I}L(x^{(i)}) = L^{(i)}$ for each i.
  - $\mathcal{I}L(x) \in \mathcal{L}$ for every $x \in \Omega$.
  - If $Q \in O(1,3)$ and $L^{(i)} \leftarrow QL^{(i)}Q^T$, then $\mathcal{I}L(x) \leftarrow Q\mathcal{I}L(x)Q^T$.



- Here, $O(1,3) = \{Q \in \mathbb{R}^{4\times 4} \mid QJQ^T = J\}$ is the **indefinite orthogonal group**, where $J = \mathrm{diag}(-1,1,1,1)$.

Interpolation of Lorentzian Metrics

Componentwise interpolation

- Not signature-preserving, in general. For instance,

$$\frac{1}{2}\underbrace{\begin{pmatrix}0&4&0&0\\4&0&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}}_{\in\mathcal{L}\text{ since }\lambda=-4,1,1,4}+\frac{1}{2}\underbrace{\begin{pmatrix}2&-4&0&0\\-4&2&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}}_{\in\mathcal{L}\text{ since }\lambda=-2,1,1,6}=\underbrace{\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}}_{\notin\mathcal{L}\text{ since }\lambda=1,1,1,1}$$

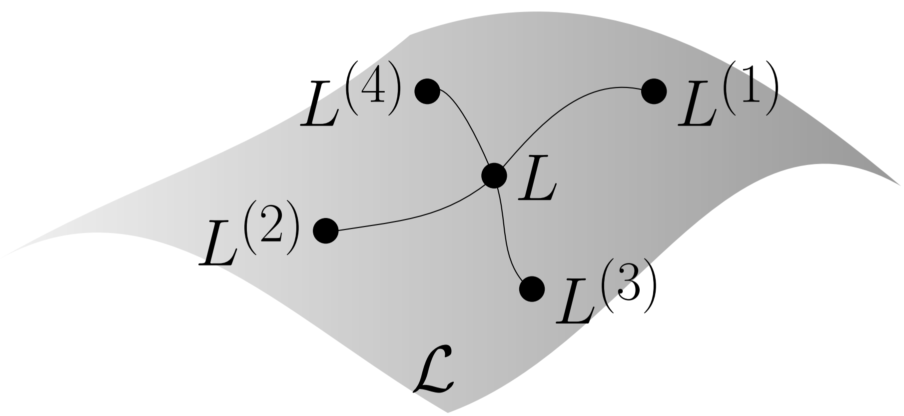
Interpolation of Lorentzian Metrics

Geodesic interpolation[6] [7]

- A **geodesic finite element** is given by

$$\mathcal{I}L(x) = \arg\min_{L\in\mathcal{L}} \sum_{i=1}^{m} \phi_i(x)\,\mathrm{dist}(L^{(i)}, L)^2,$$

where $\{\phi_i\}_{i=1}^m$ are scalar-valued shape functions satisfying $\phi_i(x^{(j)}) = \delta_{ij}$. Also known as the **weighted Riemannian mean**.

