Variational Discretizations of Gauge Field Theories using Group-equivariant Interpolation

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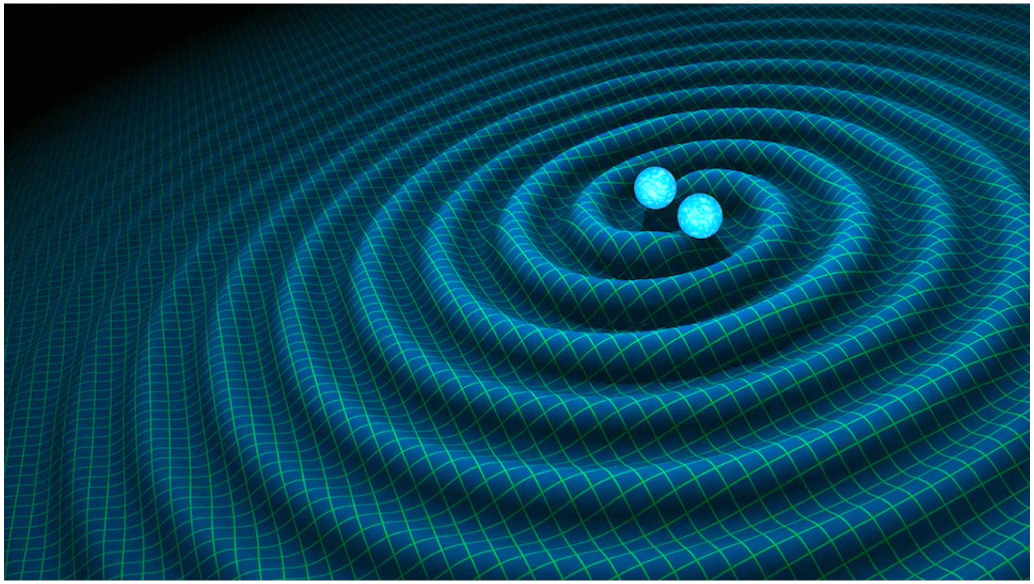
Gravitational Waves, LIGO, and Numerical Relativity



- **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,

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

- 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

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

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

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

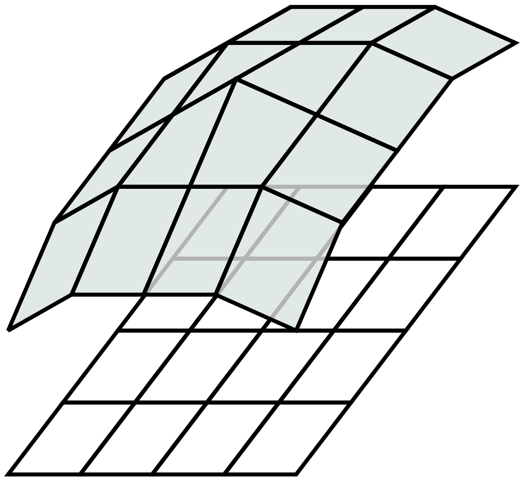
where we used integration by parts, and the fact that the variation δq vanishes at the endpoints.

- 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, $\mathcal{S}(q) = \int_{\mathcal{X}} L(j^1q)$.
- **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.

