Variational Discretizations of Gauge Field Theories using Group-equivariant Interpolation

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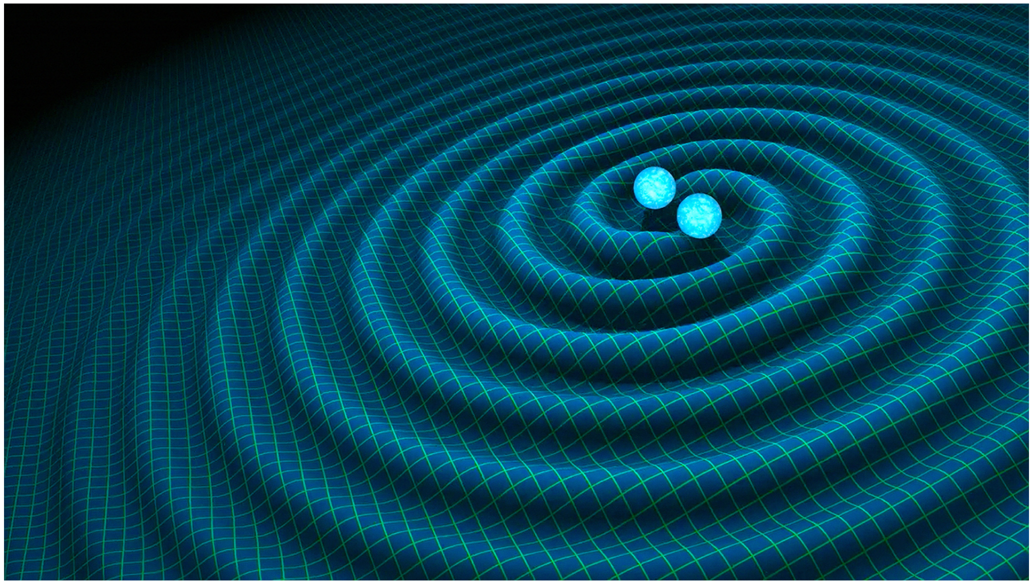
Gravitational Waves, LIGO, and Numerical Relativity



- **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**:
  - **maximal slicing gauge**, $K = \partial_t K = 0$, where $K = K_{\alpha\beta}K^{\alpha\beta}$ is the trace of the extrinsic curvature.
  - **de Donder (or harmonic) gauge**, $\Gamma^{\alpha}_{\beta\gamma} g^{\beta\gamma} = 0$, which 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**.

Dirac Geometry and Mechanics

Dirac Structures

- Dirac structures can be viewed as simultaneous generalizations of symplectic and Poisson structures.
- Implicit Lagrangian and Hamiltonian systems[1] provide a unified geometric framework for studying degenerate, interconnected, and nonholonomic Lagrangian and Hamiltonian mechanics.

Variational Principles

- The Hamilton–Pontryagin principle[2] on the Pontryagin bundle $TQ \oplus T^*Q$, unifies Hamilton's principle, Hamilton's phase space principle, and the Lagrange–d'Alembert principle.

[1] H. Yoshimura, J.E. Marsden, Dirac structures in Lagrangian mechanics. Part I: Implicit Lagrangian systems, *J. of Geometry and Physics*, **57**, 133–156, 2006.
[2] H. Yoshimura, J.E. Marsden, Dirac structures in Lagrangian mechanics. Part II: Variational structures, *J. of Geometry and Physics*, **57**, 209–250, 2006.

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

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

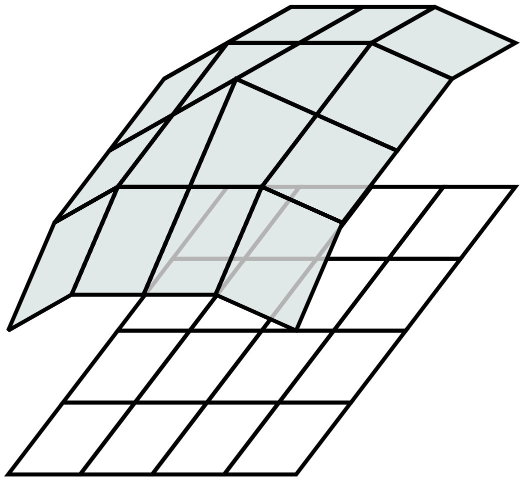
  where we used integration by parts, and the fact that the variation δq vanishes at the endpoints.

- 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[3]

- 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,

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

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

Continuous Multi-Dirac Structure

Multi-Dirac Structure[4]

- The **canonical multisymplectic $(n+2)$-form** on J^1Y^* is

$$\Omega = dy^A \wedge dp^\mu_A \wedge d^n x_\mu - dp \wedge d^{n+1}x.$$

- Consider the contraction of Ω by a $(n+1)$-multivector field,

$$\mathcal{X}_{n+1} \in \bigwedge^{n+1}(TM) \mapsto \mathbf{i}_{\mathcal{X}_{n+1}}\Omega \in \bigwedge^1(T^*M),$$

where $M = J^1Y \times_Y J^1Y^*$. The graph of this mapping defines a submanifold D_{n+1} of $\bigwedge^{n+1}(TM) \times_M \bigwedge^1(T^*M)$.

- The implicit Euler–Lagrange equations can be written as,

$$(\mathcal{X}, (-1)^{n+2}\mathbf{d}E) \in D_{n+1},$$

where $E = p + p^\mu_A v^A_\mu - L(x^\mu, y^A, v^A_\mu)$ is the generalized energy.

[4] J. Vankerschaver, H. Yoshimura, ML, *On the Geometry of Multi-Dirac Structures and Gerstenhaber Algebras*, J. Geom. Phys., 61(8), 1415-1425, 2011.