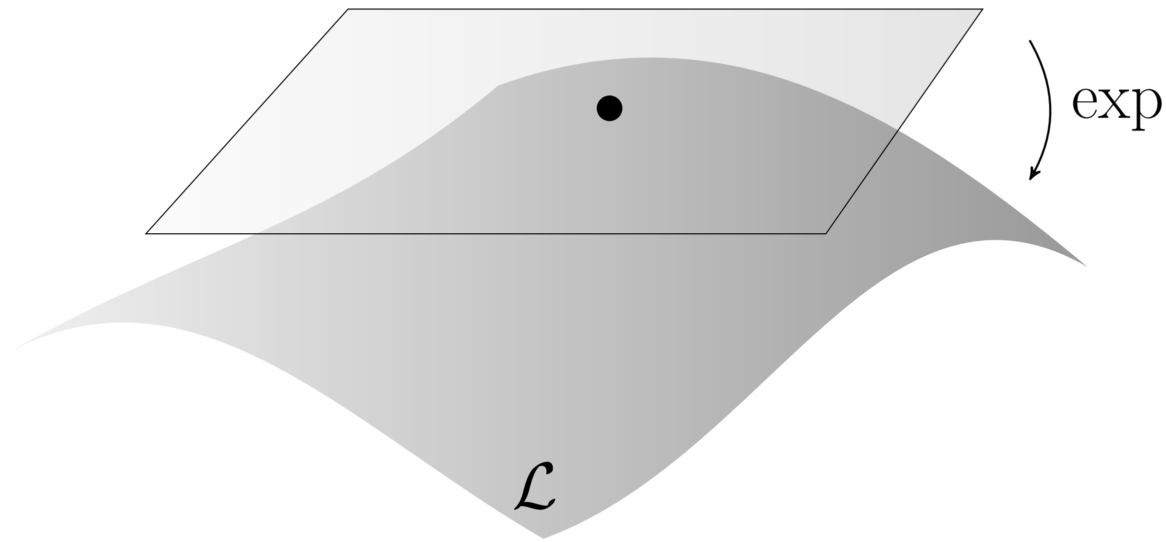


[6] O. Sander, *Geodesic finite elements on simplicial grids*, Int. J. Numer. Meth. Eng., 92(12), 999–1025, 2012.
[7] P. Grohs, *Quasi-interpolation in Riemannian manifolds*, IMA J. Numer. Anal., 33(3), 849–874, 2013.

Interpolation of Lorentzian Metrics

Our approach[8]

- **Idea:** If $\mathcal{L}$ were a Lie group, one could use the exponential map and perform all calculations on its Lie algebra, a linear space.



- In reality, $\mathcal{L}$ is not a Lie group, it is a **symmetric space**. Nonetheless, a similar construction is available.

[8] E. Gawlik, ML, *Interpolation on Symmetric Spaces via the Generalized Polar Decomposition*, Found. Comput. Math., 18(3), 757–788, 2018.

Interpolation of Lorentzian Metrics

- Notice that $\mathcal{L}$ is diffeomorphic to $GL_4(\mathbb{R})/O(1,3)$: The map

$$\begin{aligned} \bar{\varphi} : GL_4(\mathbb{R})/O(1,3) &\to \mathcal{L} \\ [A] &\mapsto AJA^T, \end{aligned}$$

  is a diffeomorphism, where $J = \text{diag}(-1,1,1,1)$.

- Every coset $[A]$ has a canonical representative Y by virtue of the **generalized polar decomposition**:

$$A = YQ, \quad Y \in Sym_J(4),\, Q \in O(1,3),$$

  where

$$Sym_J(4) = \{Y \in GL_4(\mathbb{R}) \mid YJ = JY^T\}.$$

- $\log(Y)$ lives in a linear space called a **Lie triple system**:

$$\log(Y) \in \mathfrak{sym}_J(4) = \{P \in \mathbb{R}^{4\times4} \mid PJ = JP^T\}.$$

Interpolation of Lorentzian Metrics

Summary

$$\begin{array}{ccccccc} & & & & GL_4(\mathbb{R}) & & \\ & & & \overset{\iota}{\nearrow} & \downarrow \pi & \overset{\varphi}{\searrow} & \\ \mathfrak{sym}_J(4) & \xrightarrow{\exp} & Sym_J(4) & \xrightarrow{\psi} & GL_4(\mathbb{R})/O(1,3) & \xrightarrow{\bar{\varphi}} & \mathcal{L} \end{array}$$

