Melvin Leok: Research Summary

My research is focused on developing geometric structure-preserving numerical schemes based on the approach of geometric mechanics, with a view towards obtaining more robust and accurate numerical implementations of feedback and optimal control laws arising from geometric control theory. This general approach is termed *computational geometric mechanics*, which is a subfield of *geometric integration*. It relies on a systematic and self-consistent discretization of geometry, mechanics, and control.

The approach is based on discretizing Hamilton's principle, which yields variational integrators that are automatically symplectic and momentum preserving, and exhibit good energy behavior for exponentially long times. Such discrete conservation laws typically impart long time numerical stability to computations, since they conserve exactly a discrete quantity that is always close to the continuous quantity of interest.

Manifold-Valued Approximation Theory. Classical field theories like electromagnetism and general relativity have a rich gauge symmetry, and it is important to distinguish between the physically relevant dynamics and the nonphysical gauge modes. A critical component to developing momentum-preserving discretizations of field and gauge theories is the construction of group-equivariant interpolation spaces. For functions that take values in symmetric spaces, which include important spaces such as Lorentzian metrics, positive-definite matrices, and Grassmannians, we construed a group-equivariant interpolant [30] using a local diffeomorphism between the symmetric space and its associated Lie triple system via a generalized polar decomposition, and arbitrarily-high derivatives of this interpolant can be efficiently computed [31].

Computational Geometric Mechanics. While Lagrangian systems have symplectic structures and momentum maps, they may also exhibit other important features like symmetries, nonlinear configuration spaces, or shocks and multiscale phenomena. It is desirable to preserve as many structural properties as possible, and towards this end a discrete theory of abelian Routh reduction was developed in [50] for systems with symmetry, as well as a generalization of variational integrators to flows on Lie groups and homogeneous spaces [28; 52; 57; 58; 69; 121; 130]. Two general approaches for constructing variational integrators are described in [83; 87], one based on the Galerkin approach, and the other on a boundary-value problem formulation. Examples of generalized Galerkin variational integrators that combine discrete variational mechanics with techniques from approximation theory and numerical quadrature, and yield adaptive symplectic-momentum methods for problems with multiple scales and shocks are described in [82], and the optimality of these methods is proven in [43] using a refinement of Γ-convergence, and extended to Lie groups in [44]. Related techniques that use collocation on the prolongation of the Hamiltonian vector field are described in [86]. It is also possible to handle degenerate Hamiltonian systems without resorting to the Lagrangian framework [89].

A theory of discrete Dirac mechanics and discrete Dirac structures was developed in [84; 85], which provide a unified treatment of Lagrangian and Hamiltonian mechanics, and symplectic and Poisson structures, respectively. These results are related as Hamilton–Pontryagin integrators preserve the discrete Dirac structure, and they provide the appropriate geometric framework for studying complex hierarchical interconnected systems [106]. The foundations for extending Dirac structures and Dirac integrators to the setting of Hamiltonian PDEs using generating functionals is laid forth in [122–125]. This is related in turn to extensions of Hamilton–Jacobi theory to discrete [103; 104] and degenerate [91] systems, as well as Lie algebroids [88]. Applications to semiclassical quantum mechanics are considered in [102].

Computational Geometric Control Theory. A theory of geometric control was developed that builds upon the discrete-time dynamics associated with variational integrators, and which does not introduce any additional approximations. This results in numerical control algorithms which are geometric structure-preserving and exhibit good long-time behavior. This approach allowed for the development of a discrete method of controlled Lagrangians [8–10; 12] for stabilizing relative equilibria. Motivated by applications in robotics, astrodynamics, and autonomous vehicles, discrete optimal control techniques on Lie groups were developed in [11; 46; 53; 54; 62; 67] and various extensions were studied, such as geometric phase based control [61], reconfiguration of formations of spacecraft using combinatorial optimization [59], time optimal control [63], articulated multi-body systems in space [65] and in perfect fluids [68; 71], tethered spacecraft [70; 73; 74; 79], autonomous UAVs [72; 76; 78], and underactuated chained pendula [77]. Additional applications include global state estimation [55; 60; 66] and uncertainty propagation on Lie groups [56; 64]. The geometric approach to the analysis of mechanical systems can also be used to provide important dynamical systems insights into problems evolving on nonlinear manifolds, as described in [17; 75; 80; 81].

Melvin Leok: Extended Research Statement

1. Introduction

Symmetry, and the study of invariants, has played a fundamental role in the development of modern mathematics. Many fields of mathematics can be characterized as the study of invariants of objects under a particular class of transformations. Geometry is concerned with spatial invariants under rigid transformations, topology studies spatial invariants of smooth transformations, and category theory analyzes transformations that leave a class of mathematical structures invariant. In differential equations, the methods for obtaining analytical solutions arise as special cases of symmetry techniques developed by Lie [96].

This reflects the deep and unifying role symmetry plays in a variety of mathematical fields, and indeed, symmetry techniques are a fundamental tool in the increasingly mature field of *geometric integration* [42], which is concerned with developing numerical methods that preserve geometric properties, that in turn correspond to the numerical scheme being invariant or equivariant under the action of a symmetry group.

My research is broadly concerned with developing theoretical, numerical and computational methods that are derived from differential geometric and symmetry techniques that arise in geometric integration, geometric mechanics, and geometric control theory. This is part of a longer-term effort to develop a coherent theory of *computational geometric mechanics* and *computational geometric control theory*. More precisely, my research is focused on developing a self-consistent discretization of geometry and mechanics to enable the systematic construction of geometric structure-preserving numerical schemes based on the approach of geometric mechanics, with a view towards obtaining more robust and accurate numerical implementations of feedback and optimal control laws arising from geometric control theory. This research has been been supported by single investigator grants in applied and computational mathematics and engineering, DMS-0726263, DMS-1001521, CMMI-1029445, CMMI-1334759, DMS-1411792, a *Faculty Early Career Development (CAREER) Award*, DMS-1010687, and a *Focused Research Group (FRG) Award*, DMS-1065972, and a *Research Training Grant (RTG) Award*, DMS-1345013, from the National Science Foundation.

In recognition of the growing impact of the field of computational geometric mechanics and computational geometric control theory, I gave a plenary talk at the Foundations of Computational Mathematics conference in Barcelona, Spain in July 2017. The FoCM conference, held every three years, covers the entire spectrum of mathematical computation. Recently, I also gave plenary talks at the NUMDIFF-14, Numerical treatment of differential and differential-algebraic equations conference in Halle, Germany, and the IFAC Workshop on Lagrangian and Hamiltonian Methods for Nonlinear Control in Lyon, France.

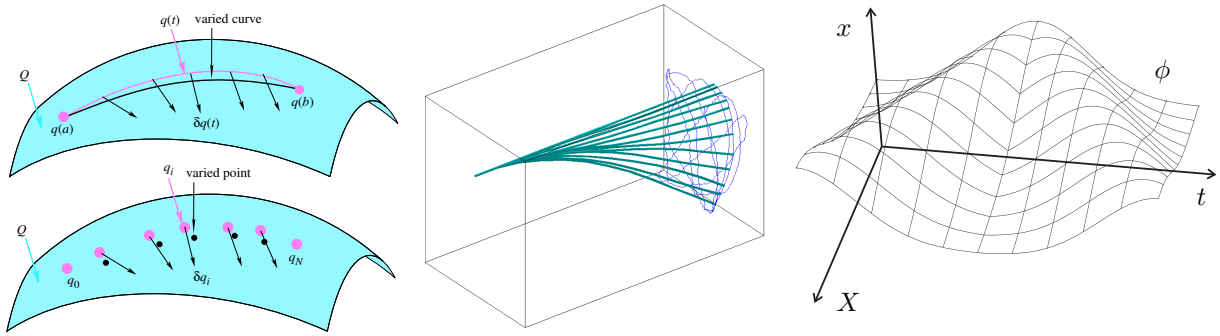
Geometric Integration. Geometric integration aims to construct numerical methods that preserve the geometric structure of a continuous dynamical system. In many problems arising from science and engineering, such as solar system dynamics and molecular dynamics, the underlying geometric structure affects the qualitative behavior of solutions, and as such, geometric integrators typically yield more qualitatively accurate simulations, and allow issues of long-time structural stability to be addressed.