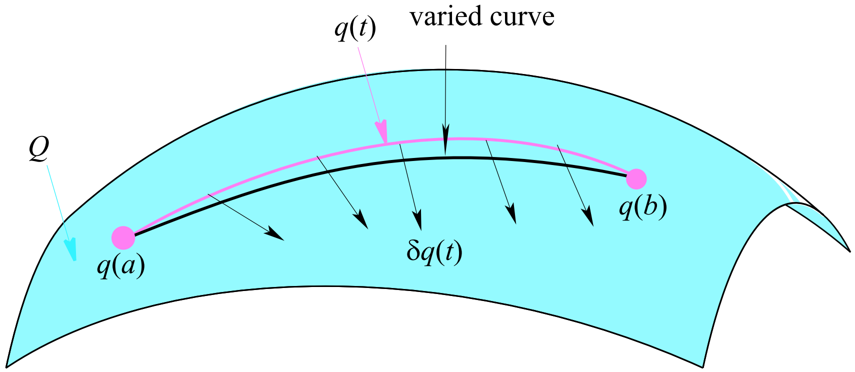
Geometric Discretizations

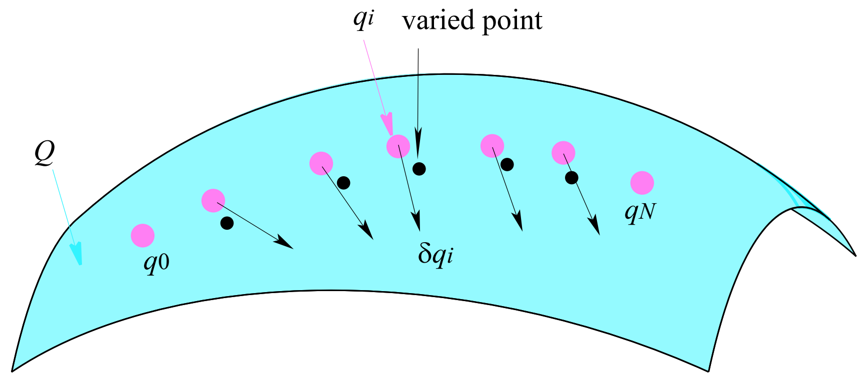
Geometric Integrators

- 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**

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

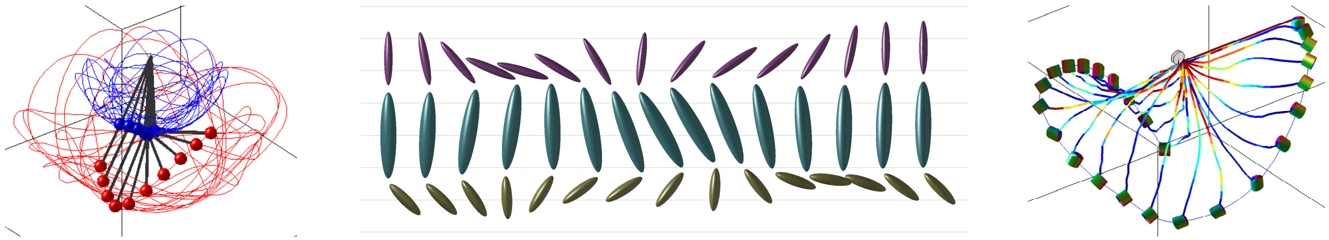
- The associated discrete flow $(q_{k-1}, q_k) \mapsto (q_k, q_{k+1})$ is automatically symplectic, since it is equivalent to,

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

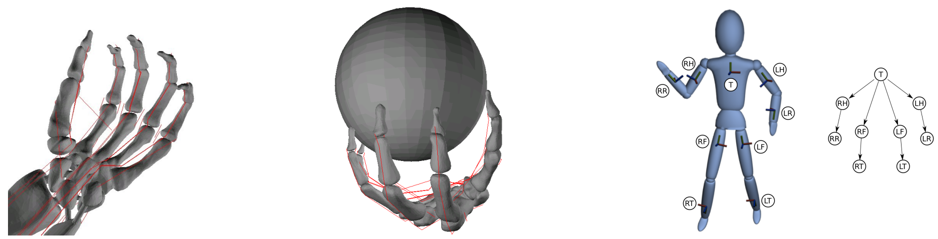
which is the characterization of a symplectic map in terms of a **Type I generating function** (discrete Lagrangian).

Examples of Variational Integrators

• Multibody Systems

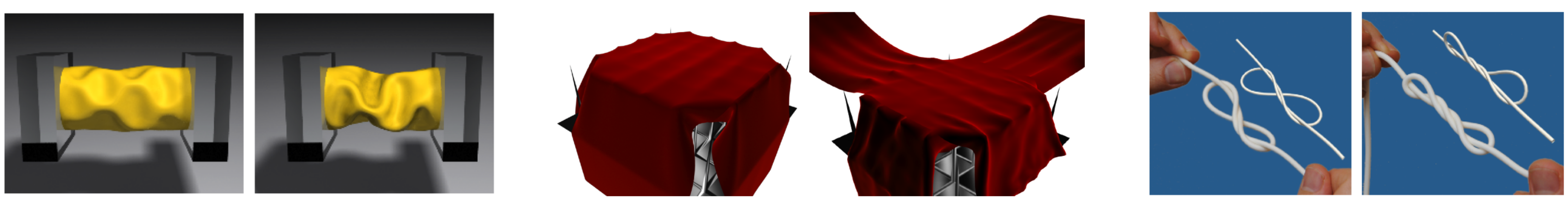


Simulations courtesy of Taeyoung Lee, George Washington University.



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**[5]
  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.

- 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 it generates an r-order accurate symplectic integrator.

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

Lagrangian Variational Integrators

Main Advantages of Variational Integrators

- **Variational Error Analysis (Sketch of Proof)**

  Consider the discrete Legendre transforms, $\mathbb{F}^{\pm}L_d : Q \times Q \to T^*Q$,

$$\begin{aligned}
\mathbb{F}^{+}L_d &: (q_k, q_{k+1}) \to (q_{k+1}, p_{k+1}) = (q_{k+1}, D_2 L_d(q_k, q_{k+1})), \\
\mathbb{F}^{-}L_d &: (q_k, q_{k+1}) \to (q_k, p_k) \qquad\quad\; = (q_k, -D_1 L_d(q_k, q_{k+1})).
\end{aligned}$$

- This yields the following commutative diagram,

$$\begin{tikzcd}
 & (q_k, p_k) \arrow[rr, "\tilde{F}_{L_d}"] & & (q_{k+1}, p_{k+1}) & \\
(q_{k-1}, q_k) \arrow[ur, "\mathbb{F}^{+}L_d"] \arrow[rr, "F_{L_d}"'] & & (q_k, q_{k+1}) \arrow[ul, "\mathbb{F}^{-}L_d"'] \arrow[ur, "\mathbb{F}^{+}L_d"] \arrow[rr, "F_{L_d}"'] & & (q_{k+1}, q_{k+2}) \arrow[ul, "\mathbb{F}^{-}L_d"']
\end{tikzcd}$$

  Since $\tilde{F}_{L_d} = \mathbb{F}^{+}L_d \circ \left(\mathbb{F}^{-}L_d\right)^{-1}$, the result easily follows.