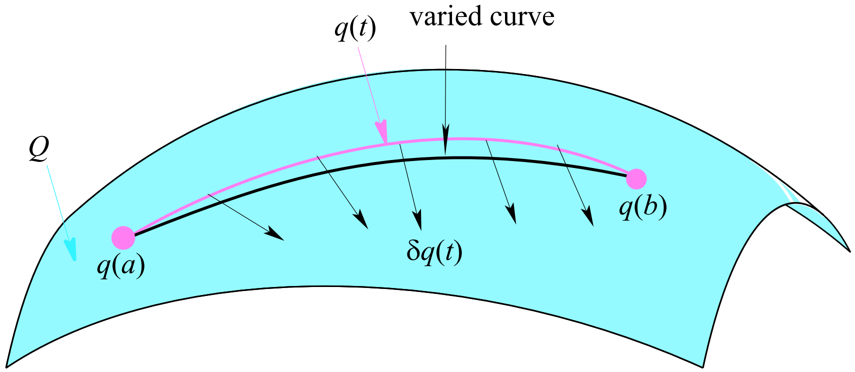
Geometric Discretizations

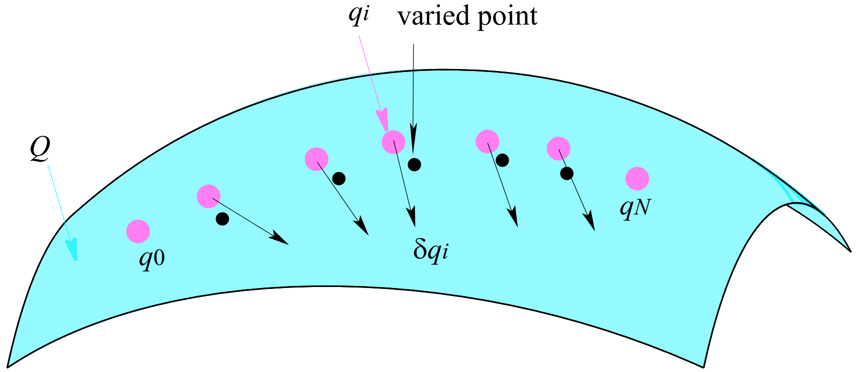
Geometric Integrators

- 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**

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

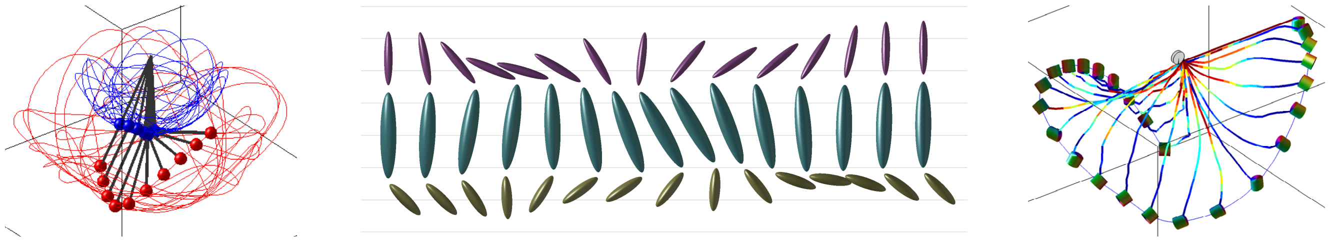
- The associated discrete flow $(q_{k-1}, q_k) \mapsto (q_k, q_{k+1})$ is automatically symplectic, since it is equivalent to,

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

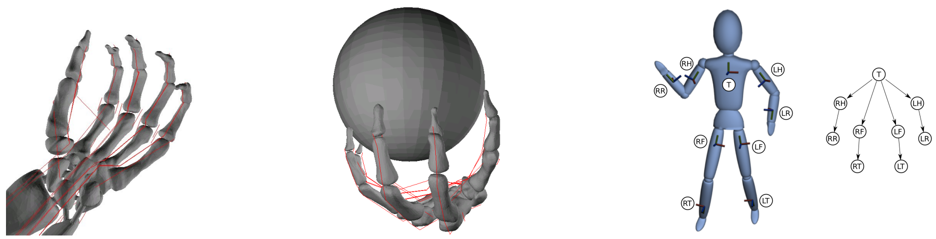
which is the characterization of a symplectic map in terms of a **Type I generating function** (discrete Lagrangian).

Examples of Variational Integrators

• Multibody Systems

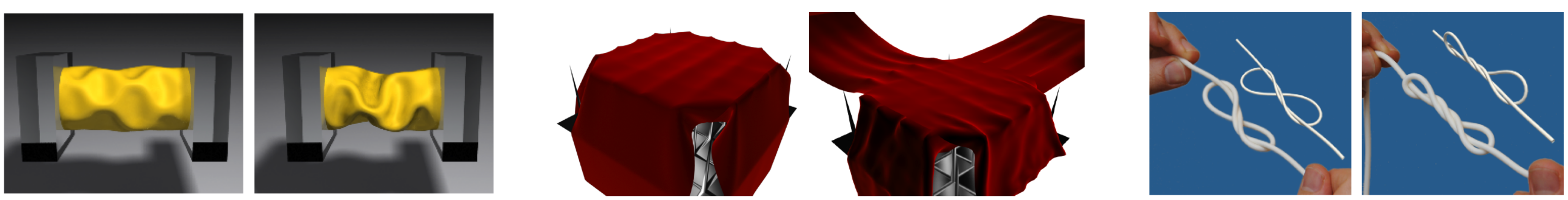


Simulations courtesy of Taeyoung Lee, George Washington University.



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

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

  is preserved by the discrete flow.

Lagrangian Variational Integrators

Main Advantages of Variational Integrators

- **Variational Error Analysis**[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.

Additional Motivations for Symplectic Discretizations

Adjoint Sensitivity Analysis

- Given a system of differential equations, the **adjoint system** has a Hamiltonian structure, even if the original system does not.
- Preserving the symplecticity is essential to maintaining the relationship between the primal and adjoint variables.

Accelerated Optimization and Machine Learning

- **Nesterov's accelerated optimization** methods can be viewed as discretizations of the flow of the time-dependent Bregman Lagrangian.
- Connections between **discrete Lagrangian mechanics** and **information geometry**, which in turn is connected to **machine learning**.

