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Variational Discretizations of Gauge Field Theories Using Group-Equivariant Interpolation

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Abstract

We describe a systematic mathematical approach to the geometric discretization of gauge field theories that is based on Dirac and multi-Dirac mechanics and geometry, which provide a unified mathematical framework for describing Lagrangian and Hamiltonian mechanics and field theories, as well as degenerate, interconnected, and nonholonomic systems. Variational integrators yield geometric structure-preserving numerical methods that automatically preserve the symplectic form and momentum maps, and exhibit excellent long-time energy stability. The construction of momentum-preserving variational integrators relies on the use of group-equivariant function spaces, and we describe a general construction for functions taking values in symmetric spaces. This is motivated by the geometric discretization of general relativity, which is a second-order covariant gauge field theory on the symmetric space of Lorentzian metrics.

Keywords Geometric numerical integration · Variational integrators · Symplectic integrators · Hamiltonian field theories · Manifold-valued data · Gauge field theories · Numerical relativity

Mathematics Subject Classification 37M15 · 53C35 · 65D05 · 65M70 · 65P10 · 70H25

1 Introduction

Geometric numerical integration [30] is concerned with the construction of numerical methods that preserve geometric properties of the flow of a dynamical system. These

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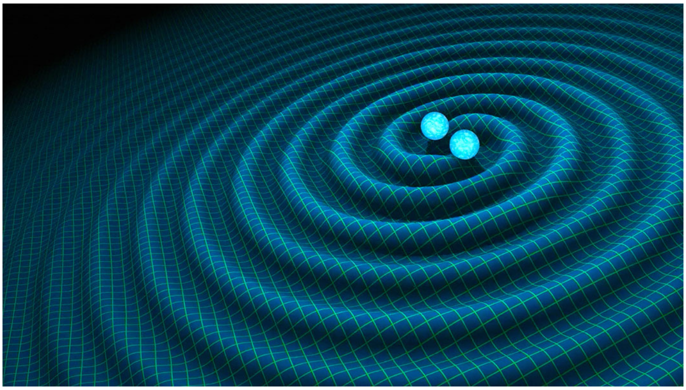


Fig. 1 An artist's impression of gravitational waves generated by binary neutron stars. Credits: R. Hurt/Caltech-JPL

geometric properties constrain the trajectories of the dynamical system, and consequently, geometric structure-preserving numerical methods typically yield numerical solutions that are qualitatively more accurate, particularly for long-time simulations. In addition to geometric invariants, dynamical systems often evolve on nonlinear manifolds, and numerical methods that are able to handle manifold-valued data and functions are important in a variety of applications, including mechanics [17,32,53], computer vision and graphics [14,16,22,35,38,59], medical imaging [11], and numerical relativity [9].

The development of geometric structure-preserving discretizations of covariant field theories with manifold-valued data is motivated by the application to numerical general relativity. There has been a renewed interest in numerical relativity due to the pivotal role it plays in realizing the promise of gravitational wave astronomy. Gravitational waves are ripples in the fabric of spacetime (see Fig. 1) that were predicted by Einstein [19], and the 2017 Nobel Prize in Physics honored Barry Barish, Kip Thorne, and Rainer Weiss, the founders of the LIGO (Laser Interferometer Gravitational-Wave Observatory) project, the precursor of the Advanced LIGO project that was responsible for the first gravitational-wave detections [2].

The first few gravitational waves detected involved binary black hole mergers [1–4], but the most recent observation involved a binary neutron star collision [5] that was also observable by optical telescopes. The simultaneous observation of gravitational and electromagnetic waves emanating from this cosmic event provided compelling independent validation of the Advanced LIGO observations of gravitational waves. The numerical simulation of Einstein's equations is critical to solving the inverse problem that relates gravitational-wave observations to the underlying astronomical event. Given the deeply geometric nature of the Einstein equations, and the fundamental role that spacetime covariance plays in the physics of gravitation, it is natural to explore geometric discretizations of general relativity that respect its numerous geometric conservation properties.

In this paper, we will describe the general framework and the underlying mathematical techniques we have developed as part of an ongoing program to systematically discretize covariant field theories with manifold-valued data.

2 Discrete Canonical Formulation of Gauge Field Theories

There are two equivalent methods for describing field theories: (1) the covariant multisymplectic approach, where the solution is a section of the configuration bundle over spacetime; (2) the canonical (or instantaneous) approach [24], where one chooses a spacetime slicing that foliates spacetime with a parametrized family of Cauchy surfaces, and the solution is described by time-parameterized sections of the instantaneous configuration spaces. It is important to relate these at the discrete level, since the covariant approach is relevant to general spacetime discretizations of PDEs, and the instantaneous approach provides an initial-value formulation of PDEs.

Relating these two approaches is more subtle in the presence of symmetries. One particularly important class of Lagrangian field theories is that of *gauge field theories*, where the Lagrangian density is equivariant under a *gauge symmetry*, which is a local symmetry action. Examples include electromagnetism, Yang–Mills, and general relativity. A consequence of gauge symmetries is that when the field theory is formulated as an initial-value problem, the evolution of the field theory is not uniquely specified by the initial conditions, that is to say that they are underdetermined. In particular, the fields can be decomposed into *dynamic fields*, whose evolution is described by well-posed equations, and *kinematic fields* which have no physical significance. In relativity, the former are the metric and extrinsic curvature on a spatial hypersurface, and the latter are the lapse and shift. Besides the indeterminacy in the evolution equations, there are initial-value constraints (typically elliptic) on the Cauchy data. *Noether's first theorem* applied to the nontrivial rigid subgroup of the gauge group implies that there exists a *Noether current* that obeys a continuity equation, and integrating this over a Cauchy surface yields a conserved quantity called a *Noether charge*. What is more interesting for gauge field theories is *Noether's second theorem*, where the gauge symmetry implies that the equations of motion are not functionally independent, and this has important implications for covariant field theories, such as general relativity.

Electromagnetism as a Gauge Field Theory

Let $\mathbf{E}$ and $\mathbf{B}$ denote the electric and magnetic fields, respectively. Maxwell's equations in terms of the scalar and vector potentials ϕ and $\mathbf{A}$ are,

$$\mathbf{E} = -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t}, \quad \nabla^2\phi + \frac{\partial}{\partial t}(\nabla\cdot\mathbf{A}) = 0, \quad \mathbf{B} = \nabla\times\mathbf{A},$$
$$\Box\mathbf{A} + \nabla\left(\nabla\cdot\mathbf{A} + \frac{\partial\phi}{\partial t}\right) = 0,$$

where $\Box$ denotes the d'Alembert or wave operator, which is the Laplace operator of Minkowski space. The gauge transformation $\phi \mapsto \phi - \frac{\partial f}{\partial t}$ and $\mathbf{A} \mapsto \mathbf{A} + \nabla f$, where f is a scalar function, leaves the equations invariant. The associated Cauchy initial data constraints are $\nabla \cdot \mathbf{B}^{(0)} = 0$ and $\nabla \cdot \mathbf{E}^{(0)} = 0$, and the Noether currents are $j_0 = \mathbf{E} \cdot \nabla f$ and $\mathbf{j} = -\mathbf{E}\frac{\partial f}{\partial t} + (\mathbf{B} \times \nabla) f$.

The gauge freedom is typically addressed by fixing a gauge condition. For example, the Lorenz gauge is $\nabla \cdot \mathbf{A} = -\frac{\partial \phi}{\partial t}$, which yields $\Box\phi = 0$ and $\Box\mathbf{A} = 0$, and the Coulomb gauge is $\nabla \cdot \mathbf{A} = 0$, which yields $\nabla^2\phi = 0$ and $\Box\mathbf{A} + \nabla\frac{\partial \phi}{\partial t} = 0$. Given different initial and boundary conditions, appropriately choosing the gauge can dramatically simplify the problem, but there is no systematic way of doing this for a given problem.

General Relativity as a Gauge Field Theory

We now describe the salient aspects of the Einstein equations that motivate our proposed research. The *Einstein–Hilbert action* for general relativity is defined on Lorentzian metrics,

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

where $g = \det g_{\mu\nu}$, $R_{\mu\nu} = R^{\alpha}_{\mu\alpha\nu}$ is the Ricci tensor, and $\mathcal{L}_M$ describes the matter fields, which vanishes in the vacuum case. The action is second-order with respect to derivatives of the metric and describes a second-order gauge field theory, with the spacetime diffeomorphisms as the gauge group. The corresponding Euler–Lagrange equations are 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, which is also the Noether current associated with the spacetime diffeomorphism symmetry.