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**.

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,

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

  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.
- 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[6] [7]

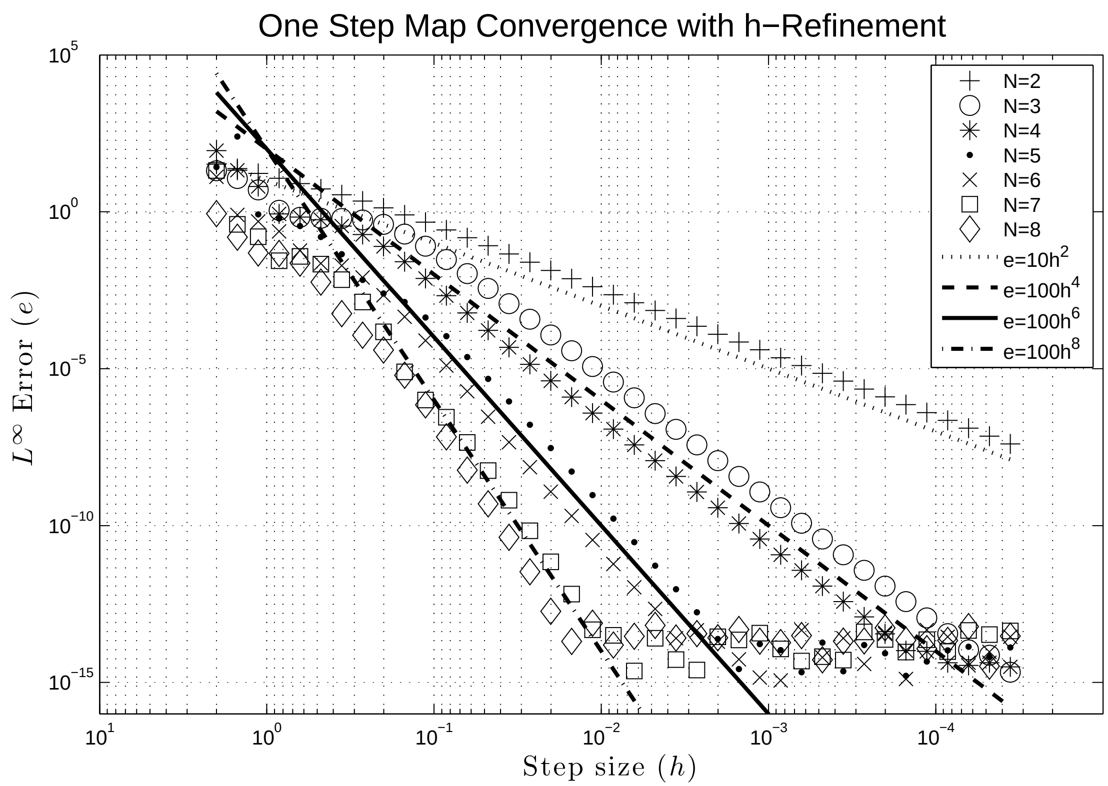
- Under suitable technical hypotheses:
  - Regularity of L in a closed and bounded neighboorhood;
  - The quadrature rule is sufficiently accurate;
  - The discrete and continuous trajectories *minimize* their actions;

  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**.

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

Ritz Variational Integrators

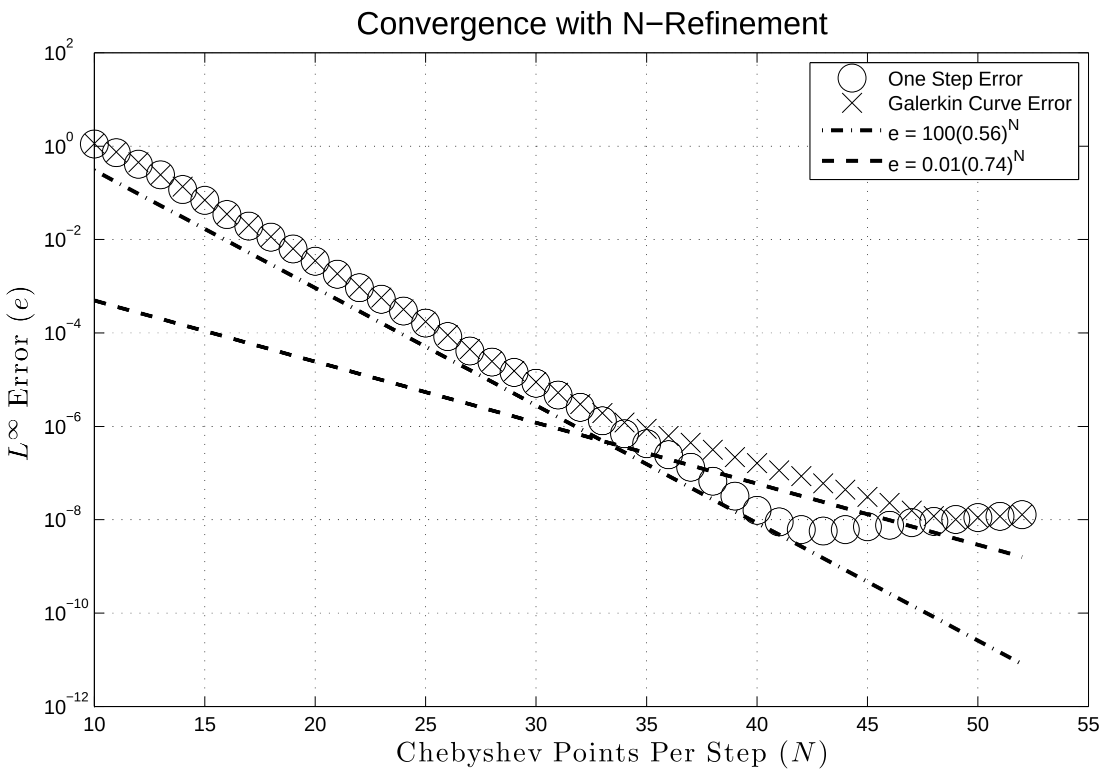
Numerical Results: Order Optimal Convergence