$$\log(Y) \longmapsto Y \longmapsto [Y] \longmapsto YJY^T$$

- $\mathcal{L}$ is locally diffeomorphic to the **Lie triple system**

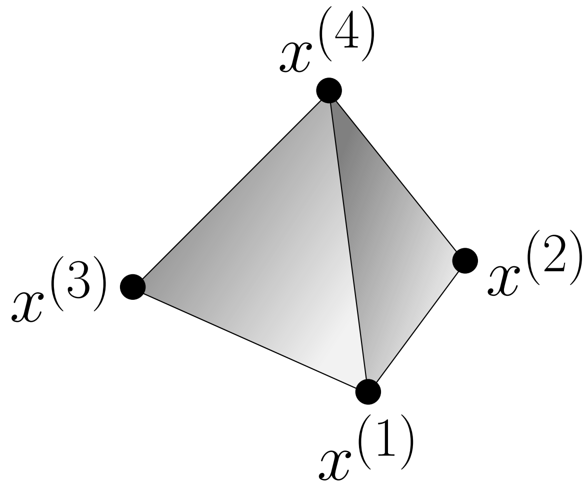
$$\mathfrak{sym}_J(4) = \{P \in \mathbb{R}^{4\times 4} \mid PJ = JP^T\},$$

which is a **linear space**.

- Interpolation on a linear space is easy.

Interpolation of Lorentzian Metrics

Interpolation Formula



- The resulting interpolation formula reads

$$\mathcal{I}L(x) = J \exp\left(\sum_{i=1}^{m} \phi_i(x) \log(JL^{(i)})\right),$$

where $J = \text{diag}(-1, 1, 1, 1)$, and $\{\phi_i\}_{i=1}^{m}$ are scalar-valued shape functions satisfying the Kronecker delta property $\phi_i(x^{(j)}) = \delta_{ij}$.

Interpolation of Lorentzian Metrics

Signature preservation

- The interpolant $\mathcal{I}L$ is signature-preserving; that is,

$$\mathcal{I}L(x) \in \boldsymbol{\mathcal{L}}$$

for every $x \in \Omega$.

Frame invariance

- Let $Q \in O(1,3)$. If $\tilde{L}^{(i)} = QL^{(i)}Q^T$, $i = 1, 2, \ldots, m$, and if Q is sufficiently close to the identity matrix, then

$$\mathcal{I}\tilde{L}(x) = Q\,\mathcal{I}L(x)\,Q^T$$

for every $x \in \Omega$.

Interpolation of Lorentzian Metrics

Symmetry under inversion

- If $\tilde{L}^{(i)} = (L^{(i)})^{-1}$, $i = 1, 2, \ldots, m$, then

$$\mathcal{I}\tilde{L}(x) = (\mathcal{I}L(x))^{-1}$$

for every $x \in \Omega$.

Determinant averaging

- If $\sum_{i=1}^{m} \phi_i(x) = 1$ for every $x \in \Omega$, then

$$\det \mathcal{I}L(x) = \prod_{i=1}^{m} \left(\det L^{(i)}\right)^{\phi_i(x)}$$

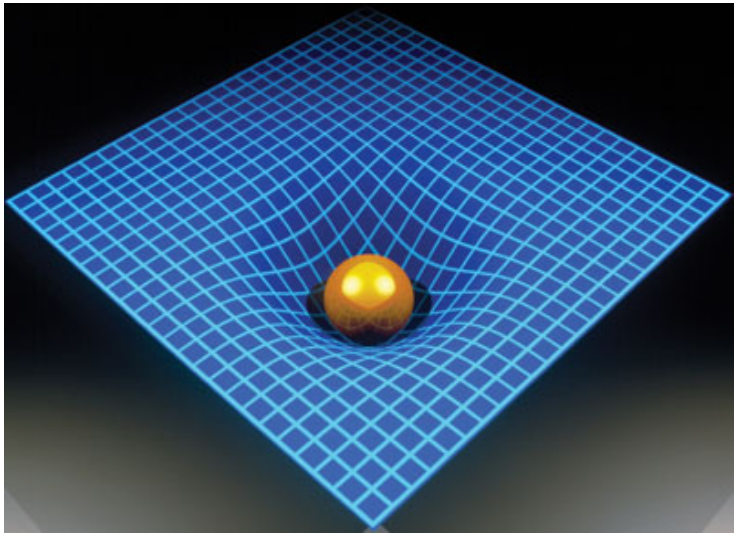
for every $x \in \Omega$.