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,

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

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]

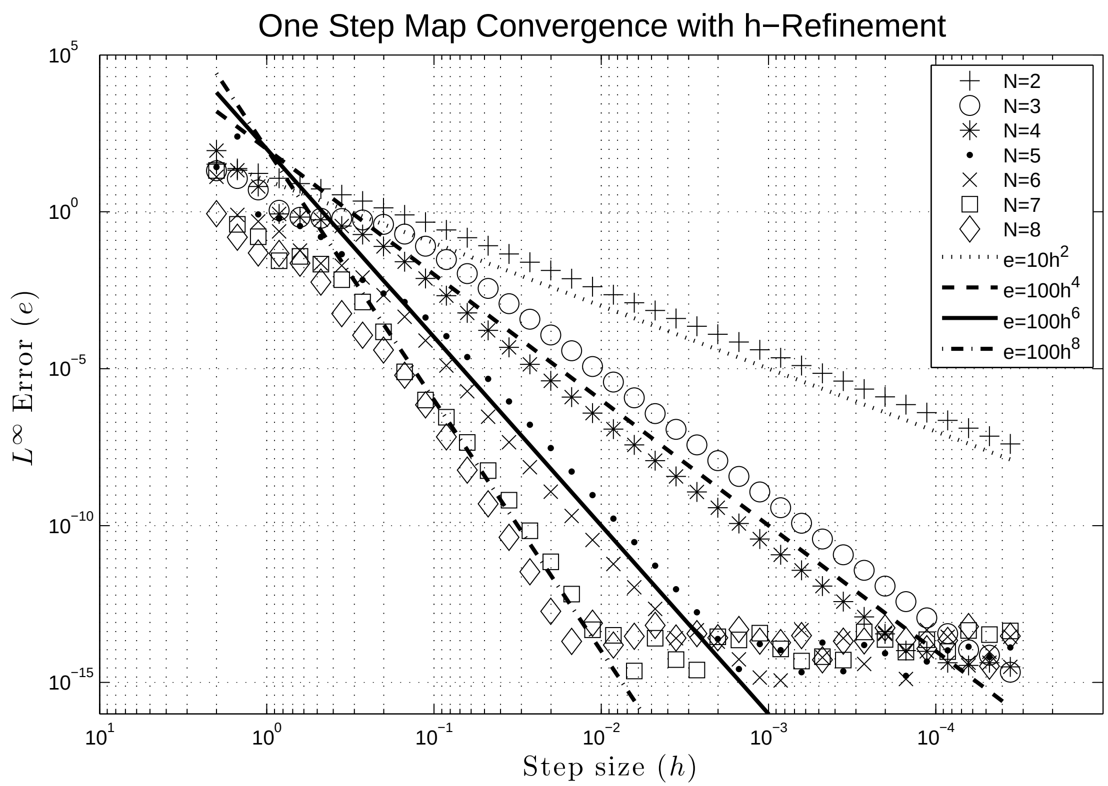
- Under suitable technical hypotheses:
  - Regularity of L in a closed and bounded neighborhood;
  - The quadrature rule is sufficiently accurate;
  - The discrete and continuous trajectories *minimize* their actions;

  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

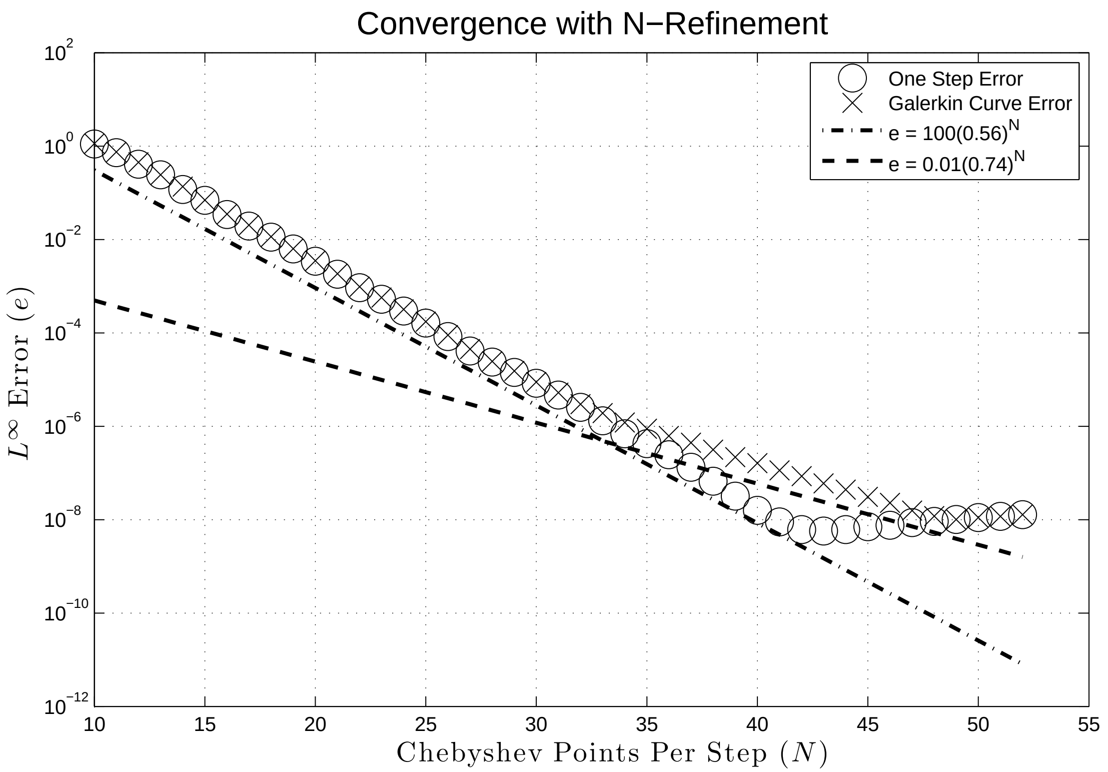
Numerical Results: Order Optimal Convergence