Geometric Mechanics. Geometric mechanics had its roots in the pioneering works of Abraham and Marsden [1]; Arnold [5]; Smale [118, 119], which elucidated the role of differential geometry and symmetry in the study of mechanical systems. Today, these techniques play an important role in the mathematical theory of fluid mechanics [18; 26], elasticity [97], field theory, and geometric control theory [14].

Computational Geometric Mechanics. Computational geometric mechanics is concerned with constructing geometric integrators for Lagrangian and Hamiltonian mechanical systems. Variational integrators [98], obtained by discretizing Hamilton's principle (see Figure 1), are automatically symplectic and momentum preserving, and exhibit good energy behavior for exponentially long times. Such discrete conservation laws typically impart long time numerical stability to computations, since the structure-preserving algorithm exactly conserves a discrete quantity that is always close to the continuous quantity of interest.

Classical field theories like electromagnetism and general relativity have a rich gauge symmetry, and it is important to distinguish between physically relevant dynamics and nonphysical gauge modes. By symmetry reduction, one obtains a reduced system of equations that evolve on a lower dimensional shape space, which yield insights into phenomena like relative equilibria that would otherwise remain obscured without reduction.

More generally, there is a need to understand numerical methods applied to the simulation of complex dynamical systems as intrinsically discrete dynamical systems, which leads to the question of how to construct canonical discretizations that preserve, at a discrete level, the important properties of the continuous system.



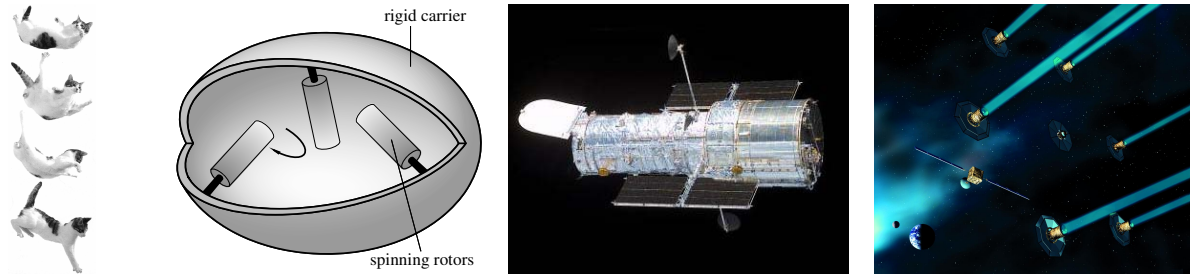
(a) Comparison of Hamilton's principle and the discrete variational principle.

(b) Generalizations to homogeneous spaces yield geometrically exact discretizations of elastic rods.

(c) PDE solutions represented as sections of a configuration bundle. Basis of multisymplectic discretizations of Hamiltonian PDEs.

Figure 1: Variational discretizations of Hamiltonian ODEs and PDEs, which yield symplectic, momentum preserving numerical schemes with excellent long time energy behavior.

Computational Geometric Control Theory. The accurate and efficient simulation of mechanical systems is an integral aspect of controlling modern engineering systems, such as robotic arms, spacecrafts, and underwater vehicles. Geometric control allows the attitude of a satellite to be controlled by changing its shape, in the same way that a cat flexing its body while falling allows it to always land on its feet (see Figure 2). Curiously, while geometry plays a critical role in geometric control, controllers are typically implemented using numerical methods that do not preserve the geometry. By developing a theory of geometric control that is predicated on the discrete-time dynamics associated with computational geometric mechanics, and does not introduce any additional approximations, one obtains numerical control algorithms which are geometric structure-preserving and exhibit good long-time behavior. Furthermore, by characterizing the configuration spaces of articulated multi-body systems using products of Lie groups and homogeneous spaces, one obtains control algorithms that are global and singularity-free, which are essential for constructing the non-trivial and highly aggressive global maneuvers that often yield the most efficient control strategies.



(a) Geometric phases and the falling cat.

(b) Mathematical model of a satellite involving a rigid body with internal rotors.

(c) Applicable to geometric control of satellites such as the Hubble space telescope. Courtesy NASA.

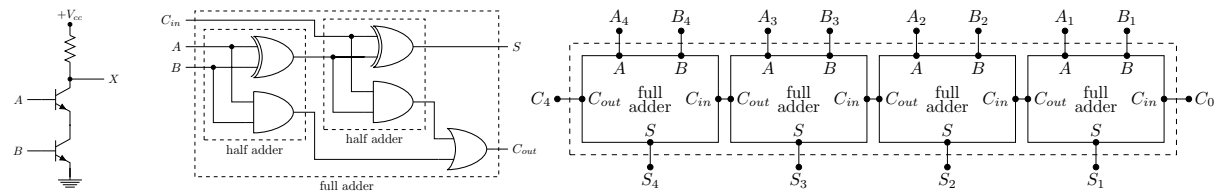
(d) ESA Darwin flotilla, which yield a large effective aperture space telescope. Courtesy ESA.

Figure 2: Computational geometric control theory. Learning from falling cats to construct geometric controllers for satellite attitude dynamics through the use of shape changes.

Extensions to Gauge Field Theories and Interconnected Systems. An important class of field theories are those that admit a symmetry under a continuous group of local transformations, which are referred to as ***gauge field theories***. One of the main goals of the proposed research is to develop a systematic framework for constructing and analyzing structure-preserving discretizations that respect the

gauge symmetries and preserve the associated conserved quantities for gauge field theories, such as Maxwell's equations of electromagnetism, and Einstein's equations of general relativity. In addition to developing the abstract mathematical theory of discrete gauge field theories, we will also develop novel finite-element approximation spaces, including spacetime generalizations of finite-element exterior calculus for discrete electromagnetism, and Lorentzian metric-valued geodesic finite-elements for discrete general relativity.

Another ubiquitous class of problems are ***interconnected systems***, which allow for the construction of complex, hierarchical, multiphysics and multiscale models by the interconnection of simpler subsystems. A typical example of a hierarchical interconnected system is an integrated circuit, which consists of components such as the multi-bit adder in Figure 3, which can be further decomposed sequentially into a full adder, half adders, logical gates, and then transistors and resistors. An important observation is that this kind of layered complexity, where the interconnections at each level of abstraction is sparse, is typical of complex engineered systems.



(a) NAND gate (b) Half and full adders using gates (c) 4-bit adder using 1-bit full adders

Figure 3: Hierarchical interconnected model of a multi-bit adder.

The surprising aspect about gauge field theories and interconnected systems is that they can both be described using the unified mathematical framework of Dirac and multi-Dirac mechanics and geometry. In particular, (multi-)Dirac mechanics and geometry provide a natural setting for describing degenerate, interconnected, holonomic and nonholonomic constrained systems.