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

Spectral Ritz Variational Integrators

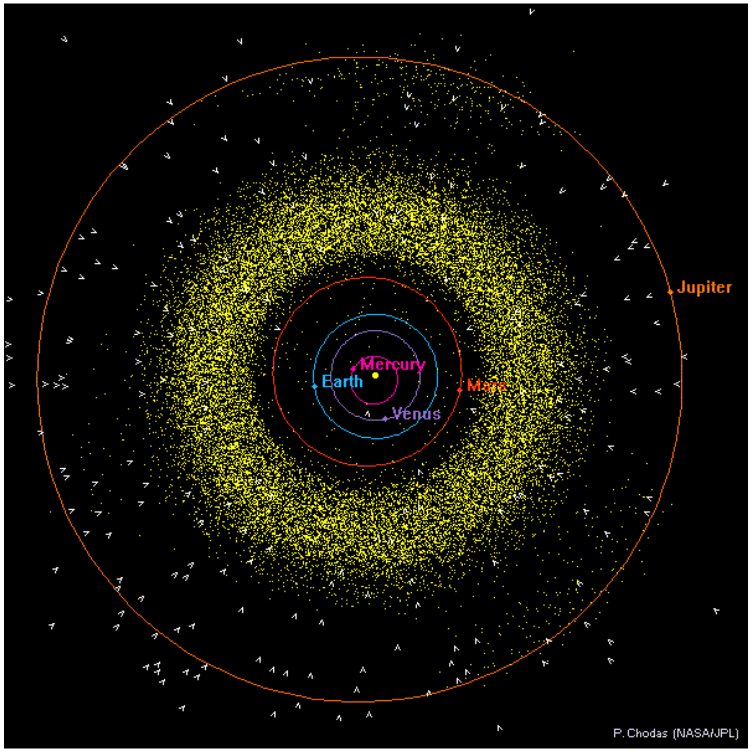
Numerical Results: Geometric Convergence

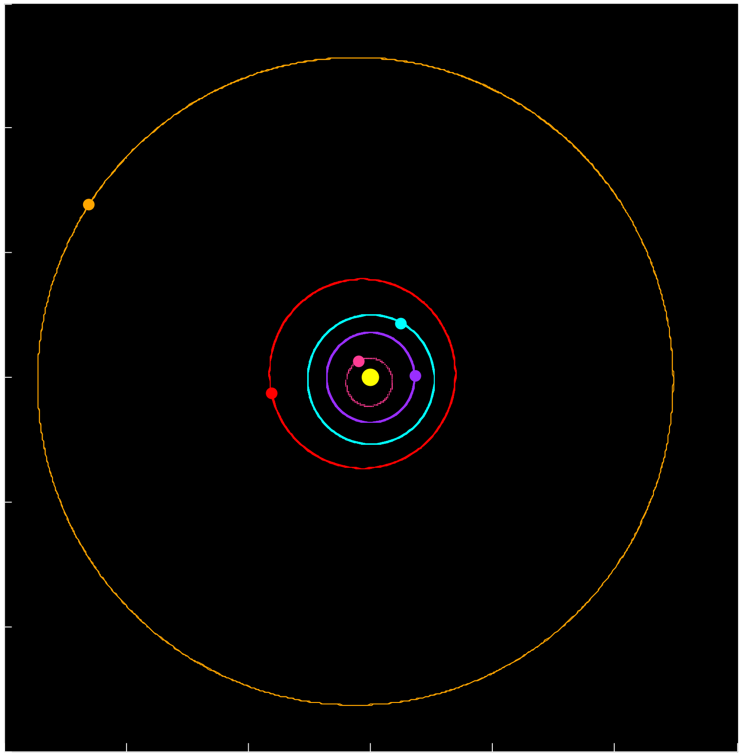


- Geometric convergence of the Kepler 2-body problem with eccentricity 0.6 over 100 steps of $h = 2.0$.