The gauge symmetry renders the Lagrangian degenerate, and as a consequence, the solutions are not unique. For example, consider the vacuum Einstein equation, $G_{\mu\nu} = 0$, when $\mathcal{L}_M = 0$, with initial conditions $g(0) = \mathrm{diag}(-1, 1, 1, 1)$, $\dot{g} = 0$, which clearly has flat spacetime $g(t) = \mathrm{diag}(-1, 1, 1, 1)$ as a solution. But, it is easy to verify that $g(t) = \mathrm{diag}(-(f'(t))^2, 1, 1, 1)$ is also a solution for any f satisfying $f'(0) = 1$ and $f''(0) = 0$.

Another consequence of the spacetime diffeomorphism symmetry is that Noether's second theorem implies that the Einstein equations are functionally dependent and can be viewed as 6 dynamical equations, together with 4 constraint equations that are automatically satisfied. To overcome the underdetermined nature of the Einstein equations, one typically chooses a gauge condition, such as the maximal slicing gauge, $K = \partial_t K = 0$, where $K = K_{\alpha\beta}K^{\alpha\beta}$ is the trace of the extrinsic curvature, or the de Donder (or harmonic) gauge, $\Gamma^{\alpha}_{\beta\gamma} g^{\beta\gamma} = 0$, which is Lorentz invariant and useful for gravitational waves. Additionally, when the Einstein equations are formulated as an initial-value problem, the Cauchy data are constrained and must satisfy the Gauss–Codazzi equations.

Covariant Field Theories

In particular, we are concerned with *covariant field theories*, which are gauge theories where the gauge group contains the spacetime diffeomorphism group. Covariance is of fundamental importance in, for instance, elasticity and general relativity, and moreover ensures (through Noether's theorem) that the *stress-energy-momentum tensor* is well-defined [25]. Covariance can be built into a field theory by augmenting the configuration bundle with a second copy of the base space [13]. Then, the spacetime variables appear as new fields on the same footing as the original fields. Computationally, this corresponds to using distinct computational and physical meshes, which allows one to construct mesh-adapting algorithms.

By Noether's theorem, there are conserved momentum maps associated with the spacetime diffeomorphism invariance of a covariant field theory. These are best analyzed in the multisymplectic formulation as the instantaneous formulation depends on the spacetime slicing, but the spacetime diffeomorphisms do not preserve slicings. Covariant momentum maps manifest themselves in the instantaneous formulation as an *energy-momentum map*, which is the instantaneous shadow of the covariant momentum map with respect to a spacetime slicing. This provides an explicit characterization of the initial-value constraints, which are equivalent to the energy-momentum map vanishing, and as such, the constraint functions can be viewed as components of the energy-momentum map.

The instantaneous Hamiltonian with respect to a spacetime slicing depends linearly on the *atlas fields* and the constraints, which yields the *adjoint form* of the evolution equations for the dynamic fields, and clarifies the relationship between the dynamics, initial-value constraints, and the gauge freedom [24]. In relativity, the adjoint formulation reduces to the familiar ADM equations of relativity [10].

Implications of Gauge Symmetries for Discretization

When the Einstein equations are discretized, the constraints are not automatically satisfied. Constrained evolution methods [8] explicitly impose the constraints but are computationally prohibitive. Instead, free evolution methods monitor the constraint violations and refine the spacetime mesh, but exponential growth of the constraint violations limit their applicability. The first successful computation of binary black hole merger [52] was only made possible by introducing constraint damping [29]. But, like all penalty term-based methods, a carefully tuned damping parameter is essential to avoid undesirable constraint growth and qualitatively incorrect solutions [63].

Given the fundamental role of general covariance and their associated constraint equations in the Einstein equations, it is natural to consider numerical methods that respect these geometric properties. Tensor product discretizations presuppose a slicing of spacetime, and constrain the allowable spacetime topologies, but the spacetime diffeomorphism symmetries do not leave slicings of spacetime invariant, so we will instead consider discretizations of general relativity that are based on *simplicial space-time meshes*.

The gauge symmetry implies that the Einstein–Hilbert action is degenerate, and we will adopt the approach of *multi-Dirac mechanics*, which is based on a Hamilton–Pontryagin variational principle for field theories that is well-adapted to degenerate field theories. The preservation of the conservation laws under discretization can be achieved by considering variational integrators that exhibit momentum conservation properties. It was demonstrated in [21] that variational integrators could be applied to numerical relativity without needing constraint damping. We propose to generalize discrete Dirac mechanics [40] and Hamiltonian variational integrators [42,60] to higher-order field theories, and combine these with group-equivariant spline approximation spaces [23] to construct geometric discretizations of general relativity. This will also serve to clarify the relationship between the covariant and instantaneous approaches.

3 Dirac Geometry and Mechanics

The Lagrangian densities for gauge field theories, such as electromagnetism, Yang-Mills, and general relativity, which are invariant under a gauge or local symmetry, are degenerate. While Lagrangian variational integrators can be constructed for degenerate Lagrangian systems, they can exhibit parasitic modes [20] as the continuous Euler–Lagrange equations degenerate from a second-order equation to a first-order one, and the primary constraint that the momentum is in the image of the Legendre transform needs to be enforced for the equations to be well-posed.

Traditionally, the construction of a well-posed formulation of a degenerate Lagrangian system is based on the geometric constraint algorithm of Gotay and Nester [26] in the context of the Dirac theory of constraints [18]. Intuitively, this involves finding a submanifold $P \subset TQ$ using an alternating projection method, such that (1) the Euler–Lagrange equations are consistent; (2) they define a vector field that is tangent to P. This was applied to geometric numerical integration in [47], but the construction, as in the continuous setting, is computationally involved and cumbersome.

An alternative approach is based on discrete Dirac mechanics which we developed in [40], and we will describe this below. In particular, the discrete analogue of the primary constraint arises naturally in the implicit discrete Euler–Lagrange equations that define the Dirac variational integrator, thereby allowing them to perform more robustly on degenerate problems.

3.1 Continuous Dirac Variational Mechanics

Dirac mechanics generalizes Lagrangian and Hamiltonian mechanics and can be described using either Dirac structures or the Hamilton–Pontryagin variational principle [64,65]. Dirac structures are the simultaneous generalization of symplectic and Poisson structures, and can encode Dirac constraints that arise in degenerate

Lagrangian systems, interconnected systems [37], and nonholonomic systems, and thereby provide a unified geometric framework for studying such problems.

Hamilton–Pontryagin Variational Principle

Consider a configuration manifold Q with associated tangent bundle TQ and phase space T^*Q. Dirac mechanics is described on the *Pontryagin bundle* $TQ \oplus T^*Q$, which has position, velocity and momentum (q, v, p) as local coordinates. The dynamics on the Pontryagin bundle is described by the *Hamilton–Pontryagin* variational principle,

$$\delta \int_{t_1}^{t_2} L(q, v) - p(\dot{q} - v)\mathrm{d}t = 0, \tag{2}$$

for variations δq that vanish at the endpoints, and where the Lagrange multiplier (and momentum) p imposes the second-order condition $v = \dot{q}$. It provides a variational description of both Lagrangian and Hamiltonian mechanics. Taking variations in q, v, and p, we obtain

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

where we used integration by parts, and the fact that the variation δq vanishes at the endpoints. This yields the *implicit Euler–Lagrange equations*,

$$\dot{q} = v, \qquad \dot{p} = \frac{\partial L}{\partial q}, \qquad p = \frac{\partial L}{\partial v}. \tag{3}$$

The last equation is the *Legendre transform* $\mathbb{F}L : (q, \dot{q}) \mapsto (q, \frac{\partial L}{\partial \dot{q}})$. A Lagrangian is *degenerate* if the Legendre transform is not onto. Explicitly imposing the Legendre transform in (3) is important for degenerate systems as it enforces the primary constraints and yields well-posed equations.