The proposed research involves the non-trivial generalization of continuous multi-Dirac mechanics and geometry to the discrete setting, or of discrete Dirac mechanics and geometry to the setting of Lagrangian PDEs. These will then be applied to discrete gauge theories and interconnected systems. In particular, gauge field theories exhibit a degeneracy that is naturally described using the multi-Dirac formulation, and by combining discrete multi-Dirac mechanics with novel symmetry-preserving discretizations, the resulting numerical methods will exhibit a discrete Noether theorem and discrete covariant momentum preservation. This is important, since there is a subtle relationship between covariant momentum conservation, the energy-momentum map, and a subset of the equations of motion that arises in the initial-value formulation of gauge field theories.

2. Background Material

2.1. **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 [127; 128]. Dirac structures are the simultaneous generalization of symplectic and Poisson structures, and can encode Dirac constraints that arise in degenerate Lagrangian systems, interconnected systems, 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, where the Lagrange multiplier (and momentum) p imposes the second-order condition $v = \dot{q}$,

$$\delta \int_{t_1}^{t_2} L(q, v) - p(\dot{q} - v) dt = 0. \tag{1}$$

It provides a variational description of both Lagrangian and Hamiltonian mechanics, and yields the ***implicit Euler–Lagrange equations***,

$$\dot{q} = v, \qquad \dot{p} = \frac{\partial L}{\partial q}, \qquad p = \frac{\partial L}{\partial v}. \tag{2}$$

The last equation is the ***Legendre transform*** $\mathbb{F}L : (q, \dot{q}) \mapsto (q, \frac{\partial L}{\partial \dot{q}})$. This is important for degenerate systems as it enforces the primary constraints that arise when the Legendre transform is not onto.

The implicit Euler–Lagrange flow is ***symplectic***, i.e., it preserves the canonical symplectic structure Ω on T^*Q, the pull-back symplectic structure $\mathbb{F}L^*\Omega$ 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 $\langle \mathbf{J}(\alpha_q), \xi \rangle = \langle \alpha_q, \xi_Q(q) \rangle$ and $\langle \mathbf{J}_L(v_q), \xi \rangle = \langle \mathbb{F}L(v_q), \xi_Q(q) \rangle$, 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 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 two-form is closed, or that the Poisson bracket satisfies Jacobi's identity. Dirac structures generalize symplectic and Poisson structures. In particular, the graph of the symplectic two-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. Furthermore, symplectic and Poisson structures that are related in the usual way induce the same Dirac structure. Then, the implicit Euler–Lagrange equations are related to a vector field X on T^*Q satisfying $(X, \mathfrak{D}L) \in D$, where $\mathfrak{D}$ is the Dirac differential [127], and the Hamiltonian version is given by $(X, dH) \in D$.

2.2. **Discrete Dirac Variational Mechanics.** Geometric numerical integration aims to preserve geometric conservation laws under discretization. Discrete variational mechanics [85; 98] is based on 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***,

$$L_d^E(q_0, q_1; h) = \operatorname*{ext}_{\substack{q \in C^2([0,h],Q) \\ q(0)=q_0, q(h)=q_1}} \int_0^h L(q(t), \dot{q}(t)) dt, \tag{3}$$

which is equivalent 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, in general, it cannot be computed explicitly. Instead, the variational characterization of the exact discrete Lagrangian can be approximated by the Galerkin variational integrators.

The ***discrete Hamilton–Pontryagin principle*** imposes the discrete second-order condition $q_k^1 = q_{k+1}^0$ using Lagrange multipliers p_{k+1}, which yields a variational principle on $(Q \times Q) \times_Q T^*Q$,

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

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

$$q_k^1 = q_{k+1}^0, \qquad p_{k+1} = D_2 L_d(q_k^0, q_k^1), \qquad p_k = -D_1 L_d(q_k^0, q_k^1), \tag{4}$$

where D_i denotes the partial derivative with respect to the i-th argument. Making the identification $q_k = q_k^0 = q_{k-1}^1$, we obtain the ***discrete Lagrangian map*** and ***discrete Hamiltonian map*** which are $F_{L_d} : (q_{k-1}, q_k) \mapsto (q_k, q_{k+1})$ and $\tilde{F}_{L_d} : (q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$, respectively. The last two equations of (4) define the ***discrete fiber derivatives***, $\mathbb{F}L_d^{\pm} : Q \times Q \to T^*Q$,

$$\mathbb{F}L_d^+(q_k, q_{k+1}) = (q_{k+1}, D_2 L_d(q_k, q_{k+1})),$$
$$\mathbb{F}L_d^-(q_k, q_{k+1}) = (q_k, -D_1 L_d(q_k, q_{k+1})).$$

These two discrete fiber derivatives induce a single unique ***discrete symplectic form***, $\Omega_{L_d} = (\mathbb{F}L_d^{\pm})^*\Omega$, and the discrete Lagrangian and Hamiltonian maps preserve Ω_{L_d} and Ω, respectively. The discrete Lagrangian and Hamiltonian maps can be expressed as $F_{L_d} = (\mathbb{F}L_d^-)^{-1} \circ \mathbb{F}L_d^+$ and $\tilde{F}_{L_d} = \mathbb{F}L_d^+ \circ (\mathbb{F}L_d^-)^{-1}$, respectively. This characterization allows one to relate the approximation error of the discrete flow maps to the approximation error of the discrete Lagrangian.

Variational Error Analysis and Discrete Noether's Theorem. The variational integrator approach simplifies the numerical analysis of symplectic integrators. The task of establishing the geometric conservation properties and order of accuracy of the discrete Lagrangian map F_{L_d} and discrete Hamiltonian map $\tilde{F}_{L_d}$ reduces to the simpler task of verifying certain properties of the discrete Lagrangian L_d instead.

Theorem 2.1 (Discrete Noether's theorem (Theorem 1.3.3 of [98])). *If a discrete Lagrangian L_d is invariant under the diagonal action of G on $Q \times Q$, then the single unique* ***discrete momentum map****, $\mathbf{J}_{L_d} = (\mathbb{F}L_d^{\pm})^*\mathbf{J}$, is invariant under the discrete Lagrangian map F_{L_d}, i.e., $F_{L_d}^*\mathbf{J}_{L_d} = \mathbf{J}_{L_d}$.*

Theorem 2.2 (Variational error analysis (Theorem 2.3.1 of [98])). *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 [84; 85]. 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

$$D_{\Delta_Q}^{\mathrm{d}+} \triangleq \left\{ ((z, z'), \alpha_{\hat{z}}) \in (T^*Q \times T^*Q) \times T^*(Q \times Q^*) \mid (z, z') \in \Delta_{T^*Q}^{\mathrm{d}+},\ \alpha_{\hat{z}} - \Omega_{\mathrm{d}+}^{\flat}((z, z')) \in \Delta_{Q \times Q^*}^{\circ} \right\}.$$

Alternatively, an ***implicit discrete Hamiltonian system*** satisfies $(X_d^k, dH_{d+}(q_k, p_{k+1})) \in D_{\Delta_Q}^{\mathrm{d}+}$.

2.3. Multi-Dirac Field Theories.

Multisymplectic Geometry. The geometric setting for Lagrangian PDEs is multisymplectic geometry [99; 100]. 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. The independent and field variables form the ***configuration bundle***, $\rho : Y \to X$, see Figure 1(c). The configuration of the system is specified by a section of Y over X, 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 over (t, x), which is $\rho^{-1}((t, x))$.