Spectral Ritz Variational Integrators

Numerical Experiments: Solar System Simulation

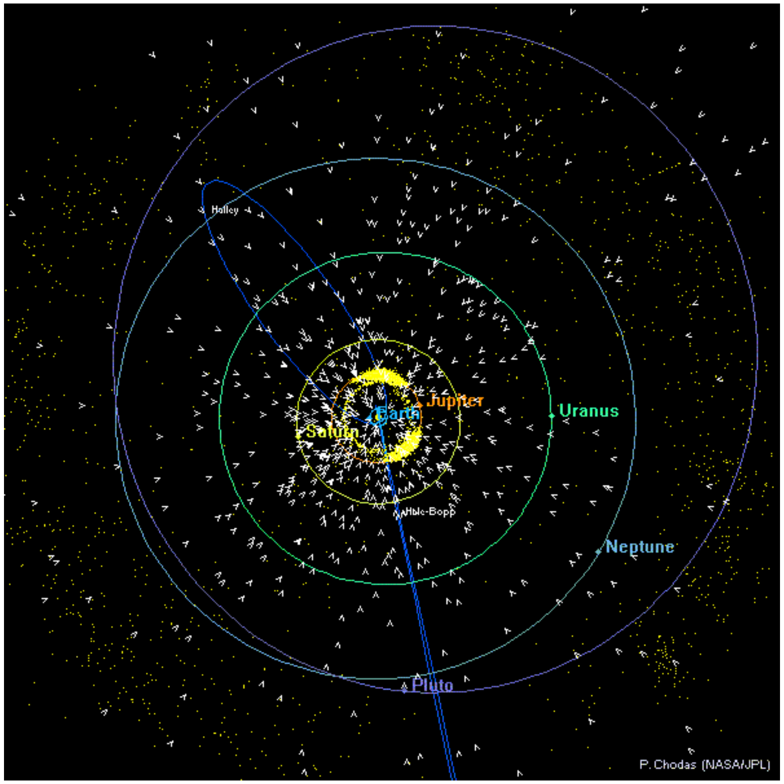


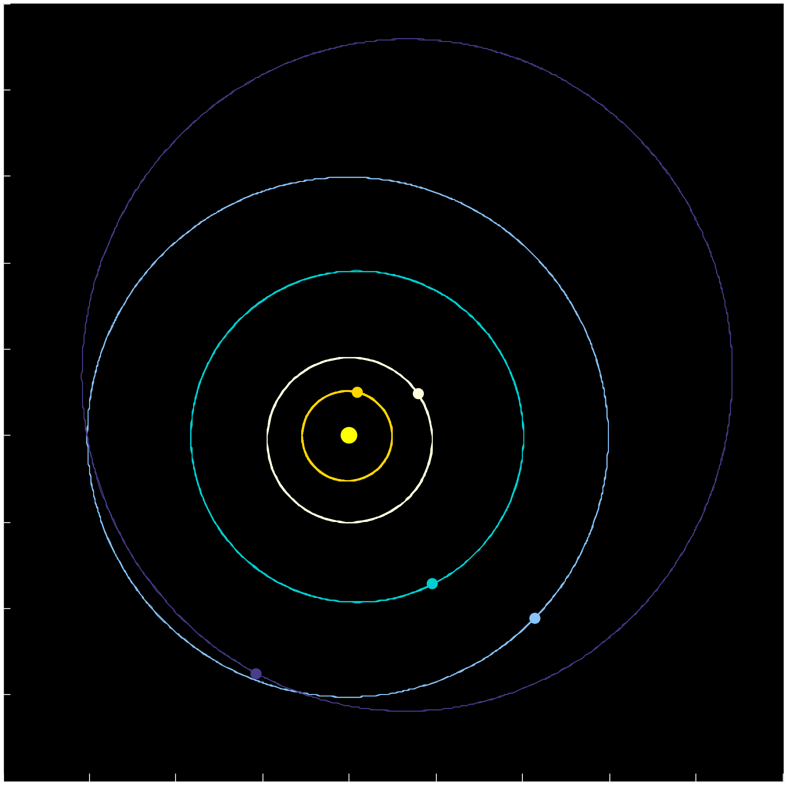


- Comparison of inner solar system orbital diagrams from a spectral variational integrator and the JPL Solar System Dynamics Group.
- $h = 100$ days, $T = 27$ years, 25 Chebyshev points per step.

Spectral Ritz Variational Integrators

Numerical Experiments: Solar System Simulation

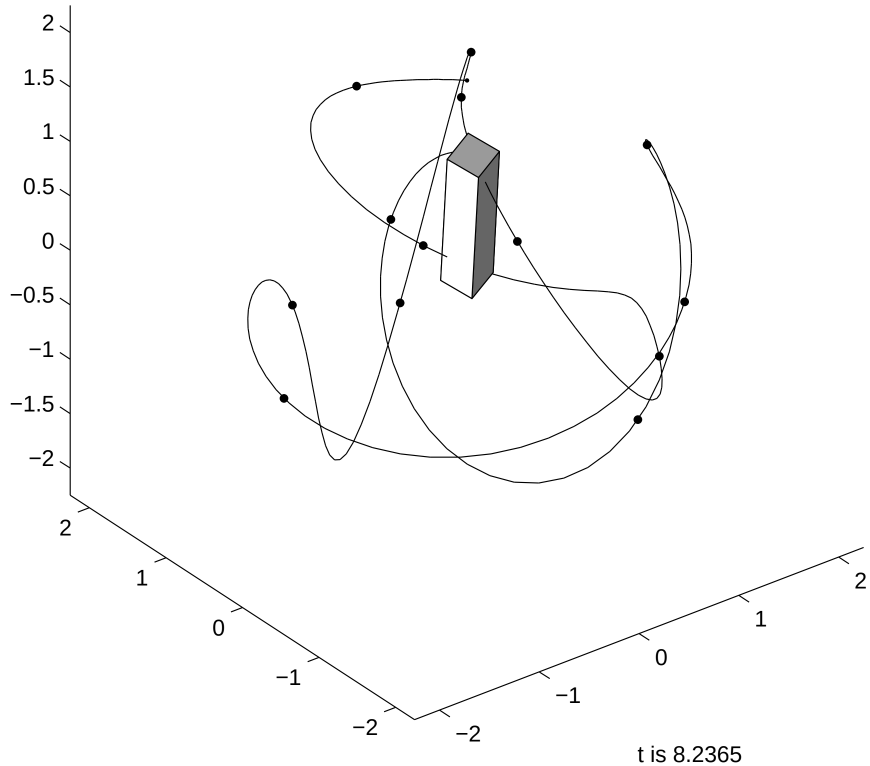




- Comparison of outer solar system orbital diagrams from a spectral variational integrator and the JPL Solar System Dynamics Group. Inner solar system was aggregated, and $h = 1825$ days.