The implicit Euler–Lagrange flow is *symplectic*, i.e., it preserves the canonical symplectic structure Ω on T^*Q, the pullback symplectic structure $\Omega_L \equiv \mathbb{F}L^*\Omega$ on TQ, and the Dirac structure described below. Given a Lie group G acting on Q, there are *momentum maps* $\mathbf{J} : T^*Q \to \mathfrak{g}^*$ and $\mathbf{J}_L : TQ \to \mathfrak{g}^*$, that are defined by $\langle \mathbf{J}(\alpha_q), \xi \rangle \equiv \langle \alpha_q, \xi_Q(q) \rangle$ and $\langle \mathbf{J}_L(v_q), \xi \rangle \equiv \langle \mathbb{F}L(v_q), \xi_Q(q) \rangle$, where $\mathfrak{g}$ is the Lie algebra of G, and ξ_Q is the infinitesimal generator of $\xi \in \mathfrak{g}$. If the Lagrangian is invariant under the tangent lifted action of G, then *Noether's theorem* states that $\mathbf{J}$ and $\mathbf{J}_L$ are conserved.

Dirac Structures

The flows of the Euler–Lagrange equations are symplectic, and those of Hamilton's equations are Poisson. The geometric structure on $TQ \oplus T^*Q$ that is preserved by the

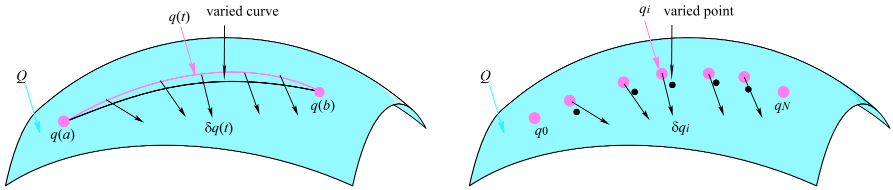


Fig. 2 A comparison of the continuous time and discrete time Hamilton's principles

Hamilton–Pontryagin flow is the *Dirac structure*, which is an n-dimensional subbundle $D \subset TM \oplus T^*M$, where $M = T^*Q$, that satisfies $\langle v_1, p_2\rangle + \langle v_2, p_1\rangle = 0$, for all $(q, v_1, p_1), (q, v_2, p_2) \in D$. An *integrable Dirac structure* has the additional property, $\langle \pounds_{X_1}\alpha_2, X_3\rangle + \langle \pounds_{X_2}\alpha_3, X_1\rangle + \langle \pounds_{X_3}\alpha_1, X_2\rangle = 0$, for all pairs of vector fields and one-forms $(X_1, \alpha_1), (X_2, \alpha_2), (X_3, \alpha_3) \in D$, where $\pounds_X$ is the Lie derivative. This generalizes the condition that the symplectic form is closed, or that the Poisson bracket satisfies Jacobi's identity. The graph of the symplectic form Ω and Poisson structure B, viewed as maps TM to T^*M, $v_q \mapsto \Omega(v_q, \cdot)$ and T^*M to TM, $\alpha_q \mapsto B(\alpha_q, \cdot)$, are Dirac structures. Then, the implicit Euler–Lagrange equations define a vector field X satisfying $(X, \mathfrak{D}L) \in D$, where $\mathfrak{D}$ is the Dirac differential [64], and Hamilton's equations are given by $(X, dH) \in D$. This also provides a natural setting for the generalized Legendre transform for degenerate systems [58].

3.2 Discrete Dirac Variational Mechanics

Geometric numerical integrators preserve geometric conservation laws. Discrete variational mechanics [40,45] involve a discretization of Hamilton's principle, where the continuous time trajectories are replaced by sampled trajectories in discrete time, as illustrated in Fig. 2. Then, the action integral is decomposed into integrals over each timestep, and this is approximated by the *discrete Lagrangian*, $L_d : Q \times Q \to \mathbb{R}$, which is a Type I generating function of a symplectic map and approximates the *exact discrete Lagrangian*,

$$L_d^E(q_0, q_1; h) \equiv \underset{\substack{q\in C^2([0,h],Q)\\ q(0)=q_0, q(h)=q_1}}{\mathrm{ext}} \int_0^h L(q(t), \dot{q}(t))\mathrm{d}t, \tag{4}$$

which is related to Jacobi's solution of the Hamilton–Jacobi equation. The exact discrete Lagrangian generates the exact discrete-time flow map of a Lagrangian system, but it cannot be computed explicitly. Instead, it can be approximated by the Ritz discrete Lagrangian (7).

We introduced the *discrete Hamilton–Pontryagin principle* on $(Q \times Q) \times_Q T^*Q$ in [40], which imposes the discrete second-order condition $q_k^1 = q_{k+1}^0$ using Lagrange multipliers p_{k+1},

$$\delta\left[\sum\nolimits_{k=0}^{n-1} L_d(q_k^0, q_k^1) + \sum\nolimits_{k=0}^{n-2} p_{k+1}(q_{k+1}^0 - q_k^1)\right] = 0. \tag{5}$$

This in turn yields the *implicit discrete Euler–Lagrange equations*,

$$q_k^1 = q_{k+1}^0, \qquad p_{k+1} = D_2 L_d(q_k^0, q_k^1), \qquad p_k = -D_1 L_d(q_k^0, q_k^1), \tag{6}$$

where D_i denotes the partial derivative with respect to the i-th argument. Making the identification $q_k = q_k^0 = q_{k-1}^1$, the last two equations define the *discrete fiber derivatives*, $\mathbb{F}L_d^{\pm} : Q \times Q \to T^*Q$,

$$\begin{aligned} \mathbb{F}L_d^{+}(q_k, q_{k+1}) &\equiv (q_{k+1}, D_2 L_d(q_k, q_{k+1})), \\ \mathbb{F}L_d^{-}(q_k, q_{k+1}) &\equiv (q_k, -D_1 L_d(q_k, q_{k+1})), \end{aligned}$$

which are the discrete analogues of the Legendre transform. These yield the *discrete Lagrangian map* $F_{L_d} \equiv (\mathbb{F}L_d^-)^{-1} \circ \mathbb{F}L_d^+ : (q_{k-1}, q_k) \mapsto (q_k, q_{k+1})$ and the *discrete Hamiltonian map* $\tilde{F}_{L_d} \equiv \mathbb{F}L_d^+ \circ (\mathbb{F}L_d^-)^{-1} : (q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$, which can be summarized by the following commutative diagram,

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

The approximation error of these discrete flow maps can be related to the approximation error of the discrete Lagrangian. Furthermore, the discrete fiber derivatives induce a *discrete symplectic form*, $\Omega_{L_d} \equiv (\mathbb{F}L_d^{\pm})^* \Omega$, and the discrete Lagrangian and Hamiltonian maps preserve Ω_{L_d} and Ω, respectively. In addition, it exhibits a discrete analogue of Noether's theorem, that relates symmetries of the discrete Lagrangian with momentum-preserving properties of the associated variational integrator.

Variational Error Analysis and Discrete Noether's Theorem

The variational integrator approach simplifies the numerical analysis of symplectic integrators by reducing the problem of establishing geometric conservation properties and order of accuracy of the discrete flow maps F_{L_d} and $\tilde{F}_{L_d}$ to the simpler task of verifying certain properties of the discrete Lagrangian L_d instead.