Interpolation of Lorentzian Metrics

Numerical example (Linear Interpolation)

- Interpolating the Schwarzschild metric, which is a spherically symmetric, vacuum solution of the Einstein equations.

$$-\left(1-\frac{1}{r}\right)dt^2+\left(1-\frac{1}{r}\right)^{-1}dr^2+r^2\left(d\theta^2+\sin^2\theta\,d\varphi^2\right)$$



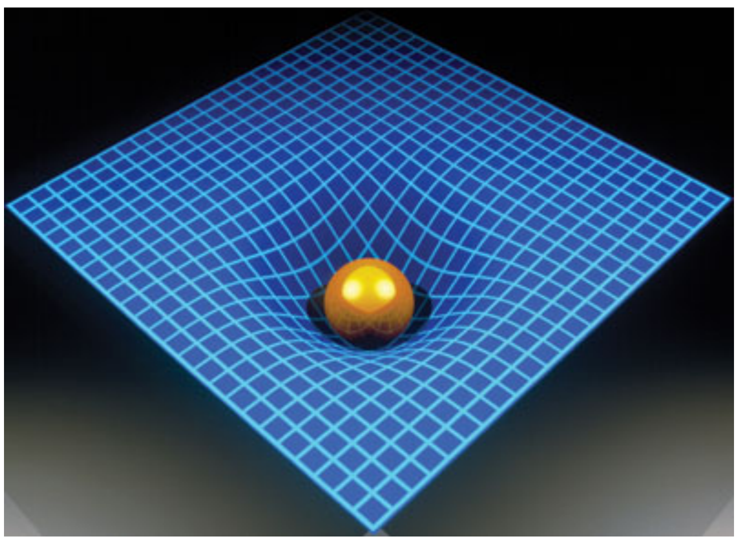
	Linear shape functions $\{\phi_i\}_i$			
N	L^2-error	Order	H^1-error	Order
2	$3.3\cdot10^{-3}$		$2.8\cdot10^{-2}$	
4	$8.4\cdot10^{-4}$	1.975	$1.4\cdot10^{-2}$	0.998
8	$2.1\cdot10^{-4}$	1.994	$7.1\cdot10^{-3}$	0.999
16	$5.3\cdot10^{-5}$	1.998	$3.6\cdot10^{-3}$	1.000

Interpolation of Lorentzian Metrics

Numerical example (Quadratic Interpolation)

- Interpolating the Schwarzschild metric, which is a spherically symmetric, vacuum solution of the Einstein equations.

$$-\left(1-\frac{1}{r}\right)dt^2+\left(1-\frac{1}{r}\right)^{-1}dr^2+r^2\left(d\theta^2+\sin^2\theta\,d\varphi^2\right)$$



	Quadratic shape functions $\{\phi_i\}_i$			
N	L^2-error	Order	H^1-error	Order
2	$1.7\cdot10^{-4}$		$2.5\cdot10^{-3}$	
4	$2.2\cdot10^{-5}$	3.001	$6.2\cdot10^{-4}$	1.993
8	$2.7\cdot10^{-6}$	3.000	$1.6\cdot10^{-4}$	1.998
16	$3.4\cdot10^{-7}$	3.000	$3.9\cdot10^{-5}$	1.999

Interpolation of Lorentzian Metrics

Relationship with other methods

- The interpolant we constructed has the form,
$$\mathcal{I}L(x) = J \exp\left(\sum_{i=1}^{m} \phi_i(x) \log(JL^{(i)})\right).$$
- An alternative interpolant is defined implicitly via
$$\mathcal{I}L(x) = \mathcal{I}L(x) \exp\left(\sum_{i=1}^{m} \phi_i(x) \log\left(\mathcal{I}L(x)^{-1} L^{(i)}\right)\right).$$
This interpolant is equivalent to the **geodesic interpolant**.
- Replacing $J = \mathrm{diag}(-1, 1, 1, 1)$ with the identity matrix, one recovers the weighted **Log-Euclidean mean**[9] of symmetric positive-definite matrices,
$$\mathcal{I}L(x) = \exp\left(\sum_{i=1}^{m} \phi_i(x) \log(L^{(i)})\right).$$

[9] V. Arsigny, P. Fillard, X. Pennec, and N. Ayache. Geometric means in a novel vector space structure on symmetric positive-definite matrices. SIAM. J. Matrix Anal. & Appl., 29(1), 328–347, 2007.