Spectral Lie Group Variational Integrators

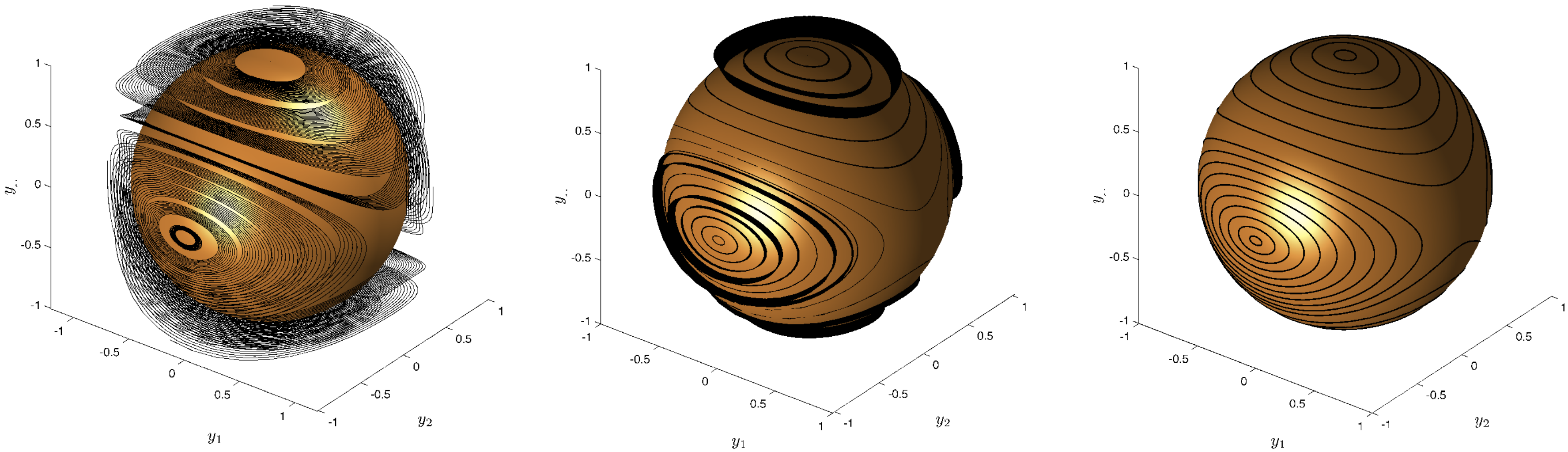
Numerical Experiments: 3D Pendulum



- $n = 20$, $h = 0.6$. The black dots represent the discrete solution, and the solid lines are the Ritz 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

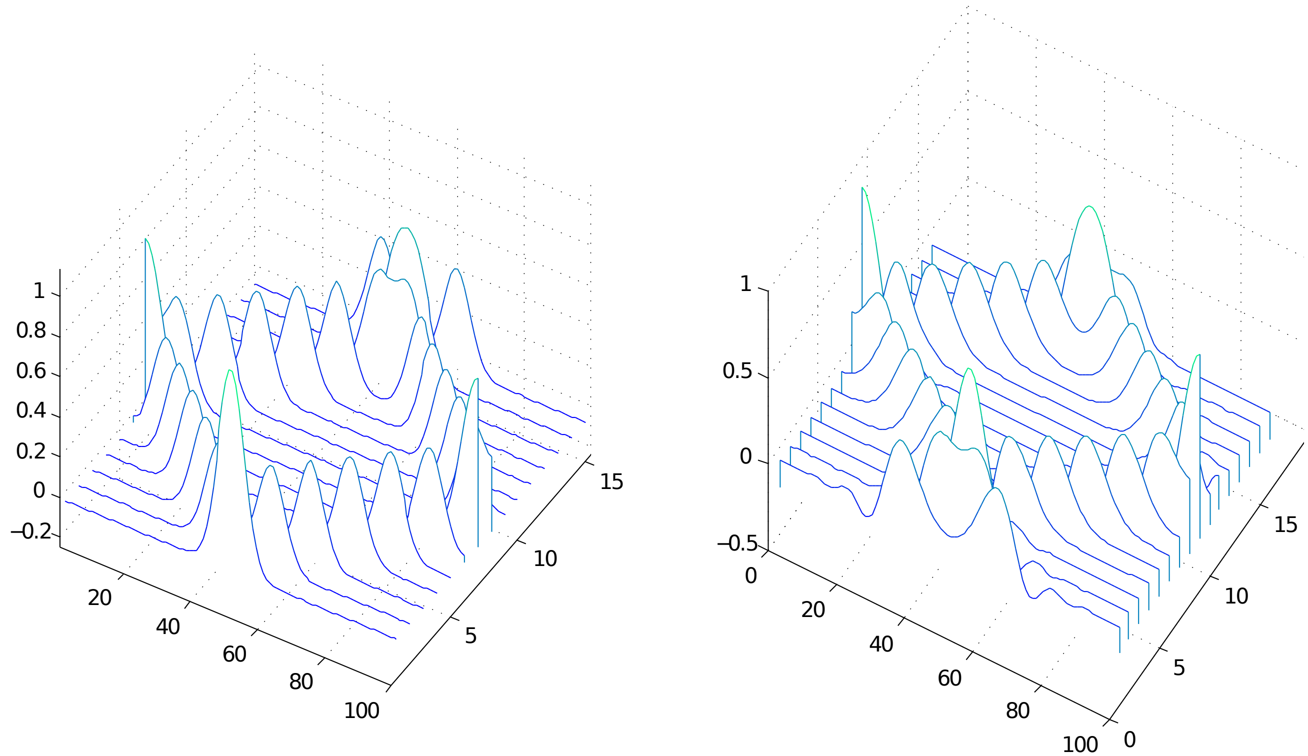


Explicit Euler | MATLAB ode45 | Lie Group Variational Integrator

- 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.

Spectral Variational Integrators

Numerical Experiments: Spectral Wave Equation



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

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**[8] 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.

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[8] 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

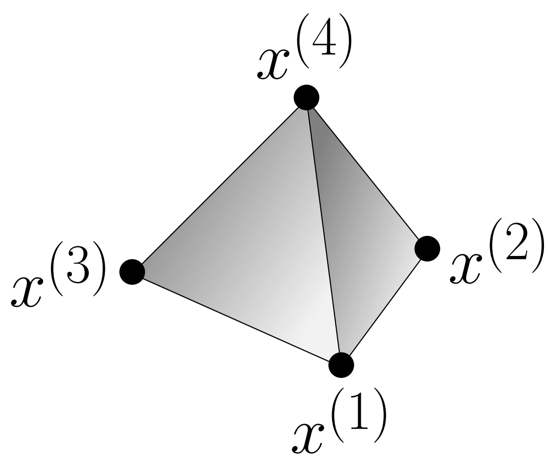
- We need finite elements that take values in the space of Lorentzian metrics that are group-equivariant.
- Two current approaches, **geodesic finite elements** and **group-equivariant interpolation on symmetric spaces**.

Interpolation of Lorentzian Metrics

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

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

- 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 $J = \text{diag}(-1,1,1,1)$.