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 $v_\mu^a = \partial y^a / \partial x^\mu$ 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_a^μ), corresponding to the affine map $v_\mu^a \mapsto (p + p_a^\mu v_\mu^a) d^{n+1}x$, 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 $\mathcal{L} : J^1Y \to \bigwedge^{n+1}(X)$, and let $\mathcal{L}(j^1\phi) = L(j^1\phi)\, dV = L(x^\mu, y^a, v_\mu^a)\, dV$, 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 $\frac{\partial y^a}{\partial x^\mu} = v_\mu^a$ replaces $v = \dot{q}$, so the ***Hamilton-Pontryagin principle*** is

$$\delta S(y^a, y_\mu^a, p_a^\mu) = \delta \int_U \left[p_a^\mu \left(\frac{\partial y^a}{\partial x^\mu} - v_\mu^a \right) + L(x^\mu, y^a, v_\mu^a) \right] d^{n+1}x = 0. \tag{5}$$

Taking variations with respect to y^a, v_μ^a and p_a^μ (where δy^a vanishes on the boundary ∂U) yields the ***implicit Euler–Lagrange equations***,

$$\frac{\partial p_a^\mu}{\partial x^\mu} = \frac{\partial L}{\partial y^a}, \quad p_a^\mu = \frac{\partial L}{\partial v_\mu^a}, \quad \text{and} \quad \frac{\partial y^a}{\partial x^\mu} = v_\mu^a, \tag{6}$$

which generalizes (2) to the case of field theories. We developed an intrinsic version of this variational principle in [124], using the geometry of the first jet bundle and its dual as the starting point. As the jet bundle is an affine bundle, the duality pairing used implicitly in (5) is more complicated.

The second equation of (6) yields the ***covariant Legendre transform***, $\mathbb{F}\mathcal{L} : J^1Y \to J^1Y^\star$,

$$p_a^\mu = \frac{\partial L}{\partial v_\mu^a}, \qquad p = L - \frac{\partial L}{\partial v_\mu^a} v_\mu^a. \tag{7}$$

This unifies the two aspects of the Legendre transform by combining the definitions of the momenta and the Hamiltonian into a single covariant entity.

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

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

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

$$\mathbf{d}^2\mathcal{S}(\phi)(V,W) = \int_{\partial U} (j^1\phi)^*(\mathbf{i}_{j^1V}\mathbf{i}_{j^1W}\Omega_L) = 0, \tag{8}$$

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 [99]).

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

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

The graph of this mapping is a submanifold 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 field equations (6) can be written as

$$(\mathcal{X}, (-1)^{n+2}\mathbf{d}E) \in D_{n+1}, \tag{9}$$

where D_{n+1} is the graph of the multisymplectic form Ω. In general, a ***Lagrange-Dirac field theory*** is a triple $(\mathcal{X}, E, D_{n+1})$ satisfying (9), where D_{n+1} belongs to a multi-Dirac structure D.

2.4. Desirable Properties of Variational Integrators.

Symplecticity. Given a discrete Lagrangian L_d, one obtains a discrete fiber derivative, $\mathbb{F}L_d : (q_0, q_1) \mapsto (q_0, -D_1L_d(q_0, q_1))$. Variational integrators are symplectic, i.e, the pullback under $\mathbb{F}L_d$ of the canonical symplectic form Ω on the cotangent bundle T^*Q, is preserved. Pushing-forward the discrete Euler–Lagrange equations yield a symplectic-partitioned Runge–Kutta method.

Momentum Conservation. Noether's theorem states that if a Lagrangian is invariant under the lifted action of a Lie group, the associated momentum is preserved by the flow. If a discrete Lagrangian is invariant under the diagonal action of a symmetry group, a discrete Noether's theorem holds, and the discrete flow preserves the discrete momentum map. For PDEs with a uniform spatial discretization, a backward error analysis implies approximate spatial momentum conservation [105].

Approximate Energy Conservation. While variational integrators do not exactly preserve energy, backward error analysis [7; 40; 41; 109] shows that it preserves a modified Hamiltonian that is close to the original Hamiltonian for exponentially long times. In practice, the energy error is bounded and does not exhibit a drift. This is the temporal analogue of the approximate momentum conservation result for PDEs, as energy is the momentum map associated with time invariance.

Applicable to a Large Class of Problems. The discrete variational approach is very general, and allows for the construction of geometric structure-preserving numerical integrators for PDEs [92], nonsmooth collisions [29], stochastic systems [13], nonholonomic systems [20], thermodynamical [27] and constrained systems [93]. Furthermore, Dirac structures and mechanics allows for interconnections between Lagrangian systems, thereby providing a unified simulation framework for multiphysics systems.

Generates a Large Class of Methods. A variational integrator can be constructed by choosing a finite-dimensional function space, and a numerical quadrature method [82]. By leveraging techniques from approximation theory, numerical analysis, and finite elements, one can construct variational integrators that are appropriate for problems that evolve on Lie groups [57; 58] and homogeneous spaces [69], or exhibit multiple timescales [92; 120].

3. Prior Research Accomplishments

Various aspects of the long-term program to develop computational geometric mechanics and geometric control theory have been completed, primarily by my collaborators and I, and are summarized below.

Computational Geometric Mechanics	
Discrete Geometry	**Discrete Mechanics**
Discrete Exterior Calculus (§3.1.1) Discrete Principal Connections (§3.1.2) Discrete Dirac Geometry (§3.2.4)	Discrete Reduction Theory (§3.2.1) Lie Group Variational Integrators (§3.2.2) Generalized Variational Integrators (§3.2.3) Discrete Dirac Mechanics (§3.2.4)

$\Downarrow$

Computational Geometric Control Theory
Discrete Optimal Control on Lie Groups (§3.3.1)
Discrete Controlled Lagrangian Systems (§3.3.2)
Discrete Optimal Attitude Estimation and Filtering (§3.3.3)
Discrete Hamilton–Jacobi Theory and Bellman Equations (§3.3.4)

3.1. **Discrete Geometry.**

3.1.1. *Discrete Exterior Calculus [23; 24].* A theory of discrete exterior calculus on simplicial complexes of arbitrary finite dimension is constructed in [23]. Discrete differential forms are expressed as cochains, and discrete vector fields are considered by introducing a circumcentric cell complex which is dual to the simplicial complex. From this, one systematically recovers discrete vector differential operators like the divergence, gradient, curl and the Laplace–Beltrami operator. Discrete harmonic maps are equivalently characterized as the kernel of the discrete Laplace–Beltrami operator or as extremizers of a discrete variational principle. The discrete Laplace–de Rham operator yields a discrete Hodge–de Rham theory that relates the discrete de Rham cohomology to simplicial cohomology. A discrete Poincaré lemma is obtained in [24], by constructing a homotopy operator for unstructured meshes.

3.1.2. *Discrete Connections on Principal Bundles [90].* Motivated by applications to discrete Lagrangian reduction, the discrete analogue of the Atiyah sequence is introduced in [90]. Splittings of the discrete Atiyah sequence yield a discrete connection, which can equivalently be represented as a discrete connection one-form, or a discrete horizontal lift. Given a discrete G-invariant Lagrangian in discrete mechanics, one obtains a discrete momentum map whose zero surface yields a discrete horizontal distribution that defines a discrete mechanical connection. This, in turn, can be represented as a discrete connection one-form, which yields a discretization of the Lagrange–Poincaré operator that encodes the reduced equations in discrete Lagrangian reduction. In the context of discrete exterior calculus, one considers the orthonormal frame bundle over a simplicial complex with piecewise constant Riemannian structure, viewed as a $SO(n)$-bundle in the sense of Cartan. Then one constructs a discrete Levi-Civita connection and obtains the discrete curvature as the exterior derivative of the connection.