Theorem 1 [Discrete Noether's theorem (Theorem 1.3.3 of [45])] *If a discrete Lagrangian L_d is invariant under the diagonal action of G on $Q \times Q$, then the discrete momentum map, $\boldsymbol{J}_{L_d} = (\mathbb{F}L_d^{\pm})^* \boldsymbol{J}$, is invariant under the discrete Lagrangian map F_{L_d}, i.e., $F_{L_d}^* \boldsymbol{J}_{L_d} = \boldsymbol{J}_{L_d}$.*

Theorem 2 [Variational error analysis (Theorem 2.3.1 of [45])] *If a discrete Lagrangian L_d approximates the exact discrete Lagrangian L_d^E to order p, i.e., $L_d(q_0, q_1; h) = L_d^E(q_0, q_1; h) + \mathcal{O}(h^{p+1})$, then the discrete Hamiltonian map $\tilde{F}_{L_d}$ is an order p accurate one-step method.*

Discrete Dirac Structures

Discrete Dirac mechanics can also be described in terms of discrete Dirac structures [39,40]. An *implicit discrete Lagrangian system* satisfies $\left(X_d^k, \mathfrak{D}^+ L_d(q_k^0, q_k^1)\right) \in D_{\Delta_Q}^{\mathrm{d}+}$, where $\mathfrak{D}^+$ is the discrete Dirac differential, and the discrete Dirac structure $D_{\Delta_Q}^{\mathrm{d}+}$ is

$$
\begin{aligned}
&D_{\Delta_Q}^{\mathrm{d}+} \\
&\equiv \left\{((z, z'), \alpha_{\tilde{z}}) \in (T^*Q \times T^*Q) \times T^*(Q \times Q^*) \mid \left(z, z'\right) \in \Delta_{T^*Q}^{\mathrm{d}+}, \alpha_{\tilde{z}} - \Omega_{\mathrm{d}+}^{\flat}\left((z, z')\right) \in \Delta_{Q \times Q^*}^{\circ}\right\}.
\end{aligned}
$$

Here, $\Delta_{T^*Q}^{\mathrm{d}+} \subset Q \times Q$ is a discrete constraint distribution that is obtained from a continuous constraint distribution $\Delta_Q \subset TQ$ and a retraction $\mathcal{R} : TQ \to Q$, and $\Delta_{Q\times Q^*}^{\circ} \subset T^*(Q \times Q^*)$ is a discrete annihilator distribution that is the pullback of the continuous annihilator distribution $\Delta_Q^{\circ} \subset T^*Q$ by the projection $\pi_Q^{\mathrm{d}+} : Q \times Q^* \to Q$. Alternatively, an *implicit discrete Hamiltonian system* satisfies $(X_d^k, dH_{d+}(q_k, p_{k+1})) \in D_{\Delta_Q}^{\mathrm{d}+}$.

3.3 Ritz Variational Integrators

A computable discrete Lagrangian can be obtained from the variational characterization of the exact discrete Lagrangian (4) by replacing the integral with a quadrature formula $\mathcal{G} : C^2([0, h], Q) \to \mathbb{R}, \mathcal{G}(f) = h \sum_{j=1}^m b_j f(c_j h) \approx \int_0^h f(t)\mathrm{d}t$, and replacing the space of C^2 curves with a finite-dimensional function space $\mathbb{M}^n([0, h]) \subset C^2([0, h], Q)$. This yields the *Ritz discrete Lagrangian*,

$$
\begin{aligned}
L_d(q_0, q_1) &\equiv \operatorname*{ext}_{\substack{q \in \mathbb{M}^n([0,h]) \\ q(0)=q_0, q(h)=q_1}} \mathcal{G}(L(q, \dot{q})) \\
&= \operatorname*{ext}_{\substack{q \in \mathbb{M}^n([0,h]) \\ q(0)=q_0, q(h)=q_1}} h \sum_{j=1}^m b_j L(q(c_j h), \dot{q}(c_j h)). \qquad (7)
\end{aligned}
$$

While Theorem 2 relates the order of accuracy of the variational integrator with the order of accuracy of the discrete Lagrangian, it does not relate the order of accuracy of the discrete Lagrangian with the approximation properties of the finite-dimensional function space $\mathbb{M}^n$. Ideally, the approximation error in the Ritz discrete Lagrangian should be bounded by a constant multiple of the best approximation error in approximating the exact solution q of the Euler–Lagrange boundary-value problem with an element of the finite-dimensional function space $\mathbb{M}^n$, i.e.,

$$\|L_d(q_0, q_1; h) - L_d^E(q_0, q_1; h)\| \leq c \inf_{\tilde{q}\in\mathbb{M}^n([0,h])} \|q - \tilde{q}\|.$$

In such an instance, we say that the Ritz method is *order-optimal*.

Given a nested sequence of approximation spaces $\mathbb{M}^1 \subset \mathbb{M}^2 \subset \ldots \subset \mathbb{M}^\infty \equiv C^2([0, h], Q)$, and a correspondingly accurate sequence of quadrature formulas, we obtain a sequence of Ritz discrete Lagrangians,

$$L_d^n(q_0, q_1) = \operatorname*{ext}_{q\in\mathbb{M}^n} h \sum\nolimits_{j=1}^{s_n} b_j^n L(q(c_j^n h), \dot{q}(c_j^n h)),$$

which arise as extremizers of a sequence of variational problems. Showing that this sequence converges to the exact discrete Lagrangian, which is the extremizer of the limiting variational problem, corresponds to proving Γ-convergence [15]. To establish order-optimality, we need to relate the rate of Γ-convergence with the best approximation properties of the sequence of approximation spaces.

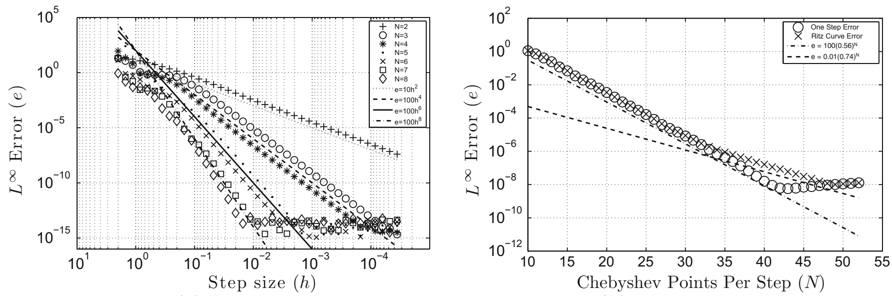
In [31], we proved an order-optimality result by carefully refining the proof of Γ-convergence of variational integrators that was presented in [48]. This relied on similar technical assumptions: (1) regularity of L in a closed and bounded neighborhood; (2) the quadrature rule is sufficiently accurate; (3) the discrete and continuous trajectories *minimize* their actions. The critical assumption is action minimization, and for Lagrangians of the form, $L = \dot{q}^T M\dot{q} - V(q)$, and sufficiently small h, this assumption holds, which yield the following results.

Theorem 3 [Order-optimality of Ritz variational integrators (Theorem 3.3 of [31])] *Given a Lagrangian of the form, $L(q, \dot{q}) = \dot{q}^T M\dot{q} - V(q)$, an $\mathcal{O}(h^{n+1})$ quadrature formula $\mathcal{G}_n$, a finite-dimensional function space $\mathbb{M}^n$ with best approximation error in position and velocity of $\mathcal{O}(h^n)$, and a sufficiently small timestep h, the Ritz discrete Lagrangian approximates L_d^E to $\mathcal{O}(h^{n+1})$.*

Theorem 4 [Geometric convergence of Spectral variational integrators (Theorem 3.4 of [31])] *Given a Lagrangian of the form, $L(q, \dot{q}) = \dot{q}^T M\dot{q} - V(q)$, $\mathcal{O}(K_1^{-n})$ quadrature formulas $\mathcal{G}_n$, function spaces $\mathbb{M}^n$ with best approximation error in position and velocity of $\mathcal{O}(K_2^{-n})$, and a sufficiently small timestep h, the Spectral discrete Lagrangian approximates L_d^E to $\mathcal{O}(K^{-n})$, where $K = \min(K_1, K_2)$.*

Figure 3 provides numerical evidence that Ritz and spectral variational integrators exhibit the theoretical rates of convergence established in Theorems 3 and 4. Figure 4 demonstrates that by using spectral variational integrators constructed using sufficiently high-degree Chebyshev polynomials, it is possible to obtain stable and qualitatively accurate simulations of orbital trajectories of the solar system, even when taking timesteps that exceed the smallest orbital periods in the problem. Figure 5 illustrates that variational integrators exhibit superior error properties, even when compared to time-adaptive methods with tight tolerances.