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

Spectral Ritz Variational Integrators

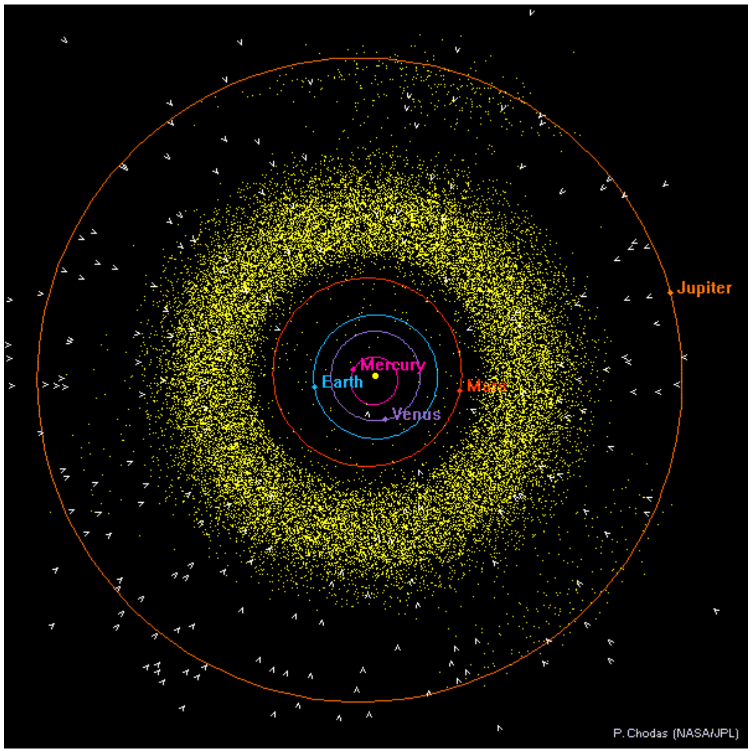
Numerical Results: Geometric Convergence

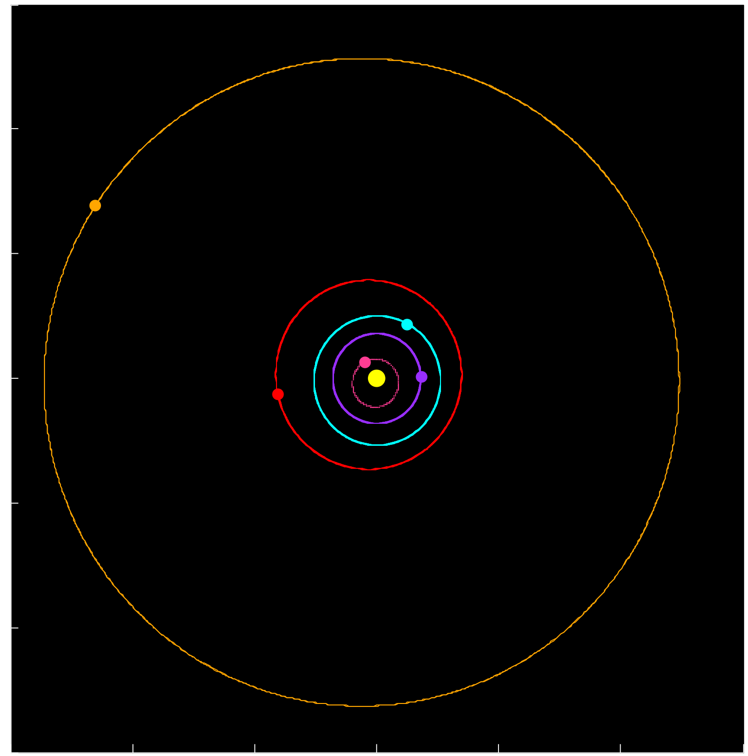


- Geometric convergence of the Kepler 2-body problem with eccentricity 0.6 over 100 steps of $h = 2.0$.