Abstraction to Symmetric Spaces

Lorentzian metrics as a Symmetric Space

- $\mathcal{S}$ – smooth manifold — $\mathcal{L}$ (Lorentzian metrics)
- η – distinguished element of $\mathcal{S}$ — $J = \mathrm{diag}(-1, 1, 1, 1)$
- G – Lie group that acts transitively on $\mathcal{S}$ — $GL_4(\mathbb{R})$
- $\sigma : G \to G$ – involutive automorphism — $\sigma(A) = JA^{-T}J$
- $G^\sigma = \{g \in G \mid \sigma(g) = g\}$ — $O(1,3)$
- $G_\sigma = \{g \in G \mid \sigma(g) = g^{-1}\}$ — $Sym_J(4)$

Abstraction to Symmetric Spaces

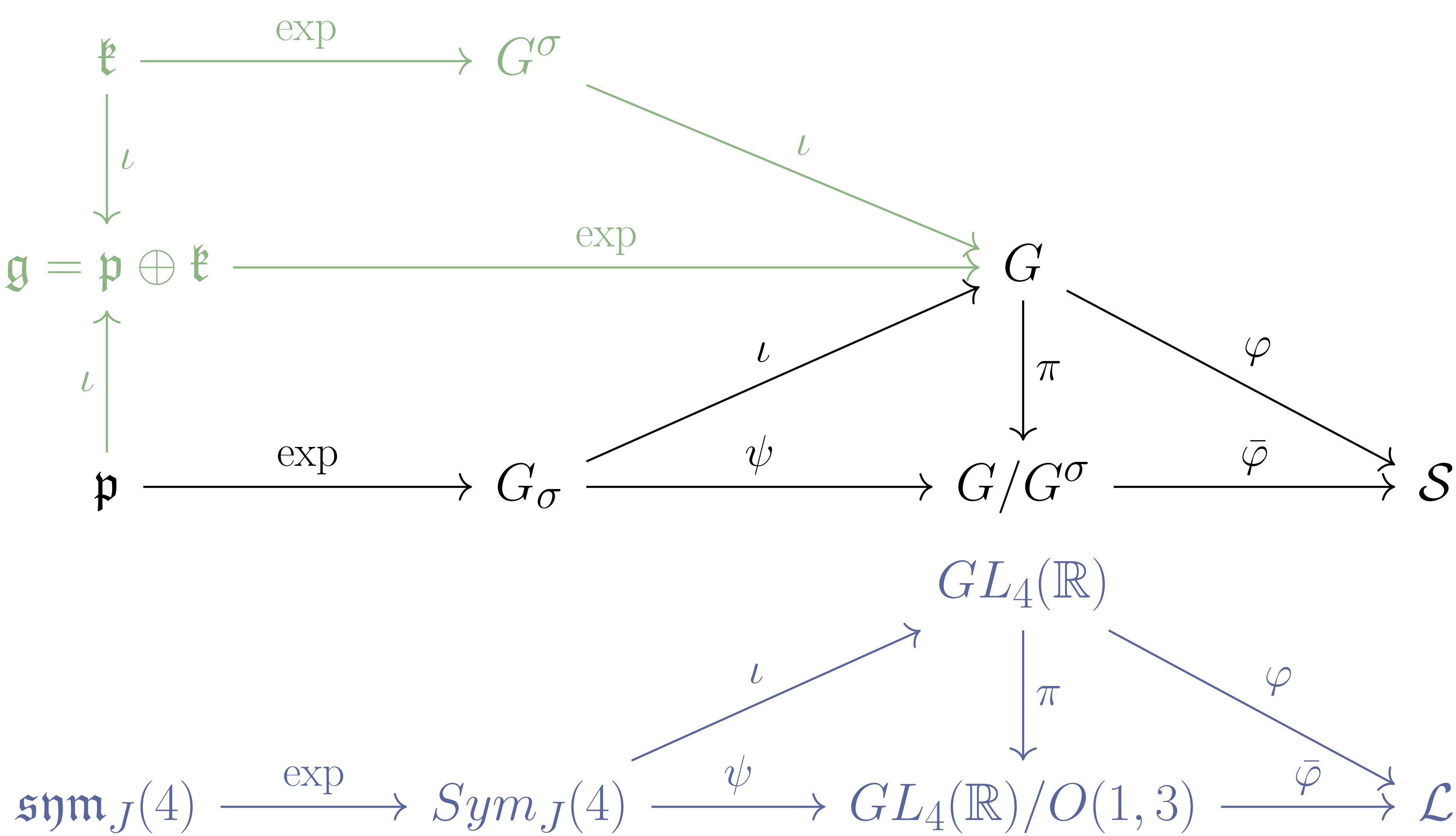
Key Assumption

- Isotropy subgroup of η coincides with the fixed set G^σ, i.e.

$$g \cdot \eta = \eta \iff \sigma(g) = g.$$
$$AJA^T = J \iff JA^{-T}J = A$$

- Then $\mathcal{S}$ is diffeomorphic to G/G^σ (a **symmetric space**) and every $[g] \in G/G^\sigma$ has a canonical representative $p \in G_\sigma$ by the **generalized polar decomposition** $g = pk$, $p \in G_\sigma$, $k \in G^\sigma$.
- This is related to the **Cartan decomposition** of the Lie algebra $\mathfrak{g} = \mathfrak{p} \oplus \mathfrak{k}$, where $\mathfrak{k}$ is the Lie algebra of the subgroup G^σ, and $\mathfrak{p} = \{P \in \mathfrak{g} \mid d\sigma(P) = -P\} \subset \mathfrak{g} = \{P \in \mathbb{R}^{4\times 4} \mid -JP^TJ = -P\}$, which is a **Lie triple system** – it is closed under the double commutator $[\cdot, [\cdot, \cdot]]$, but not under $[\cdot, \cdot]$.

Abstraction to Symmetric Spaces



Abstraction to Symmetric Spaces

Summary