By the discrete Noether's theorem (Theorem 1), a G-invariant discrete Lagrangian generates a momentum-preserving variational integrator. A G-invariant Ritz discrete Lagrangian can be constructed from a G-equivariant interpolant $\varphi : Q^s \to$



(a) Order-optimality **(b)** Geometric convergence

Fig. 3 The convergence rate of Ritz variational integrators is related to the best approximation error of the approximation spaces used. Spectral variational integrators based on Chebyshev polynomials converge geometrically

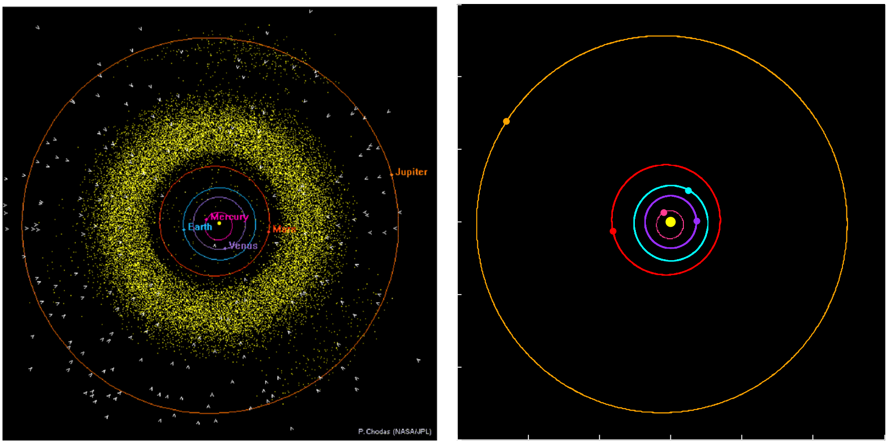
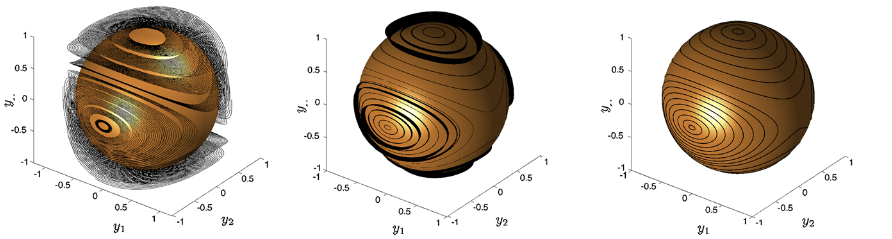


Fig. 4 The spectral variational integrator agrees qualitatively with simulations of the inner solar system from the JPL Solar System Dynamics Group using the full ephemeris, even with timesteps ($h = 100$ days) exceeding the 88-day orbital period of Mercury



(a) Euler Method **(b)** MATLAB RK45 **(c)** Lie group variational integrator

Fig. 5 Free rigid body, with the norm of the body angular momentum, $\sqrt{\Pi_1^2 + \Pi_2^2 + \Pi_3^2}$, and the energy, $\frac{1}{2}\left(\frac{\Pi_1^2}{I_1} + \frac{\Pi_2^2}{I_2} + \frac{\Pi_3^2}{I_3}\right)$, as invariants. The exact solutions lie on the intersection of the angular momentum sphere and the energy ellipsoid. This demonstrates that Lie group variational integrators exhibit excellent preservation of the invariants, even compared to adaptive numerical methods, such as RK45 in MATLAB with extremely tight tolerances

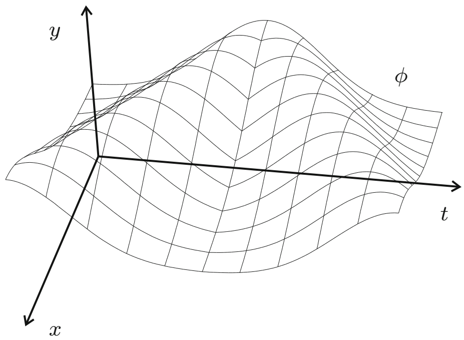


Fig. 6 A section of the configuration bundle: the horizontal axes represent spacetime, and the vertical axis represent dependent field variables. The section ϕ gives the value of the field variables at every point of spacetime

$C^1([0,1],Q)$, i.e., $\varphi(\{gq^\nu\};t) = g\cdot\varphi(\{q^\nu\};t)$. This means that the interpolant transforms in the same way as the data under the group action.

Theorem 5 [G-invariant Ritz discrete Lagrangian (Proposition 1 of [41])] *A G-equivariant interpolant and a G-invariant Lagrangian yields a G-invariant Ritz discrete Lagrangian.*

3.4 Multi-Dirac Field Theories

Multisymplectic Geometry

The geometric setting for Lagrangian PDEs is multisymplectic geometry [43,44]. The *base space* X consists of independent variables, denoted by $(x^0,\ldots,x^n)\equiv(t,x)$, where $x^0\equiv t$ is time, and $(x^1,\ldots,x^n)\equiv x$ are space variables. The dependent field variables, $(y^1,\ldots,y^m)\equiv y$, form a fiber over each spacetime basepoint, and the resulting fiber bundle is the *configuration bundle*, $\rho: Y\to X$. The configuration of the system is specified by a section of Y over X (see Fig. 6), which is a continuous map $\phi: X\to Y$, such that $\rho\circ\phi = 1_X$, i.e., for every $(t,x)\in X$, $\phi((t,x))$ is in the fiber $\rho^{-1}((t,x))$ over (t,x).

The multisymplectic analogue of the tangent bundle is the *first jet bundle* J^1Y, which is a fiber bundle over X that consists of the configuration bundle Y and the first partial derivatives $v^a_\mu = \partial y^a/\partial x^\mu$ of the field variables with respect to the independent variables. Given a section $\phi: X\to Y$, $\phi(x^0,\ldots,x^n) = (x^0,\ldots x^n, y^1,\ldots y^m)$, its *first-jet extension* $j^1\phi: X\to J^1Y$ is a section of J^1Y over X given by

$$j^1\phi(x^0,\ldots,x^n) = \left(x^0,\ldots,x^n,y^1,\ldots,y^m,{y^1}_{,0},\ldots,{y^m}_{,n}\right).$$

The *dual-jet bundle* $J^1Y^\star$ is affine, with fiber coordinates (p,p^μ_a), corresponding to the affine map $v^a_\mu\mapsto(p+p^\mu_a v^a_\mu)d^{n+1}x$, where $d^{n+1}x = dx^1\wedge\cdots\wedge dx^n\wedge dx^0$.

Hamilton–Pontryagin Principle for Field Theories

The first-order Lagrangian density is a map $\mathcal{L} : J^1Y \to \bigwedge^{n+1}(X)$. Let $\mathcal{L}(j^1\phi) = L(j^1\phi)\, d^{n+1}x = L(x^\mu, y^a, v^a_\mu)\, d^{n+1}x$, where $L(j^1\phi)$ is a scalar function on J^1Y. For field theories, the analogue of the Pontryagin bundle is $J^1Y \times_Y J^1Y^\star$, and the first-jet condition $\frac{\partial y^a}{\partial x^\mu} = v^a_\mu$ replaces $v = \dot{q}$, so the *Hamilton–Pontryagin principle* is

$$\delta S(y^a, y^a_\mu, p^\mu_a) = \delta \int_U \left[p^\mu_a \left(\frac{\partial y^a}{\partial x^\mu} - v^a_\mu \right) + L(x^\mu, y^a, v^a_\mu) \right] d^{n+1}x = 0. \tag{8}$$

Taking variations with respect to y^a, v^a_μ and p^μ_a yield the *implicit Euler–Lagrange equations*,

$$\frac{\partial p^\mu_a}{\partial x^\mu} = \frac{\partial L}{\partial y^a}, \quad p^\mu_a = \frac{\partial L}{\partial v^a_\mu}, \quad \text{and} \quad \frac{\partial y^a}{\partial x^\mu} = v^a_\mu, \tag{9}$$

which generalizes (3) to the case of field theories. We developed an intrinsic version of this variational principle in [62], using the geometry of the first-jet bundle and its dual as the starting point. As the dual-jet bundle is affine, the duality pairing used implicitly in (8) is more complicated.

The second equation of (9) yields the *covariant Legendre transform*, $\mathbb{F}\mathcal{L} : J^1Y \to J^1Y^\star$,

$$p^\mu_a = \frac{\partial L}{\partial v^a_\mu}, \qquad p = L - \frac{\partial L}{\partial v^a_\mu} v^a_\mu. \tag{10}$$

This combines the definitions of the momenta and the Hamiltonian into a single covariant entity.