Spectral Ritz Variational Integrators

Numerical Experiments: Solar System Simulation

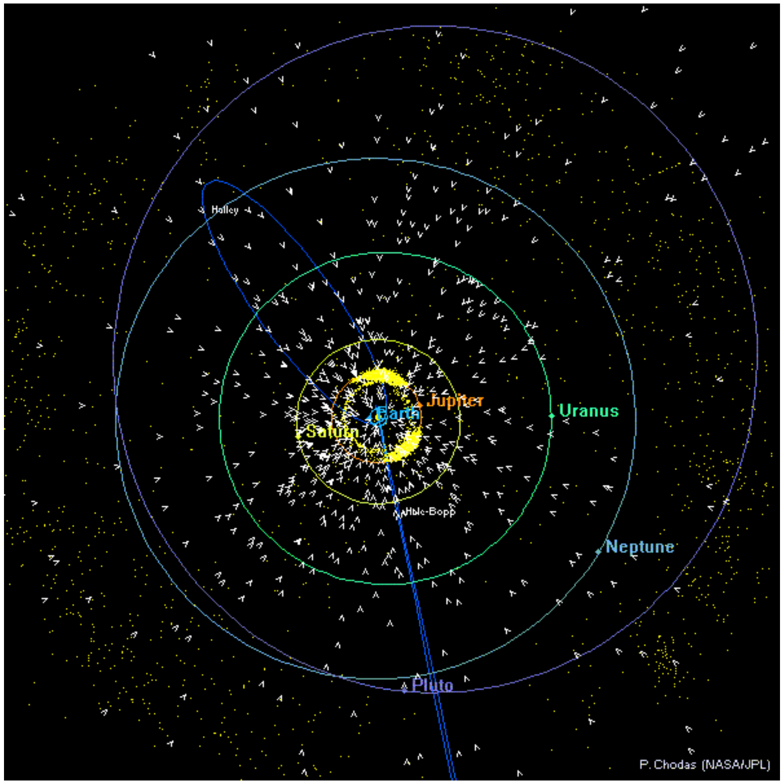


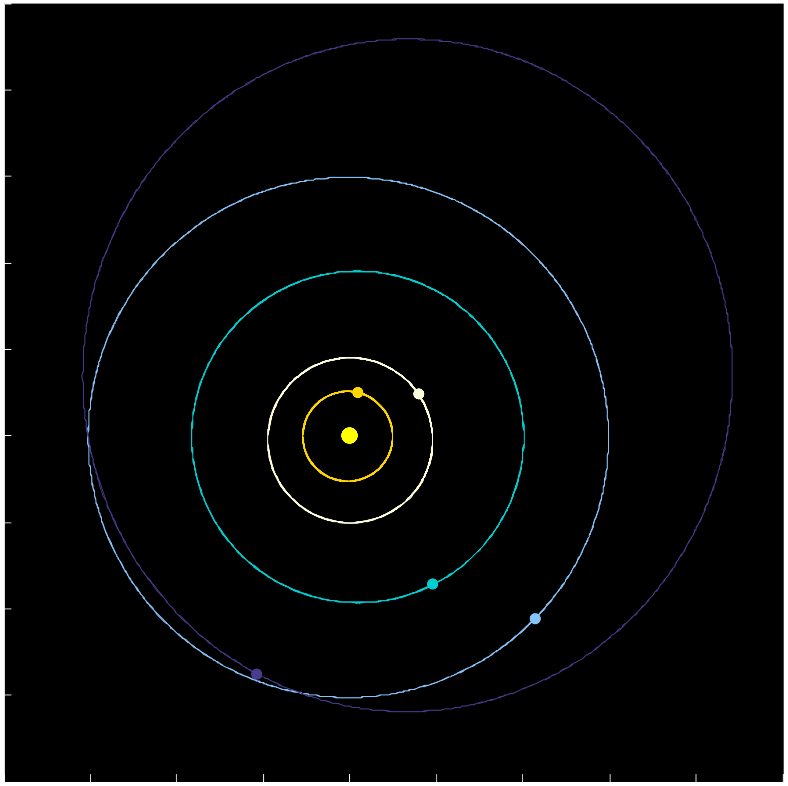


- Comparison of inner solar system orbital diagrams from a spectral variational integrator and the JPL Solar System Dynamics Group.
- $h = 100$ days, $T = 27$ years, 25 Chebyshev points per step.

Spectral Ritz Variational Integrators

Numerical Experiments: Solar System Simulation

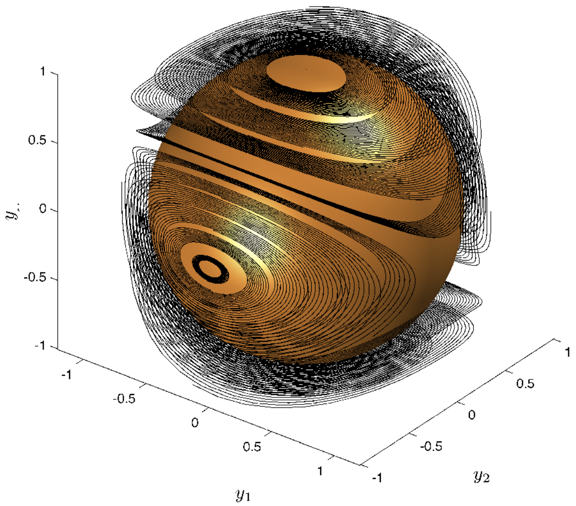




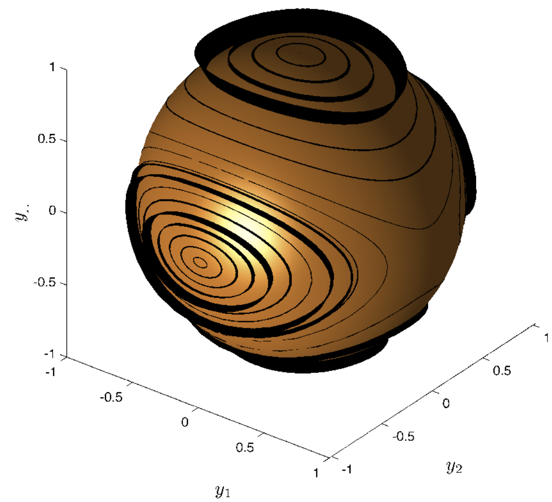
- Comparison of outer solar system orbital diagrams from a spectral variational integrator and the JPL Solar System Dynamics Group. Inner solar system was aggregated, and $h = 1825$ days.