Interpolation of Lorentzian Metrics

Componentwise interpolation

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

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

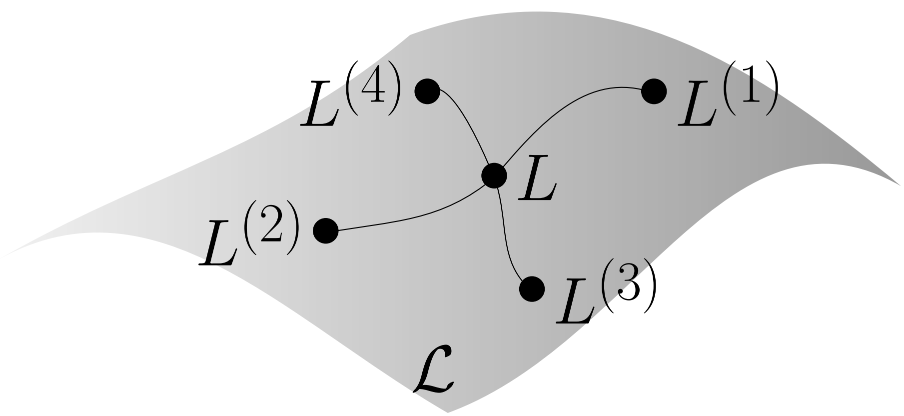
Interpolation of Lorentzian Metrics

Geodesic finite elements[9] [10]

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

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

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**.

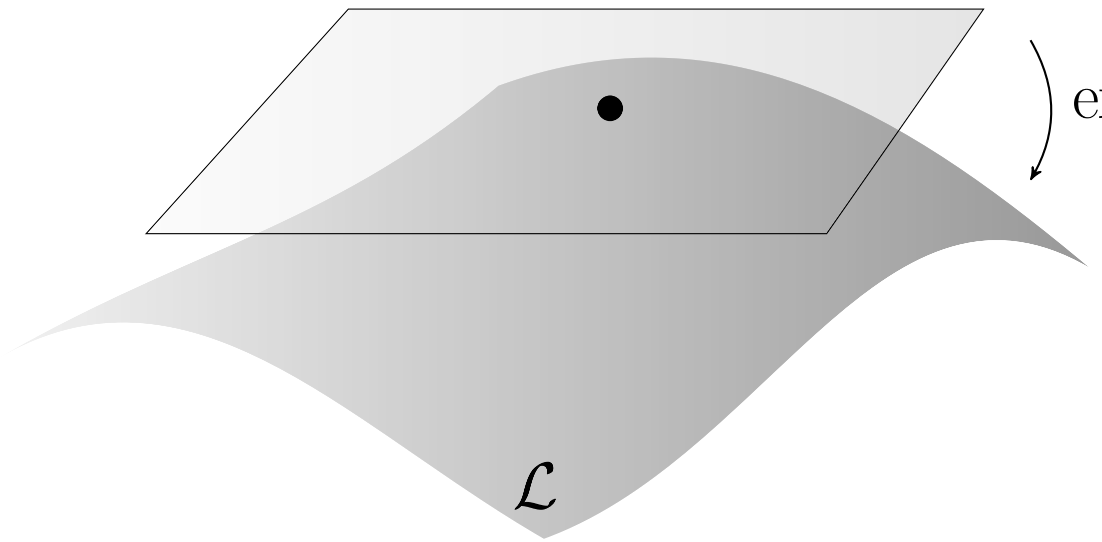


[9] O. Sander, *Geodesic finite elements on simplicial grids*, Int. J. Numer. Meth. Eng., 92(12), 999–1025, 2012.
[10] P. Grohs, *Quasi-interpolation in Riemannian manifolds*, IMA J. Numer. Anal., 33(3), 849–874, 2013.

Interpolation of Lorentzian Metrics

Our approach[11]

- **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.

[11] E. Gawlik, ML, *Interpolation on Symmetric Spaces via the Generalized Polar Decomposition*, Found. Comput. Math., Online First, 2017.

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 $J = \mathrm{diag}(-1,1,1,1)$.

- 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**:

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

Interpolation of Lorentzian Metrics

Summary

$$\begin{tikzcd}
 & & GL_4(\mathbb{R}) \arrow[d, "\pi"] \arrow[dr, "\varphi"] & \\
\mathfrak{sym}_J(4) \arrow[r, "\exp"] & Sym_J(4) \arrow[ur, "\iota"] \arrow[r, "\psi"] & GL_4(\mathbb{R})/O(1,3) \arrow[r, "\bar{\varphi}"] & \mathcal{L}
\end{tikzcd}$$

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

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

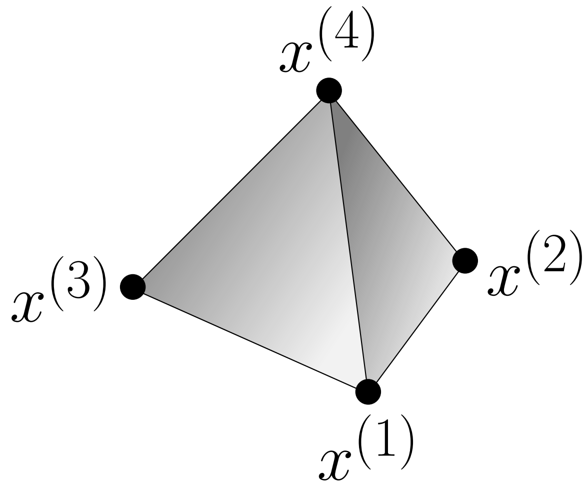
$$\mathfrak{sym}_J(4) = \{P \in \mathbb{R}^{4\times 4} \mid PJ = JP^T\},$$

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 $J = \mathrm{diag}(-1, 1, 1, 1)$, 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,

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

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

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

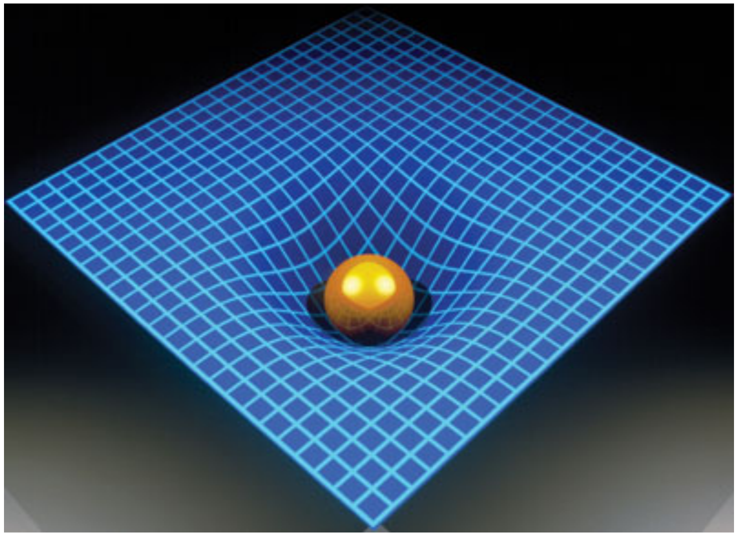
for every $x \in \Omega$.