Multi-Dirac Structures

Analogous to the canonical symplectic form on T^*Q is the canonical multisymplectic $(n+2)$-form Ω on $J^1Y^\star$, which is given in coordinates by

$$\Omega = dy^a \wedge dp^\mu_a \wedge d^n x_\mu - dp \wedge d^{n+1}x,$$

where $d^n x_\mu = \partial_\mu \lrcorner\, d^{n+1}x$, and $\lrcorner$ denotes contraction. This naturally leads to the analogue of symplecticity in a multisymplectic field theory, which is the *multisymplectic form formula*,

$$d^2\mathcal{S}(\phi)(V, W) = \int_{\partial U} (j^1\phi)^*(j^1V \lrcorner\, j^1W \lrcorner\, \Omega_L) = 0, \tag{11}$$

for all first variations V, W, where $\Omega_L = \mathbb{F}\mathcal{L}^*\Omega$. The proof of the multisymplectic form formula is analogous to the intrinsic proof of symplecticity, where one evaluates the second exterior derivative of the action integral restricted to solutions of the Euler–Lagrange equation (see [43]).

Just as the graph of a symplectic form is a Dirac structure, the graph of a multi-symplectic $(n+2)$-form Ω on a manifold M is a multi-Dirac structure, which we introduced in [61]. Consider the map from an l-multivector field $\mathcal{X}_l$ to its contraction with Ω:

$$\mathcal{X}_l \in \bigwedge^l (TM) \mapsto \mathcal{X}_l \lrcorner \Omega \in \bigwedge^{n+2-l} (T^*M), \qquad 1 \leq l \leq n+1.$$

The graph of this mapping is a subbundle D_l of $\bigwedge^l (TM) \times_M \bigwedge^{n+2-l} (T^*M)$. The direct sum of all such subbundles, $D = D_1 \oplus \cdots \oplus D_{n+1}$, is a *multi-Dirac structure* which is maximally isotropic under a graded antisymmetric version of the standard Dirac pairing. Thus, multi-Dirac structures are graded versions of standard Dirac structures. The implicit Euler–Lagrange equations (9) can be written as

$$(\mathcal{X}, (-1)^{n+2} dE) \in D_{n+1}, \tag{12}$$

where D_{n+1} is the graph of the multisymplectic form Ω, and $E = p + p^\mu_A v^A_\mu - L(x^\mu, y^A, v^A_\mu)$ is the generalized energy. In general, a *Lagrange–Dirac field theory* is a triple $(\mathcal{X}, E, D_{n+1})$ satisfying (12), where D_{n+1} belongs to a multi-Dirac structure D.

3.5 The Boundary Lagrangian and Generating Functionals of Lagrangian PDEs

Recall that the exact discrete Lagrangian is a scalar function that depends on the boundary-values at the initial and final time,

$$L_d^{\text{exact}}(q_0, q_1) \equiv \int_0^h L\left(q_{0,1}(t), \dot{q}_{0,1}(t)\right) \mathrm{d}t,$$

and yields the action along a solution of the Euler–Lagrange boundary-value problem. By analogy, we will introduce the boundary Lagrangian, which is a functional on the space of boundary data.

The Space of Boundary Data $\mathcal{Y}_{\partial U}$

Let $U \subset X$ be open with boundary ∂U. We want to prescribe boundary data along ∂U with values in Y, the total space of the configuration bundle $\rho : Y \to X$. Note that ∂U does not have to be a Cauchy surface, or even be spacelike. All the definitions below are metric independent and apply to hyperbolic and elliptic problems alike. An *element of boundary data* on U is a section $\varphi : \partial U \to Y$ of ρ, defined on ∂U. We denote by $\mathcal{Y}_{\partial U}$ the space of all boundary data. Often, there are constraints on the boundary data that depend on the type of PDE and the geometry of U. For example, in a hyperbolic PDE, since solutions are constant along characteristics, the admissible boundary data are constrained if ∂U contains a characteristic. We refer to $\mathcal{K}_{\partial U} \subset \mathcal{Y}_{\partial U}$ as the space of *admissible boundary data*.

The Boundary Lagrangian $L_{\partial U}$

To distinguish between boundary data on ∂U and fields defined on the interior of U, we denote the former by $\varphi \in \mathcal{K}_{\partial U} \subset \mathcal{Y}_{\partial U}$, and the latter by ϕ. The *boundary Lagrangian* $L_{\partial U}$ is the functional on the space of admissible boundary data $\mathcal{K}_{\partial U} \subset \mathcal{Y}_{\partial U}$ that is given by

$$L_{\partial U}(\varphi) = \operatorname*{ext}_{\phi|_{\partial U}=\varphi} \int_U \mathcal{L}(j^1\phi),$$

where we extremized the action functional over all sections ϕ that satisfy the boundary conditions. The boundary Lagrangian is a generating functional: if the boundary data are unrestricted, the image of $\mathbf{d}L_{\partial U}$ is a Lagrangian submanifold of $T^*\mathcal{Y}_{\partial U}$; otherwise, $\mathbf{d}L_{\partial U}(\mathcal{K}_{\partial U})$ is an isotropic submanifold.

Functional Derivatives and Normal Momentum

We now describe how $L_{\partial U}$ generates a multisymplectic relation. A generating function S_1 defines a symplectic map $(q_0, p_0) \mapsto (q_1, p_1)$ by

$$p_0 = -\frac{\partial S_1}{\partial q_0}(q_0, q_1), \qquad p_1 = \frac{\partial S_1}{\partial q_1}(q_0, q_1). \tag{13}$$

This relates the boundary momentum to the variation of the generating function S_1 with respect to the boundary data. Symplecticity follows as a trivial consequence of these equations, together with $\mathbf{d}^2 = 0$, as the following calculation shows,

$$\begin{aligned} 0 = \mathbf{d}^2 S_1(q_0, q_1) &= \mathbf{d}\left(\frac{\partial S_1}{\partial q_0}(q_0, q_1)dq_0 + \frac{\partial S_1}{\partial q_1}(q_0, q_1)dq_1\right) \\ &= \mathbf{d}(-p_0 dq_0 + p_1 dq_1) = -dp_0 \wedge dq_0 + dp_1 \wedge dq_1. \end{aligned}$$

We consider the functional derivative $\delta L_{\partial U}/\delta\varphi$, which is the unique element of $T^*\mathcal{Y}_{\partial U}$ such that

$$\mathbf{d}L_{\partial U}(\varphi) \cdot \delta\varphi = \int_{\partial U} \frac{\delta L_{\partial U}}{\delta\varphi} \cdot \delta\varphi,$$

for every variation $\delta\varphi \in T\mathcal{Y}_{\partial U}$. When a Riemannian or Lorentzian metric on X is given, we obtain

$$\pi = \frac{\delta L_{\partial U}}{\delta\varphi} = \frac{\partial L}{\partial v^a_\mu} n_\mu dy^a \otimes dS, \tag{14}$$

where n^μ is the outward normal to ∂U, dS is the induced metric volume form on ∂U, and indices are raised/lowered using the metric. In components, $\pi_a = p_a^\mu n_\mu$, i.e., π_a is the normal component of the covariant momentum p_a^μ, and so we refer to $\pi \in T^*\mathcal{Y}_{\partial U}$ as the *normal momentum* to the boundary ∂U. The multisymplectic generalization of (13) is that (14) holds for every point on ∂U. Furthermore, as shown in Section IV.D of [60], evaluating $\mathbf{d}^2 L_{\partial U}$ yields the *multisymplectic form formula* (11).