Spectral Lie Group Variational Integrators

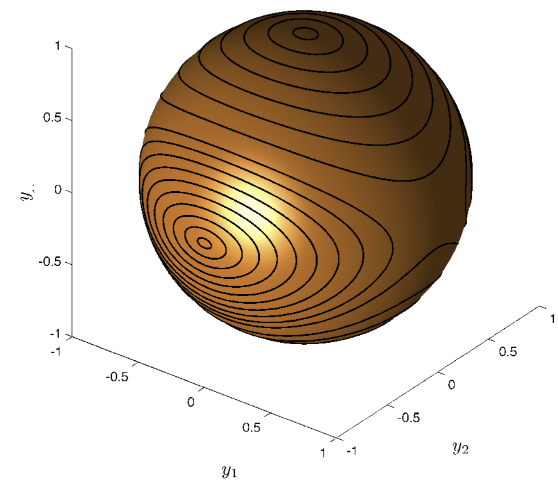
Numerical Experiments: Free Rigid Body



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.

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[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 **multisymplectic relation**, which is the PDE analogue of,

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

where the sign 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

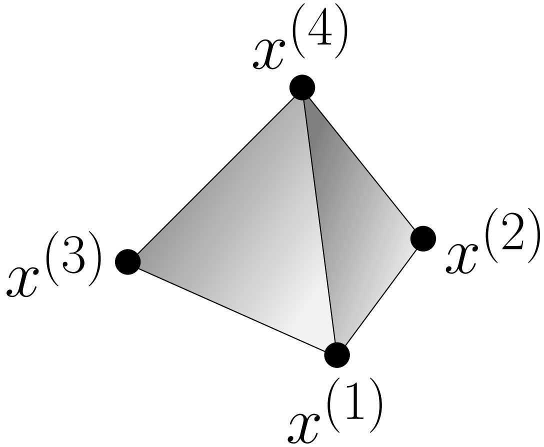
- We need finite elements that take values in the space of Lorentzian metrics that are group-equivariant.
- Two current approaches, **geodesic finite elements** and **group-equivariant interpolation on symmetric spaces**.

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,

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

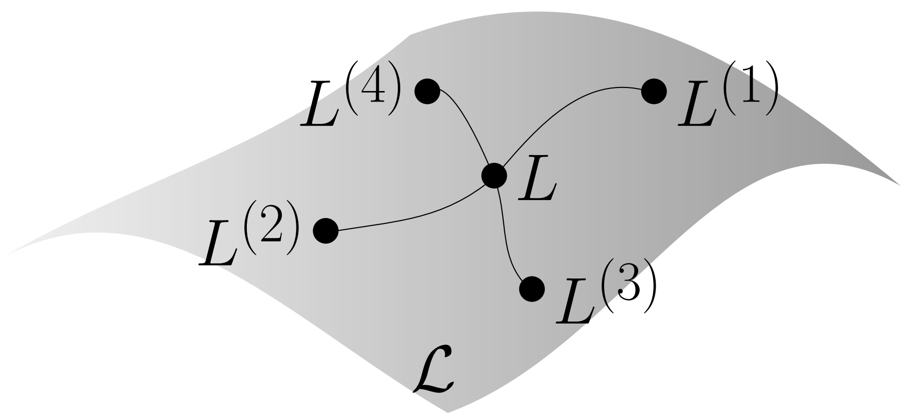
Interpolation of Lorentzian Metrics

Geodesic interpolation[6] [7]

- 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**.