3.2. **Discrete Mechanics.**

3.2.1. *Discrete Routh Reduction [50].* Abelian symmetry reduction for discrete mechanics is considered in [50]. Reducing the discrete variational principle by splitting the variations into horizontal and vertical components yields the discrete Routh equations that are symplectic with respect to the non-canonical symplectic structure of the continuous Routh equations. The push forward to the Hamiltonian side gives the Reduced Symplectic Partitioned Runge-Kutta algorithm, which is a discrete analogue of cotangent bundle reduction.

3.2.2. *Lie Group and Homogeneous Variational Integrators [28; 52; 57; 58; 69; 80; 81].* Lie group variational integrators preserve the Lie group structure of the configuration space without the use of local charts, reprojection, or constraints. Instead, the discrete solution is updated using the exponential of a Lie algebra element that satisfies a discrete variational principle. These yield highly efficient geometric integration schemes for rigid body dynamics that automatically remain on the rotation group. We avoid coordinate singularities associated with local charts, such as Euler angles, by representing the attitude globally as a rotation matrix, which is important for accurately simulating chaotic orbital motion.

These ideas were introduced in [52], and applied to a system of extended rigid bodies interacting under their mutual gravitational potential in [57; 58], wherein symmetry reduction to a relative frame is also addressed. The superior computational efficiency of Lie group variational integrators for the full body simulation of systems of extended rigid bodies in the context of astrodynamics is demonstrated in [28].

Homogeneous spaces such as the two-sphere have a transitive Lie group action, and as such, Lie group actions can be used to generate flows on homogeneous spaces. This is the approach adopted in [69] to construct a compact and global description of the dynamics of chains of spherical pendula that is dramatically simpler than spherical polar or cylindrical coordinate representations. In an analogous manner, Lie group variational integrators are adapted to homogeneous spaces, to yield a class of variational integrators for homogeneous spaces. This provides an efficient basis for modeling and simulating engineering systems such as articulated robotic arms, flexible structures, and mechanisms in a geometrically exact manner. These homogeneous space variational integrator techniques have been applied to long chains of spherical pendula [77], and a related approach based on discretizing the Hamel formalism was studied in [130].

We have been able to develop the first global variational integrator for point vortices on the sphere [121]. This task was complicated by the degenerate Lagrangian, and the homogeneous space structure of the sphere. By lifting the variational principle from S^2 to $SU(2)$ by a combination of the isomorphism between S^3 and $SU(2)$, together with the Hopf fibration, we developed a variational Lie group integrator for point vortices on the sphere that is symplectic, second-order accurate, and preserves the unit-length constraint.

In [80; 81], we introduce methods for describing in a global fashion the Lagrangian and Hamiltonian dynamics on embedded manifolds and two-spheres.

3.2.3. *Generalized Variational Integrators [43; 44; 82; 83; 87; 89; 94; 95; 116].* The order of a variational integrator can be analyzed in terms of the extent to which a computable discrete Lagrangian approximates the exact discrete Lagrangian. The two characterizations of the exact discrete naturally lead to two general methods for constructing variational integrators, which is described in [83; 87].

The exact discrete Lagrangian associated with Jacobi's solution is the action integral evaluated on a solution of a two-point boundary-value problem. As such, a computable approximation to the exact discrete Lagrangian can be obtained in two stages: (i) apply a numerical quadrature formula to the action integral, evaluated along the exact solution of the Euler–Lagrange boundary-value problem; (ii) replace the exact solution of the Euler–Lagrange boundary-value problem with a numerical solution of the boundary-value problem, in particular, by a converged shooting solution associated with a given one-step method (see [87]). More generally, the shooting-based solution of the Euler–Lagrange boundary-value problem can also be replaced with approximate solutions based on other numerical schemes, including Taylor integrators [116], and collocation methods applied to either the Euler–Lagrange vector field [94; 95] or its prolongation [86].

The variational characterization of the exact discrete Lagrangian leads to a class of Galerkin variational integrators, which involve approximating the action integral in two stages: (i) represent sections of the configuration bundle with a finite-dimensional function space; (ii) replace the integral with quadrature. In [82], concepts from numerical analysis and approximation theory, such as adaptivity, approximability, and accuracy are incorporated into discrete mechanics by an appropriate choice of function space and quadrature.

By considering piecewise interpolatory functions, and enforcing continuity using Lagrange multipliers, one obtained a constrained extremal problem whose dual yields discrete Hamiltonian dynamics, wherein the Lagrange multipliers are the discrete momenta. Fourier-Chebyshev expansions in space-time yield pseudospectral variational integrators that are appropriate for quantum mechanical simulations. Nonlinear approximation spaces, wherein the space-time mesh points are allowed to vary, provide spatio-temporal adaptivity in variational integrators and naturally generalize Symplectic-Energy-Momentum integrators. In multiscale problems, the function space is augmented with solutions of the cell problem, which solve for

the fast dynamics while keeping the slow variables fixed. The highly oscillatory action integral is evaluated using an exponentially fitted quadrature scheme such as Filon–Lobatto. This yields a multiscale variational integrator with convergence rates that are independent of the ratio of fast and slow timescales.

In [89], we consider the case of degenerate Hamiltonian systems, where there is no corresponding Lagrangian formulation. This necessitates the development of discrete variational mechanics that is expressed directly in terms of the Hamiltonian, and relies on discretizing Hamilton's phase space variational principle, expressed in terms of Type II generating functions. In the case of nondegenerate Hamiltonians, the construction commutes with the Lagrangian formulation via the Legendre transformation, and one recovers the standard Galerkin variational integrators, but expressed in terms of the continuous Hamiltonian.

A particularly subtle issue is the relationship between the order of accuracy of Galerkin variational integrators and the best approximation properties of the underlying finite-dimensional function spaces. In [43], we proved that Galerkin variational integrators are order-optimal by carefully refining a proof of Γ-convergence of variational integrators [101]. Furthermore, we also showed that a Galerkin variational integrator based on spectral basis functions is geometrically convergent. Galerkin variational integrators also provide analytical approximations on the interior of a time interval, and we showed that these approximations converge at half the rate of the solutions at the discrete timesteps. More significantly, this subtle analysis was extended to the case of Galkerin variational integrators for dynamical systems that evolve on Lie groups in [44].

3.2.4. *Discrete Dirac Mechanics and Geometry [84; 85].* The discrete variational characterization of discrete Dirac mechanics is described using the discrete Hamilton–Pontryagin principle, and encompasses discrete analogues of Lagrangian, Hamiltonian, and nonholonomic mechanics, and allows for the arbitrary interconnection of such systems. In addition, discrete Dirac structures provide a unification of discrete analogues of symplectic and Poisson structures, while incorporating the Dirac theory of constraints, which is of importance in relativistic systems, as well as nonholonomic (nonintegrable) constraints. In addition to providing an alternative discrete geometric description of the associated discrete mechanics, it also explicitly characterizes the discrete geometric structures that are preserved by Dirac integrators. Existing research directions in discrete Dirac mechanics and geometry include the issue of discrete reduction theory for discrete Dirac mechanics, generalizations to degenerate Lagrangian and Hamiltonian systems, and a complete discrete interconnection theory for discrete Dirac systems.

3.3. **Computational Geometric Control Theory.**

3.3.1. *Discrete Optimal Control on Lie Groups [11; 46; 53; 54; 59; 61–63; 65; 67; 68; 70–74; 76; 78].* The discrete optimal control problem is derived as a two stage discrete variational problem. First, a forced Lie group variational integrator [52] is derived from the discrete Lagrange–d'Alembert principle, and imposed as constraints in the discrete optimal control problem. Necessary optimality conditions are derived in [11; 46] that are group-equivariant, thereby ensuring that the resulting discrete optimal trajectories are frame-independent. More accurate solutions are obtained, as the discrete dynamics faithfully approximates the continuous equations of motion, as compared to traditional discretization techniques like collocation.