Hamiltonian Variational Integrators

Given a degenerate Hamiltonian, there is no equivalent Lagrangian formulation. Thus, a characterization of variational integrators directly in terms of the continuous Hamiltonian is desirable. This was addressed in [42] by considering the Type II analogue of Jacobi's solution, given by

$$H_d^{+,E}(q_k, p_{k+1}) = \underset{\substack{(q,p)\in C^2([t_k,t_{k+1}],T^*Q)\\ q(t_k)=q_k,\, p(t_{k+1})=p_{k+1}}}{\operatorname{ext}} p(t_{k+1})q(t_{k+1}) - \int_{t_k}^{t_{k+1}} [p\dot{q} - H(q,p)]\,\mathrm{d}t.$$

A computable Ritz discrete Hamiltonian H_d^+ is obtained by choosing a finite-dimensional function space and a quadrature formula. Then, the *discrete Hamilton's equations* are given by

$$q_{k+1} = D_2 H_d^+(q_k, p_{k+1}), \qquad p_k = D_1 H_d^+(q_k, p_{k+1}). \tag{15}$$

Type II Generating Functional and Boundary Hamiltonian

The initial-value formulation of a gauge field theory involves constructing an instantaneous Hamiltonian with respect to a slicing of spacetime. To understand the connection between the instantaneous and covariant approaches, we will construct a discrete covariant Hamiltonian formulation by discretizing the *boundary Hamiltonian*, which is the exact Type II generating functional

$$H_{\partial U}(\varphi_A, \pi_B) = \underset{\substack{\phi_{|A}=\varphi_A,\\ \pi_{|B}=\pi_B}}{\operatorname{ext}} \int_B p_a^\mu \phi^a\, d^n x_\mu - \int_U (p_a^\mu \phi^a_{,\mu} - H(\phi^a, p_a^\mu))\, d^{n+1}x, \tag{16}$$

where the fields are specified on $A \subset \partial U$, and the normal momenta are specified on the complement $B = \partial U \setminus A$. The associated variational derivatives, which generalize (15), are given by

$$\frac{\delta H_{\partial U}}{\delta \varphi_A} = -\pi_{|A}, \quad \text{and} \quad \frac{\delta H_{\partial U}}{\delta \pi_B} = \phi_{|B}.$$

4 Group-Equivariant Interpolation on Symmetric Spaces

4.1 Interpolation on Symmetric Spaces

In order to construct momentum-preserving variational integrators for field theories with symmetries, it is necessary to construct finite element spaces that are group-equivariant. Motivated by the application to general relativity, we developed group-equivariant approximation spaces taking values in symmetric spaces, and in particular, the space of Lorentzian metrics.

A Riemannian symmetric space inherits a well-defined Riemannian structure, which allows one to apply *geodesic finite elements* [27,53,54] to construct group-equivariant approximation spaces. Given a Riemannian manifold (M, g), the geodesic finite element $\varphi : \Delta^n \to M$ associated with a set of linear space finite elements $\{v_i : \Delta^n \to \mathbb{R}\}_{i=0}^n$, and manifold-valued data m_i at the nodes, is given by the Fréchet (or Karcher) mean,

$$\varphi(x) = \arg\min_{p \in M} \sum\nolimits_{i=0}^{n} v_i(x)(\operatorname{dist}(p, m_i))^2,$$

which is computable using algorithms for optimization on manifolds [6], and the derivatives can be expressed in terms of an associated optimization problem [55]. Geodesic finite elements inherit the approximation properties of the underlying linear space finite element [28], but they are expensive to compute. We proposed a novel alternative based on the generalized polar decomposition that reduces to geodesic finite elements in some cases, and can be efficiently computed using iterative methods.

4.2 Interpolation via the Generalized Polar Decomposition

In [23], we introduced an efficiently computable group-equivariant interpolation method for functions taking values in symmetric spaces through an application of the generalized polar decomposition. This relies on a correspondence between symmetric spaces and Lie triple systems [33,49,50].

Let G be a Lie group and let $\sigma : G \to G$ be an involutive automorphism, i.e., a non-identity group homomorphism such that $\sigma^2 = 1_G$. Let $G^\sigma = \{g \in G \mid \sigma(g) = g\}$ be the subgroup of fixed points of σ. Suppose that G acts transitively on a smooth manifold $\mathcal{S}$ with a distinguished element $\eta \in \mathcal{S}$ whose stabilizer coincides with G^σ, i.e., $g \cdot \eta = \eta$ if and only if $\sigma(g) = g$. Then, there is a bijection between the homogeneous space G/G^σ and $\mathcal{S}$. But, the cosets in G/G^σ have canonical representatives, since the *generalized polar decomposition* [49,50] yields, for any near to identity $g \in G$,

$$g = pk, \quad p \in G_\sigma,\ k \in G^\sigma, \tag{17}$$

where $G_\sigma = \{g \in G \mid \sigma(g) = g^{-1}\}$. This decomposition is locally unique [49, Theorem 3.1], and there is a bijection between a neighborhood of the identity $e \in G_\sigma$ and a neighborhood of the coset $[e] \in G/G^\sigma$. The space G_σ is not a subgroup but is a symmetric space, which is closed under a non-associative symmetric product

$g \cdot h = gh^{-1}g$. Its tangent space at the identity is the space

$$\mathfrak{p} = \{Z \in \mathfrak{g} \mid d\sigma(Z) = -Z\},$$

where $\mathfrak{g}$ is the Lie algebra of G. Since G_σ is not a subgroup of G, $\mathfrak{p}$ is not a subalgebra of $\mathfrak{g}$. Rather, it is a *Lie triple system*, which is a vector space closed under the double commutator $[\cdot, [\cdot, \cdot]]$. The Lie algebra of $G^\sigma \leq G$ is $\mathfrak{k} = \{Z \in \mathfrak{g} \mid d\sigma(Z) = Z\}$, which is a subalgebra of $\mathfrak{g}$. The generalized polar decomposition (17) has a manifestation at the Lie algebra level called the *Cartan decomposition*,

$$\mathfrak{g} = \mathfrak{p} \oplus \mathfrak{k}. \tag{18}$$

All of these observations lead to the conclusion that the following diagram commutes:

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

where ι denotes the canonical inclusion, $\pi : G \to G/G^\sigma$ is the canonical projection, and $\varphi : G \to \mathcal{S}$ is the map $\varphi(g) = g \cdot \eta$. The maps ψ and $\bar{\varphi}$ are defined by commutativity of the diagram. Critically, the maps along its bottom row are local diffeomorphisms [33] in neighborhoods of the neutral elements $0 \in \mathfrak{p}$, $e \in G_\sigma$, $[e] \in G/G^\sigma$, and the distinguished element $\eta \in \mathcal{S}$. In particular,

$$F = \bar{\varphi} \circ \psi \circ \exp \tag{19}$$

provides a diffeomorphism from a neighborhood of $0 \in \mathfrak{p}$ to a neighborhood of $\eta \in \mathcal{S}$, given by $F(P) = \exp(P) \cdot \eta$ for $P \in \mathfrak{p}$. Since $\mathfrak{p}$ is a vector space, it is a more convenient space than $\mathcal{S}$ to perform averaging, interpolation, extrapolation, and the numerical solution of differential equations.

Given a smooth function $u : \Omega \to \mathcal{S}$, our goal is to construct a function $\mathcal{I}u : \Omega \to \mathcal{S}$ that satisfies $\mathcal{I}u(x^{(i)}) = u(x^{(i)}) \equiv u_i$, $i = 1, \ldots, m$, and has a desired level of regularity. Assume that for each $x \in \Omega$, $u(x)$ belongs to the range of the map (19). We may then interpolate $u_1, \ldots, u_m \in \mathcal{S}$ by interpolating $F^{-1}(u_1), \ldots, F^{-1}(u_m) \in \mathfrak{p}$ and mapping the result back to $\mathcal{S}$ via F. More precisely, let $\mathcal{I}u(x) = F(\hat{\mathcal{I}}P(x))$, where $P(x) = F^{-1}(u(x))$ and $\hat{\mathcal{I}}P : \Omega \to \mathfrak{p}$ is an interpolant of $F^{-1}(u_1), \ldots, F^{-1}(u_m)$. Then, $\mathcal{I}u$ is an interpolant that satisfies the following important property:

Proposition 1 (Proposition 3.1 of [23]) *Suppose that $\hat{\mathcal{I}}$ commutes with Ad_g for every $g \in G^\sigma$, i.e., $\hat{\mathcal{I}}(gPg^{-1})(x) = g\hat{\mathcal{I}}P(x)g^{-1}$ for every $x \in \Omega$ and every $g \in G^\sigma$. Then $\mathcal{I}$ is G^σ-equivariant, i.e., $\mathcal{I}(g \cdot u)(x) = g \cdot \mathcal{I}u(x)$ for every $x \in \Omega$ and every $g \in G^\sigma$ sufficiently close to the identity.*