Interpolation of Lorentzian Metrics

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 $\{\phi_i\}_i$

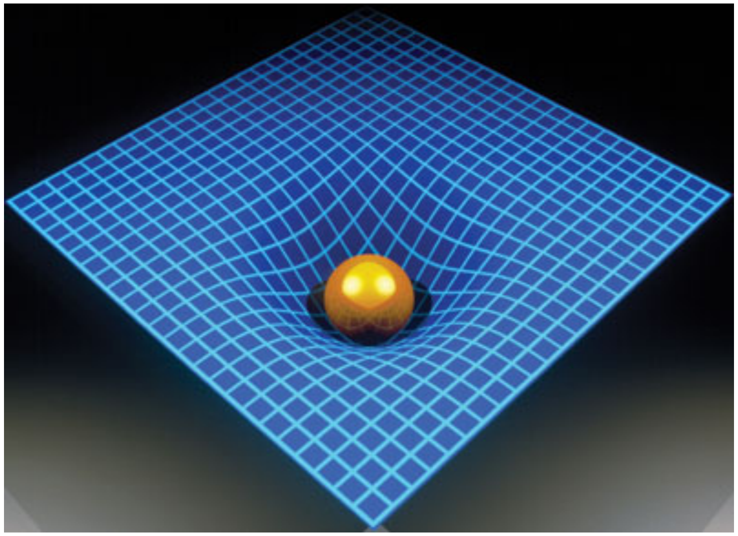
N	L^2-error	Order	H^1-error	Order
2	$3.3 \cdot 10^{-3}$		$2.8 \cdot 10^{-2}$	
4	$8.4 \cdot 10^{-4}$	1.975	$1.4 \cdot 10^{-2}$	0.998
8	$2.1 \cdot 10^{-4}$	1.994	$7.1 \cdot 10^{-3}$	0.999
16	$5.3 \cdot 10^{-5}$	1.998	$3.6 \cdot 10^{-3}$	1.000

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	$1.7\cdot 10^{-4}$		$2.5\cdot 10^{-3}$	
4	$2.2\cdot 10^{-5}$	3.001	$6.2\cdot 10^{-4}$	1.993
8	$2.7\cdot 10^{-6}$	3.000	$1.6\cdot 10^{-4}$	1.998
16	$3.4\cdot 10^{-7}$	3.000	$3.9\cdot 10^{-5}$	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 finite element**.

- Replacing $J = \mathrm{diag}(-1, 1, 1, 1)$ with the identity matrix, one recovers the weighted **Log-Euclidean mean**[12] of symmetric positive-definite matrices,

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

[12] 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

$$
\begin{tikzcd}
\mathfrak{k} \arrow[r, "\exp"] \arrow[d, "\iota"] & G^\sigma \arrow[dr, "\iota"] & & \\
\mathfrak{g} = \mathfrak{p} \oplus \mathfrak{k} \arrow[rr, "\exp"] & & G \arrow[d, "\pi"] \arrow[dr, "\varphi"] & \\
\mathfrak{p} \arrow[u, "\iota"] \arrow[r, "\exp"] & G_\sigma \arrow[ur, "\iota"] \arrow[r, "\psi"] & G/G^\sigma \arrow[r, "\bar{\varphi}"] & \mathcal{S}
\end{tikzcd}
$$

$$
\begin{tikzcd}
& & GL_4(\mathbb{R}) \arrow[d, "\pi"] \arrow[dr, "\varphi"] & \\
\mathfrak{sym}_J(4) \arrow[r, "\exp"] & Sym_J(4) \arrow[ur, "\iota"] \arrow[r, "\psi"] & GL_4(\mathbb{R})/O(1,3) \arrow[r, "\bar{\varphi}"] & \mathcal{L}
\end{tikzcd}
$$

Abstraction to Symmetric Spaces

Summary

- $\mathcal{S}$ is locally diffeomorphic to the Lie triple system $\mathfrak{p}$, which is a *linear space.*
- Interpolation on a linear space is easy.
- The resulting formula for interpolating $\{u^{(i)}\}_{i=1}^{m} \subset \mathcal{S}$ reads
$$\mathcal{I}u(x) = F\left(\sum\nolimits_{i=1}^{m} \phi_i(x) F^{-1}(u^{(i)})\right),$$
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
$$\begin{aligned} F : \mathfrak{p} &\to \mathcal{S} \\ P &\mapsto \exp(P) \cdot \eta. \end{aligned}$$
- The interpolant is **G^σ-equivariant**, and can be used to construct **multimomentum preserving variational integrators**.

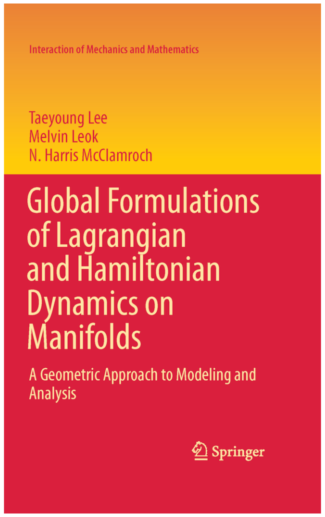
Summary

- 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.

Commericals

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. \$89.99 | €79,99 | £59.99



Another talk on interpolation on symmetric spaces

- *Interpolation of Manifold-Valued Functions via the Generalized Polar Decomposition*, Evan Gawlik, Session A5 – Geometric Integration and Computational Mechanics, 16:00–16:30, Room 111.

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