Optimal control problems with impulsive controls, in a relative frame prescribed by a nominal trajectory, are studied in [53] and solved using sequential quadratic programming. For continuously actuated control problems, this approach is prohibitively expensive. In [62], we adopt an adjoint formulation, with a forward trajectory computation, and a backward computation of the sensitivity of the cost functional with respect to the initial control, which yields a three orders of magnitude improvement in computational efficiency. The generalization of this technique to the case of non-compact Lie groups, such as $SE(3)$, is considered in [54]. An alternative approach is to parametrize the discrete controls using a lower-dimensional function space, and this is adopted in [65] to develop optimal control strategies for articulated rigid bodies. In addition, we have applied these techniques to articulated multi-body systems in perfect fluids [68; 71], tethered spacecraft [70; 73; 74; 79], autonomous UAVs [72; 76; 78], and underactuated chained pendula [77].

In control problems with symmetry, such as satellites with internal momentum wheels, wherein only the shape variables are directly actuated, geometric phase effects yield controllability of the group variables. The symmetry induces numerical ill-conditioning that is addressed by encoding the reduced geometry in the numerics, thereby yielding a well-conditioned method for geometric phase based optimal control which is described in [61], that is not constrained to small amplitude maneuvers in shape space. We also address the

reconfiguration of formations of satellites, by adopting techniques from combinatorial optimization in [59], and study discrete time-optimal control problems in [63].

3.3.2. *Discrete Controlled Lagrangian Systems [8–10; 12].* The method of controlled Lagrangian systems is based on the idea of adopting a feedback control to realize a modification of either the potential energy, or the kinetic energy of a mechanical system, referred to as potential shaping, or kinetic shaping, respectively. Since the closed-loop system dynamics correspond to a modified mechanical system, the energy is a Lyapunov function, and asymptotic feedback stabilization results can be obtained. A real-time digital feedback controller is constructed that stabilizes the inverted equilibrium of the cart-pendulum system using kinetic shaping in [8], and the extension to the case of potential shaping is considered in [9]. The general case of one actuated and one uncontrolled direction was addressed in [10; 12].

3.3.3. *Discrete Optimal Attitude Estimation and Filtering [55; 56; 60; 64; 66].* Attitude estimation is formulated as an optimization problem on the rotation group in [55], wherein the uncertainty ellipsoids representing the estimate of the attitude are propagated by a discrete flow given by a Lie group variational integrator for the forced Euler's equations in the presence of an attitude-dependent potential. Our procedure for assimilating new directional measurements with measurement uncertainty is more robust than extended Kalman filters when the satellite undergoes large rotations between measurements. Convergence of the algorithm is studied in [66], the degenerate case of single directional measurements is addressed in [60], and a careful comparison of uncertainty propagation methods is conducted in [56]. A global uncertainty propagation method that synthesizes techniques from polynomial chaos, noncommutative harmonic analysis, and Lie group variational integrators is developed in [64], which allows for probability densities with global support.

3.3.4. *Discrete Hamilton–Jacobi Theory and Bellman Equations [103; 104].* Hamilton–Jacobi theory provides a framework for studying integrable Hamiltonian systems, and we developed the corresponding discrete Hamilton–Jacobi theory in the context of discrete mechanics by considering the discrete Jacobi's solution. We also developed a discrete analogue of the geometric Hamilton–Jacobi theorem of Abraham and Marsden.

In addition, important connections between discrete Hamilton–Jacobi theory and discrete optimal control (Hamilton–Jacobi–Bellman and discrete Riccati) are established, which in turn allows one to export the general framework for discrete Hamiltonian mechanics developed in [89] to the discrete-time optimal control setting. In particular, this provides a rigorous and systematic method of deriving arbitrarily high-order generalization of the Bellman equations which are first-order accurate.

3.4. **Continuous Geometric Mechanics and Dynamical Systems.**

3.4.1. *Hamilton–Pontryagin Principle and Stokes–Dirac and Multi-Dirac Structures for Field Theories [122–124].* In [122], we derived the Stokes-Dirac structures that arise in boundary control theory by considering the symmetry reduction of a canonical Dirac structure, and in particular obtain the non-canonical advection terms that arise in the Euler equations. This geometric structure could be combined with Lagrange–Dirac interconnection theory to provide a geometric framework for describing fluid-structure interactions.

Recall that Dirac structures generalize symplectic and Poisson structures, and in particular, the graph of a symplectic structure is a Dirac structure. In the covariant approach to field theories, the multisymplectic structure plays a pivotal role, and the graph of the multisymplectic structure is a multi-Dirac structure. In [123], we elucidate the geometry of multi-Dirac structures, and introduce a multi-Courant bracket on the space of sections of a multi-Dirac structure, which endows the space with the structure of a Gerstenhaber algebra. This provides the geometric counterpart to the variational Hamilton–Pontryagin approach to Lagrangian field theories that is described in [124].

3.4.2. *Hamilton–Jacobi Theory for Degenerate Lagrangian Systems [91].* In [91], we generalize Hamilton–Jacobi theory to the setting of implicit Lagrangian systems with both holonomic and nonholonomic constraints by starting with the approach of Dirac variational mechanics. This generalizes the Hamilton–Jacobi theory for nonholonomic systems, and we consider a new class of weakly Chaplygin systems, which are degenerate nonholonomic Lagrangian systems with symmetry that arise naturally as reduced order models of mechanical systems when small masses or moments of inertia in a multibody system are neglected.

3.4.3. *Dynamical Systems Analysis on Lie Groups [17; 75].* In [17], geometric mechanics and reduction theory are used to analyze the stability properties of equilibria and relative equilibria of the 3D pendulum. This provides a systematic and unified analysis that incorporates existing results and new insights within the framework of geometric mechanics. Novel numerical techniques for computing and visualizing the stable manifolds of saddle points of pendulum dynamics on S^2 and $SO(3)$ are discussed in [75].

3.4.4. *Semiclassical Quantum Mechanics [102].* In [102], we obtained insight into semiclassical approximations of quantum mechanics based on wave packet dynamics. By including non-spherical wave packets into the Hilbert space of square-integrable functions, one could pullback the symplectic structure of quantum mechanics to non-spherical wave packet dynamics, and thereby provide a symplectic description of the model reduced dynamics.

4. Prior Computational Results

Many mechanisms arising in engineering design, such as interconnected rigid bodies with universal joint constraints, have configuration manifolds that involve Lie groups such as the group of rotations, $SO(3)$, and homogeneous spaces such as the two-sphere, S^2. Such nonlinear manifolds pose a challenge to standard numerical techniques that construct approximations using linear operations. In practice, this results in either the use of coordinate charts that are local due to coordinate singularities, or the use of constraints on an embedding space. The disadvantage of such approaches is that they either fail to preserve structure globally, or involve additional degrees of freedom and are therefore computationally inefficient. We have developed global, minimal-dimensional variational integrators for problems that naturally evolve on Lie groups [57; 58] or homogeneous spaces [69], that have been applied to a variety of applications (Figure 4).

While variational integrators are generally implicit for non-separable Lagrangians, most mechanical systems have separable Lagrangians, for which explicit variational integrators can be constructed with superior error properties at lower computational cost (Figure 5). My former Ph.D. student, Dr. Hall, and I developed provably geometrically convergent spectral variational integrators (Figures 6, 7) in [43] to address computational efficiency for non-separable Lagrangians.