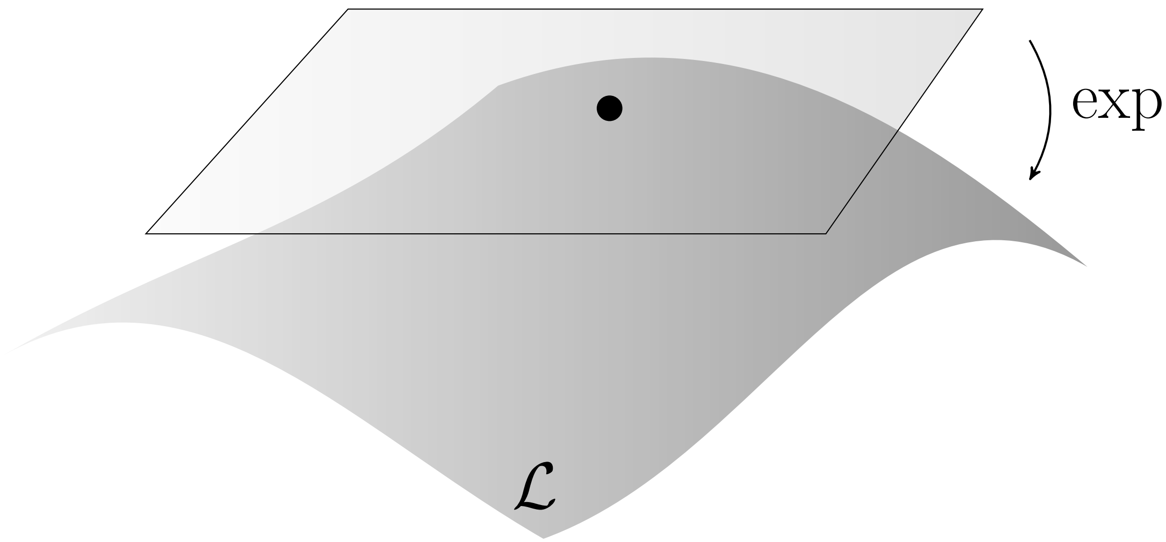


[6] O. Sander, *Geodesic finite elements on simplicial grids*, Int. J. Numer. Meth. Eng., 92(12), 999–1025, 2012.
[7] P. Grohs, *Quasi-interpolation in Riemannian manifolds*, IMA J. Numer. Anal., 33(3), 849–874, 2013.

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

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

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

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

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

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

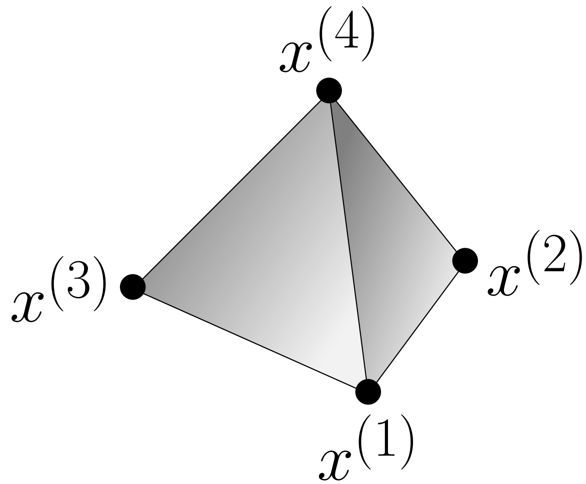
$$\mathfrak{sym}_J(4) = \{P \in \mathbb{R}^{4\times 4} \mid PJ = JP^T\},$$

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

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

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

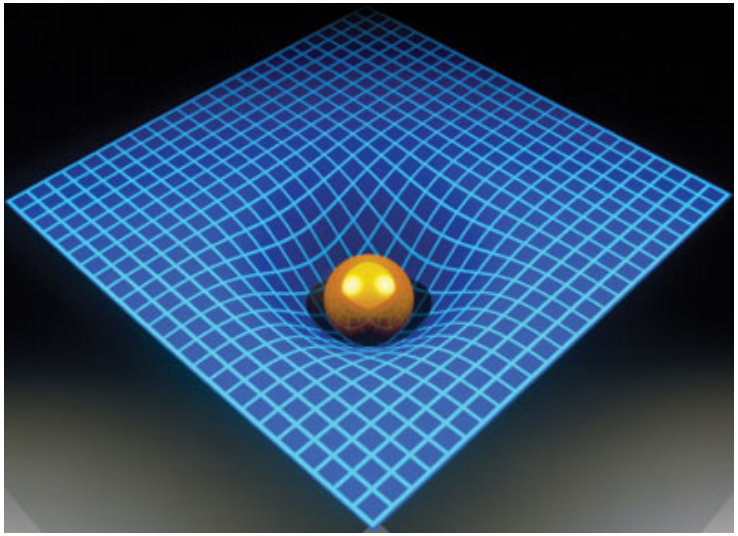
for every $x \in \Omega$.

Interpolation of Lorentzian Metrics

Numerical example (Linear Interpolation)

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

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



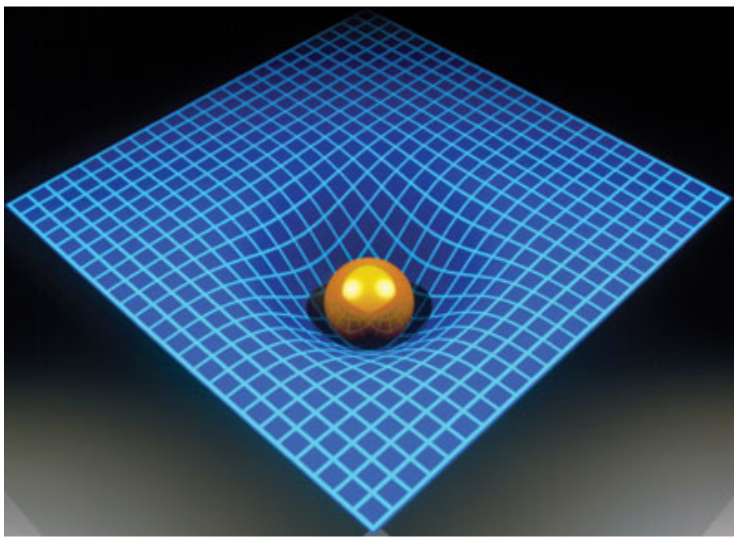
	Linear shape functions $\{\phi_i\}_i$			
N	L^2-error	Order	H^1-error	Order
2	$3.3\cdot10^{-3}$		$2.8\cdot10^{-2}$	
4	$8.4\cdot10^{-4}$	1.975	$1.4\cdot10^{-2}$	0.998
8	$2.1\cdot10^{-4}$	1.994	$7.1\cdot10^{-3}$	0.999
16	$5.3\cdot10^{-5}$	1.998	$3.6\cdot10^{-3}$	1.000