This applies to any interpolant of the form $\hat{\mathcal{I}}P(x) = \sum_{i=1}^m \phi_i(x)P(x^{(i)})$, with scalar-valued shape functions $\phi_i : \Omega \to \mathbb{R}, i = 1, 2, \ldots, m$, satisfying $\phi_i(x^{(j)}) = \delta_{ij}$. By the proposition above, such an interpolant gives rise to a G^σ-equivariant interpolant $\mathcal{I}u : \Omega \to \mathcal{S}$, given by,

$$\mathcal{I}u(x) = F\left(\sum_{i=1}^m \phi_i(x)F^{-1}(u_i)\right). \tag{20}$$

More explicitly, $\mathcal{I}u(x) = \exp(P(x))\cdot\eta$, where $P(x) = \sum_{i=1}^m \phi_i(x)F^{-1}(u_i)$. This can be generalized by replacing $\exp : \mathfrak{p} \to G_\sigma$ in (19) with another local diffeomorphism, such as $P \mapsto \psi^{-1}([\bar{g}\exp(P)])$, for a fixed $\bar{g} \in G$, which yields $p \in G_\sigma$ in the generalized polar decomposition $\bar{g}\exp(P) = pk$. This gives,

$$F_{\bar{g}}(P) = \bar{g}\exp(P)\cdot\eta, \tag{21}$$

which is a diffeomorphism between a neighborhood of $0 \in \mathfrak{p}$ and a neighborhood of $\bar{g}\cdot\eta \in \mathcal{S}$. When $\bar{g} = e$, this reduces to (19). By adopting the map (21), we obtain interpolation schemes of the form

$$\mathcal{I}_{\bar{g}}u(x) = F_{\bar{g}}\left(\sum_{i=1}^m \phi_i(x)F_{\bar{g}}^{-1}(u_i)\right) = \bar{g}\exp\left(\sum_{i=1}^m \phi_i(x)F_{\bar{g}}^{-1}(u_i)\right)\cdot\eta. \tag{22}$$

There is no canonical choice for $\bar{g}$, but an interesting option is to define $\bar{g}(x)$ implicitly via

$$\bar{g}(x)\cdot\eta = \mathcal{I}_{\bar{g}(x)}u(x). \tag{23}$$

In the case that G^σ is compact, we showed in [23, Lemma 3.3] that the generalized construction is equivalent to geodesic finite elements on G/G^σ, as described in [27, 28,53–55].

In addition to the interpolant being efficiently computable, arbitrarily high-order derivatives can also be efficiently computed,

$$\frac{\partial\mathcal{I}u}{\partial x_j}(x) = \mathrm{dexp}_{P(x)}\frac{\partial P}{\partial x_j}(x)\cdot\eta, \tag{24}$$

where $\frac{\partial P}{\partial x_j}(x) = \sum_{i=1}^m \frac{\partial\phi_i}{\partial x_j}(x)F^{-1}(u_i)$, $\mathrm{dexp}_X Y = \exp(X)\sum_{k=0}^\infty \frac{(-1)^k}{(k+1)!}\mathrm{ad}_X^k Y$, and $\mathrm{ad}_X Y = [X, Y]$ denotes the adjoint action of $\mathfrak{g}$ on itself. In practice, one truncates this series to approximate $\mathrm{dexp}_X Y$. While the exact value of $\mathrm{dexp}_X Y$ belongs to $\mathfrak{p}$ whenever $X, Y \in \mathfrak{p}$, the truncated approximation may contain spurious $\mathfrak{k}$-components, but these are inconsequential as they act trivially on η in (24).

Table 1 Approximation error of generalized polar decomposition-based Lorentzian metric-valued interpolant for the Schwarzschild metric, which is an exact solution of the Einstein equations

N	L^2-error	Order	H^1-error	Order
Linear shape functions				
2	3.3×10^{-3}		2.8×10^{-2}	
4	8.4×10^{-4}	1.975	1.4×10^{-2}	0.998
8	2.1×10^{-4}	1.994	7.1×10^{-3}	0.999
16	5.3×10^{-5}	1.998	3.6×10^{-3}	1.000
Quadratic shape functions				
2	1.7×10^{-4}		2.5×10^{-3}	
4	2.2×10^{-5}	3.001	6.2×10^{-4}	1.993
8	2.7×10^{-6}	3.000	1.6×10^{-4}	1.998
16	3.4×10^{-7}	3.000	3.9×10^{-5}	1.999

When G is a matrix group, $\mathrm{dexp}_X Y$ can be more efficiently computed using the identity [34,46]

$$\exp\begin{pmatrix} X & Y \\ 0 & X \end{pmatrix} = \begin{pmatrix} \exp(X) & \mathrm{dexp}_X Y \\ 0 & \exp(X) \end{pmatrix}. \tag{25}$$

More sophisticated approaches with better numerical properties can be found in [7,34]. This approach can be generalized to higher-order derivatives as well.

4.3 Numerical Simulations

It is established in Proposition 3.4 of [23] that the error in $\mathcal{I}u$ is controlled pointwise by the error in $\hat{\mathcal{I}}P$, and the error in $D\mathcal{I}u$ is controlled pointwise by the error in $D\hat{\mathcal{I}}P$. To verify this numerically, we realize Lorentzian metrics as a symmetric space $GL_4(\mathbb{R})/O_{1,3}$, where $GL_4(\mathbb{R})$ acts by $A \cdot L = ALA^T$, and the involution $\sigma : GL_4(\mathbb{R}) \to GL_4(\mathbb{R})$ is given by $\sigma(A) = JA^{-T}J$, where $J = \mathrm{diag}(-1, 1, 1, 1)$. When the Schwarzschild metric, $g = -\left(1 - \frac{1}{r}\right)\mathrm{d}t^2 + \left(1 - \frac{1}{r}\right)^{-1} dr^2 + r^2\left(d\theta^2 + \sin^2\theta\, d\varphi^2\right)$, which is an exact, spherically symmetric, vacuum solution of the Einstein equations, is interpolated using our interpolation method, the L^2 and H^1 errors (see Table 1) converge at the expected rates. The interpolant is guaranteed to stay in the space of Lorentzian metrics, unlike componentwise interpolants that may violate the metric signature condition.

5 Conclusion

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. We have described a systematic framework for constructing and analyzing Ritz variational integrators, and the extension to Hamiltonian partial differential equations. Group-equivariant finite element spaces yield multimomentum-conserving variational integrators via a discrete Noether's theorem. Such spaces can be constructed efficiently for finite elements taking values in symmetric spaces, in particular, Lorentzian metrics, by using a generalized polar decomposition. This lays the foundation for constructing geometric structure-preserving discretizations of general relativity that respect the spacetime diffeomorphism symmetry.

In order to realize the approach proposed in this paper, we need to further develop variational integrators for higher-order variational problems. At the continuous level, the most natural setting for dealing with higher-order Lagrangian field theories involves a generalization introduced in [12] of the Skinner–Rusk approach [56,57], which provides an unambiguous formalism for describing higher-order Lagrangian field theories. This would be an interesting basis for constructing multi-Dirac variational integrators for higher-order gauge field theories, and for developing a corresponding theory of variational error analysis.

An alternative approach is to consider the Einstein–Palatini formulation [51] of general relativity, where the Einstein–Hilbert action, which is second-order in the spacetime metric $g_{\mu\nu}$, is viewed as first-order in the spacetime metric $g_{\mu\nu}$ and the (torsion-free) affine connection $\Gamma^{\lambda}_{\mu\nu}$, where the Ricci tensor is a function of the connection, $R_{\mu\nu} = \partial_\lambda \Gamma^\lambda_{\mu\nu} - \partial_\mu \Gamma^\lambda_{\lambda\nu} + \Gamma^\rho_{\mu\nu}\Gamma^\lambda_{\lambda\rho} - \Gamma^\rho_{\lambda\nu}\Gamma^\lambda_{\mu\rho}$. This will involve developing a multi-Dirac variational discretization based on the Einstein–Palatini formulation using group-equivariant interpolants on Lorentzian metrics, and a compatible discretization of the affine connection.

Finally, it would be desirable to develop a discrete version of Noether's second theorem [36] in the context of variational spacetime discretizations of gauge field theories, and determine the functional relationship between the discrete dynamical and constraint equations.

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