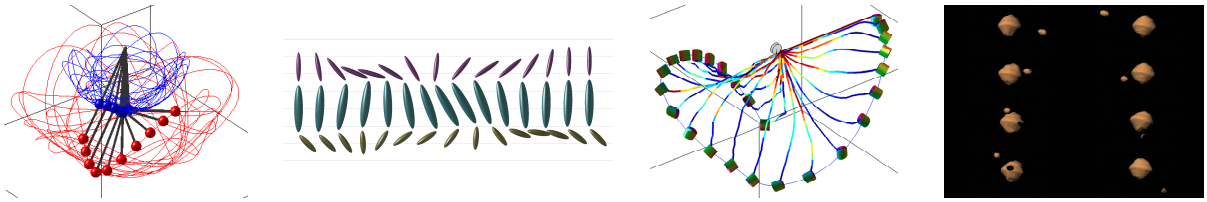
5. Current research

5.1. **Construction and Analysis of Multi-Dirac Variational Integrators.** The exact discrete Lagrangian plays a fundamental role in the construction and analysis of variational integrators for Lagrangian ODEs. We will first review how the characterization of the exact discrete Lagrangian yield Galerkin methods [87] for constructing variational integrators based on suitable choices of numerical quadrature formulas and approximation spaces. Then, we recall some results in [43] by my former Ph.D. student, Dr. Hall, and I which relates the error of the resulting variational integrators to the best approximation properties of the approximation spaces.

Our aim is to extend this from the case of ODEs to the more challenging case of PDEs, and obtain a systematic framework for constructing and analyzing multi-Dirac variational integrators for Lagrangian PDEs. This will rely upon the boundary Lagrangian that was introduced in [125] by my former postdoc, Dr. Vankerschaver, and I and its interpretation as the exact generating functional for a multisymplectic field theory, which is described below. Additionally, it will also rely on the work described in the background material, such as the continuous Dirac theory developed in [127; 128] by my collaborator, Prof. Yoshimura, the discrete Dirac theory developed in [84; 85] by my former postdoc, Prof. Ohsawa, and I and the continuous multi-Dirac theory developed in [123; 124] by my collaborator, Prof. Yoshimura, my former postdoc, Dr. Vankerschaver, and I.

We intend to construct a discrete Hamilton–Pontryagin and multi-Dirac formulation of field theories, and to apply it to degenerate and gauge field theories, such as electromagnetism and general relativity, as they provide a systematic alternative to the Dirac theory of constraints [25] and the Gotay–Nester–Hinds constraint algorithm [33–35] for dealing with the primary constraints.

5.1.1. *Analysis of Variational Integrators for Lagrangian ODEs [43; 87].*



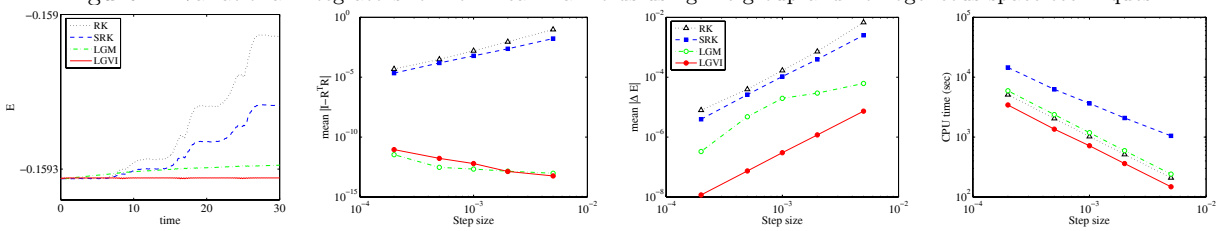
(a) Double spherical pendulum ($S^2 \times S^2$) [69]

(b) Model fish in a perfect fluid ($SO(3) \times SO(3)$) [73]

(c) Rigid body interacting with elastic string [71]

(d) Binary asteroid simulation of 1999 KW4 [115]

Figure 4: Variational integrators for nonlinear manifolds using Lie group and homogeneous space techniques.



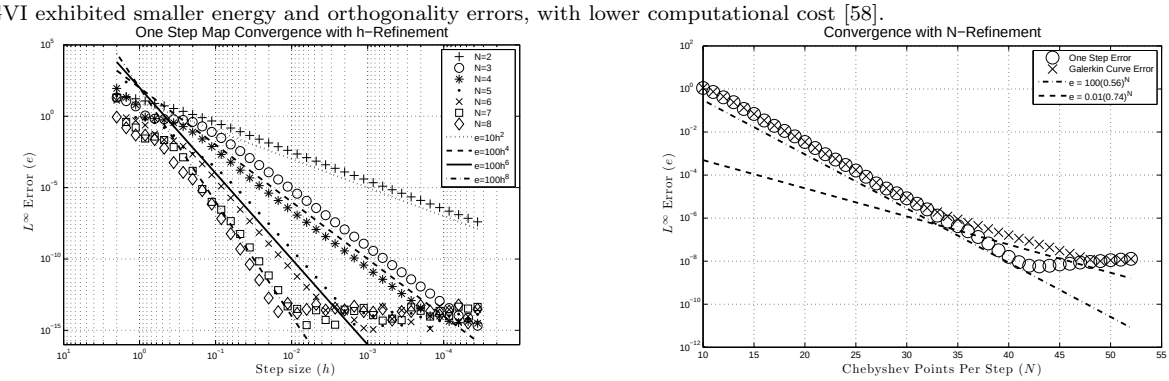
(a) Computed total energy for 30 seconds

(b) Mean orthogonality error $\|I - R^T R\|$ vs. step size

(c) Mean total energy error $|E - E_0|$ vs. step size

(d) CPU time vs. step size

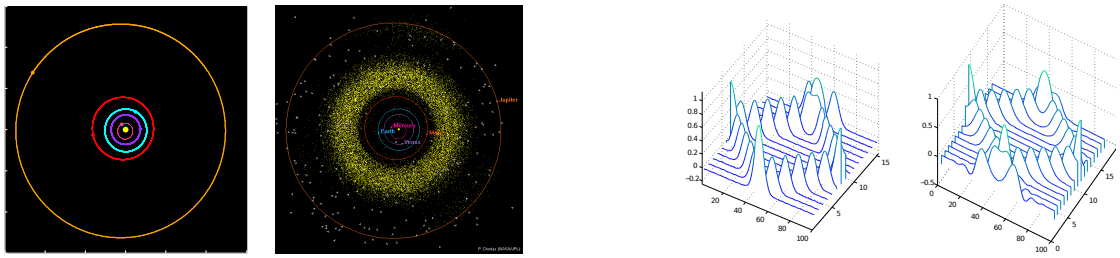
Figure 5: Comparison of a Lie group variational integrator (LGVI) with a Lie group method (LGM), symplectic Runge–Kutta method (SRK) and non-symplectic Runge–Kutta method (RK), all with second-order accuracy. This demonstrated that the LGVI exhibited smaller energy and orthogonality errors, with lower computational cost [58].



(a) Order optimality of Galerkin variational integrators.

(b) Geometric convergence of spectral variational integrators.

Figure 6: The convergence rate of Galerkin variational integrators is related to the best approximation error of the approximation spaces used. Spectral variational integrators based on Chebyshev polynomials converge geometrically.



(a) Simulation of inner solar system using a spectral variational integrator and a full ephemeris NASA simulation.

(b) Variational integrator for the wave equation, using a spectral in space and linear in time discretization.

Figure 7: The spectral variational integrator agrees qualitatively with NASA JPL simulations of the inner solar system, even with timesteps ($h = 100$ days) exceeding the orbital period of Mercury. The spectral multisymplectic discretization of the wave equation exhibits excellent coherence of the wave packets, even after hundreds of interactions.