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	$1.7 \cdot 10^{-4}$		$2.5 \cdot 10^{-3}$	
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 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 $\mathcal{S}$ — $J = \text{diag}(-1, 1, 1, 1)$
- G – Lie group that acts transitively on $\mathcal{S}$ — $GL_4(\mathbb{R})$
- $\sigma : G \rightarrow G$ – 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

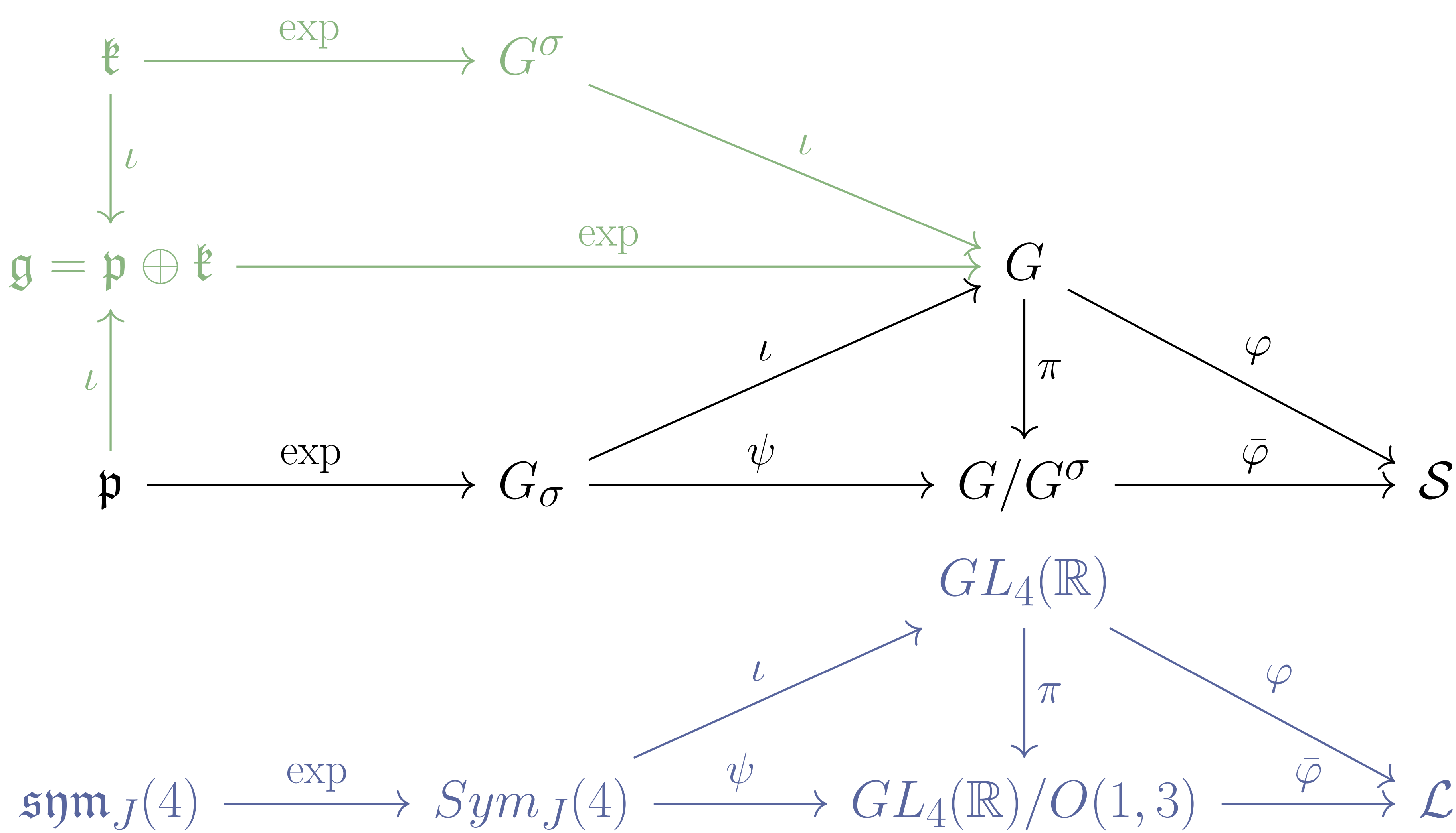
- Isotropy subgroup of η coincides with the fixed set G^σ, i.e.

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

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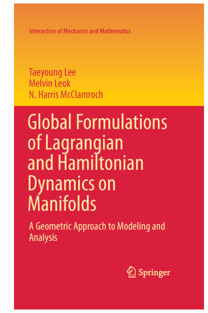
[10] D. Amsallem and C. Farhat. Interpolation method for adapting reduced-order models and application to aeroelasticity. AIAA Journal, 46(7), 1803–1813, 2008.

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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