- $\mathcal{S}$ is locally diffeomorphic to the Lie triple system $\mathfrak{p}$, which is a *linear space*, and interpolation on a linear space is easy.
- The resulting formula for interpolating $\{u^{(i)}\}_{i=1}^m \subset \mathcal{S}$ reads

$$\mathcal{I}u(x) = F\left(\sum_{i=1}^m \phi_i(x) F^{-1}(u^{(i)})\right),$$

where $\phi_i : \Omega \to \mathbb{R}$, $i = 1, 2, \ldots, m$, are scalar-valued shape functions satisfying $\phi_i(x^{(j)}) = \delta_{ij}$, and $F : \mathfrak{p} \to \mathcal{S}$, $P \mapsto \exp(P) \cdot \eta$.

- The resulting interpolant is **G^σ-equivariant**.
- Recovers interpolation formulas on the **Grassmannian**[10].

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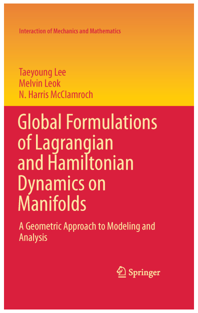
[10] D. Amsallem and C. Farhat. Interpolation method for adapting reduced-order models and application to aeroelasticity. AIAA Journal, 46(7), 1803–1813, 2008.

Summary

- Gauge field theories exhibit gauge symmetries that impose Cauchy initial value constraints, and are also underdetermined.
- These result in degenerate field theories that can be described using multi-Dirac mechanics and multi-Dirac structures.
- Described a systematic framework for constructing and analyzing Ritz variational integrators, and the extension to Hamiltonian PDEs.
- Multimomentum conserving variational integrators can be constructed from group-equivariant finite element spaces.
- These spaces can be constructed efficiently for finite elements taking values in symmetric spaces, in particular, Lorentzian metrics, by using a generalized polar decomposition.

New Monograph



- *Global Formulations of Lagrangian and Hamiltonian Dynamics on Manifolds*, Taeyoung Lee, ML, N. Harris McClamroch, Interactions of Mechanics and Mathematics, Springer, XXVII+539 pages, ISBN: 978-3-319-56951-2.

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Variational discretizations of gauge field theories using group-equivariant interpolation spaces - Talk by Melvin Leok

Lecture notes - Ori S. Katz

October 10, 2018

Abstract

Variational integrators are geometric structure-preserving numerical methods that preserve the symplectic structure, satisfy a discrete Noether's theorem, and exhibit exhibit excellent long-time energy stability properties. An exact discrete Lagrangian arises from Jacobi's solution of the Hamilton-Jacobi equation, and it generates the exact flow of a Lagrangian system. By approximating the exact discrete Lagrangian using an appropriate choice of interpolation space and quadrature rule, we obtain a systematic approach for constructing variational integrators. The convergence rates of such variational integrators are related to the best approximation properties of the interpolation space. Many gauge field theories can be formulated variationally using a multisymplectic Lagrangian formulation, and we will present a characterization of the exact generating functionals that generate the multisymplectic relation. By discretizing these using group-equivariant spacetime finite element spaces, we obtain methods that exhibit a discrete multimomentum conservation law. We will then briefly describe an approach for constructing group-equivariant interpolation spaces that take values in the space of Lorentzian metrics that can be efficiently computed using a generalized polar decomposition. The goal is to eventually apply this to the construction of variational discretizations of general relativity, which is a second-order gauge field theory whose configuration manifold is the space of Lorentzian metrics.

1 Lecture notes

Geometric structure-preserving variations.

Context: Gravitational waves detection, enabled by computational advancements, specifically numerical relativity in order to solve the inverse problem.

Einstein equations can be written in Lagrangian formulation, it's a 2nd order gauge field theory.

Gauge symmetry - local continuous transformation, a consequence is that the E-L equations are underdetermined. Therefore, constraints are required.

The E-L equations are overdetermined, since initial conditions cannot be chosen freely.

Example: Electromagnetism. Box operator is the wave operator. The transformation is an example of a gauge symmetry, and there are constraints on the associated initial data.

Gauges must be chosen carefully depending on the problem being solved. This is an issue in computations, because in computations we don't normally know what the solution will look like, and in fact a global gauge may not be the best choice.

One consequence of symmetry is conserved quantities. In gauge theory, every local symmetry has a Noether current associated with it. Integrating this current, obtain the Noether charge; in general relativity the Noether charge is the stress-energy tensor.

Since Noether's second theorem implies only 6 out of 10 components of the Einstein equation, usually people solve for 6 and use the remaining 4 components as error indicators.

There is no canonical choice of a global slice of space-time, and this is an issue in the required discretization in numerical approaches. Thus, we consider simplicial spacetime meshes. The discretization should respect the symmetry in order for the Noether discrete theorem to apply, therefore we study gauge-invariant discretization.

Continuous Hamilton-Pontryagin principle - relax the condition of $\dot{q} = v$. Obtain the implicit E-L equations.

If, for example, the Lagrangian is not hyper-regular, the equation for p becomes a primary constraint condition.

Relaxing the relation between time derivatives of spatial coordinates and the velocities, yields the implicit E-L equations.

When extracting information from numerical simulations, since they can be viewed as exact solutions of a modified equation set, the information extracted has some notion of structural stability.

One way to construct such a symplectic integrator is to approximate the path between two specified points, and allow the computed points in the path to vary. In order to approximate the path, a discrete Lagrangian is constructed.

Discrete E-L equations - two-step method. The discrete Lagrangian is essentially a Type I generating function.

Advantaged of constructing such variational integrators:

- Respects symmetries.

- Variational error analysis

Numerical experiments - On the left, the real system, on the right, the computed approximation.

Another example - the free rigid body. Comparing numerical methods, the Lie Group variational integrator keeps the constraints.

Note: The geodesic interpolation of Lorentzian metrics is very computationally expensive. We present a new approach using group diffeomorphisms.