Galerkin Variational Integrators. The variational characterization of the exact discrete Lagrangian leads to Galerkin variational integrators, where the integral is replaced with a quadrature formula, and the space of C^2 curves is replaced with a finite-dimensional function space. Given a finite-dimensional function space $\mathbb{M}^n([0,h]) \subset C^2([0,h],Q)$ and a quadrature formula $\mathcal{G} : C^2([0,h],Q) \to \mathbb{R}$, $\mathcal{G}(f) = h\sum_{j=1}^m b_j f(c_j h) \approx \int_0^h f(t)dt$, the ***Galerkin discrete Lagrangian*** is

$$L_d(q_0,q_1) = \operatorname*{ext}_{\substack{q\in\mathbb{M}^n([0,h])\\ q(0)=q_0,q(h)=q_1}} \mathcal{G}(L(q,\dot q)) = \operatorname*{ext}_{\substack{q\in\mathbb{M}^n([0,h])\\ q(0)=q_0,q(h)=q_1}} h\sum\nolimits_{j=1}^m b_j L(q(c_j h),\dot q(c_j h)).$$

While Theorem 2.2 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 Galerkin discrete Lagrangian should be bounded by a constant multiple of the best approximation error in approximating the exact solution of the Euler–Lagrange equations with an element of the finite-dimensional function space $\mathbb{M}^n$. In such an instance, we say that the Galerkin method is ***order-optimal***. Order-optimality was proved in [43] by my former Ph.D. student, Dr. Hall, and I. This required a careful refinement of the proof of Γ-convergence of variational integrators presented in [101], and relied upon similar technical assumptions.

Theorem 5.1 (Order-optimality of Galerkin variational integrators (Theorem 3.3 of [43]))**.** *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 Galerkin discrete Lagrangian approximates L_d^E to $\mathcal{O}(h^{n+1})$.*

Theorem 5.2 (Geometric convergence of Spectral variational integrators (Theorem 3.4 of [43]))**.** *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 $K = \min(K_1,K_2)$.*

5.1.2. *The Boundary Lagrangian and Generating Functionals of Lagrangian PDEs [125].* The discrete Lagrangian is a scalar function that depends on the boundary-values at the initial and final time. By analogy, the boundary Lagrangian 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 is 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 $\varphi \in \mathcal{Y}_{\partial U}$, and the latter by ϕ. The ***boundary Lagrangian*** $L_{\partial U}$ is the functional on the space of boundary data $\mathcal{Y}_{\partial U}$ 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 is 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

$$p_0 = -\frac{\partial S_1}{\partial q_0}(q_0,q_1), \qquad p_1 = \frac{\partial S_1}{\partial q_1}(q_0,q_1). \tag{10}$$

This relates the boundary momentum to the variation of S_1 with respect to the boundary data. 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

$$\pi = \frac{\delta L_{\partial U}}{\delta\varphi} = \frac{\partial L}{\partial v^a_\mu} n_\mu dy^a \otimes dS, \tag{11}$$

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, $\pi_a = p^\mu_a n_\mu$, i.e., π_a is the normal component of the covariant momentum p^μ_a, and so we refer to $\pi \in T^*\mathcal{Y}_{\partial U}$ as the ***normal momentum*** to the boundary ∂U. The multisymplectic generalization of (10) is that (11) holds for every point on ∂U.

5.1.3. *Specific Research Goals.*

Discrete Boundary Lagrangians and Multi-Dirac Variational Integrators. We aim to develop a discrete theory of multi-Dirac integrators for field theories and discrete multi-Dirac structures by discretizing boundary Lagrangians and the Hamilton–Pontryagin principle for field theories (5). The proposed approach is as follows: given a spacetime finite-element discretization of the configuration bundle, we introduce a space of discrete boundary data by taking the trace of the finite-element space to the boundary of each element. For simplicity, we assume that the discrete boundary data is parametrized by boundary degrees of freedom, and we impose the equality of the boundary degrees of freedom on a common face to two elements with a Lagrange multiplier, where the Lagrange multiplier can be viewed as the normal momentum defined in (11). This yields a discrete Hamilton–Pontryagin principle for field theories. For the mesh in Figure 8, it has the form

$$\delta \sum\nolimits_{i,j} \pi_{i+\frac{1}{2},j}(\varphi^E_{i,j} - \varphi^W_{i+1,j}) + \pi_{i,j+\frac{1}{2}}(\varphi^N_{i,j} - \varphi^S_{i,j+1}) + L^d_{\partial U}(\varphi^{\{N,S,E,W\}}_{i,j}) = 0.$$

A Galerkin discrete boundary Lagrangian $L^d_{\partial U}$ is obtained by extremizing a quadrature approximation of the action integral over finite-element sections satisfying the discrete boundary conditions. While these methods are derived in terms of a spacetime variational principle, the causality of the field theory allows the solution to be computed in an implicit (in time) time-marching fashion.

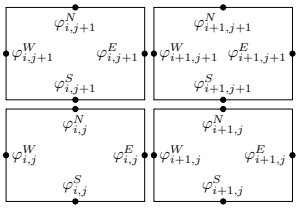


Figure 8: A $(1+1)$-spacetime mesh with boundary degrees of freedom.

Discrete Covariant Legendre Transforms and Discrete Multi-Dirac Structures. We will construct a discrete analogue of the covariant Legendre transform (7) that is generated by a discrete boundary Lagrangian. This will allow us to discretize my work on characterizing multi-Dirac mechanics in terms of multi-Dirac structures [124] by pulling back the Tulczyjew's triple for field theories [37] via the discrete covariant Legendre transform.

Variational Error Analysis of Discrete Boundary Lagrangians. We aim to develop a PDE analogue of variational error analysis (Theorem 2.2). If $\mathcal{C} = C^\infty(Y)$ is the set of smooth sections of the configuration bundle $\rho : Y \to X$, and X_d is a spacetime mesh that covers the domain U_d, consider a spacetime finite-element space $\mathcal{C}_d \subset \mathcal{C}$ that is subordinate to the spacetime mesh X_d. Taking the trace of $\mathcal{C}_d$ to the boundary ∂U_d induces a natural discretization $\mathcal{Y}^{\mathcal{C}_d}_{\partial U_d}$ of boundary data. We also introduce a projection $\mathrm{pr} : \mathcal{Y}_{\partial U} \to \mathcal{Y}^{\mathcal{C}_d}_{\partial U_d}$, and an inclusion $i_d : \mathcal{Y}^{\mathcal{C}_d}_{\partial U_d} \to \mathcal{Y}_{\partial U}$, which are compatible, i.e., $\mathrm{pr}\circ i_d = 1_{\mathcal{Y}^{\mathcal{C}_d}_{\partial U_d}}$. Given a boundary Lagrangian

$L_{\partial U} : \mathcal{Y}_{\partial U} \to \mathbb{R}$, and a discrete boundary Lagrangian $L^d_{\partial U_d} : \mathcal{Y}^{\mathcal{C}_d}_{\partial U_d} \to \mathbb{R}$, we decompose the error into

$$|L_{\partial U}(\varphi) - L^d_{\partial U_d}(\mathrm{pr}(\varphi))| \leq |L_{\partial U}(\varphi) - L_{\partial U}(i_d(\mathrm{pr}(\varphi)))| \\ + |L_{\partial U}(i_d(\mathrm{pr}(\varphi)) - L_{\partial U_d}(\mathrm{pr}(\varphi))| + |L_{\partial U_d}(\mathrm{pr}(\varphi)) - L^d_{\partial U_d}(\mathrm{pr}(\varphi))|.$$

The first term can be bounded in terms of the sensitivity with respect to the boundary data, the second term is associated with the variational crime of replacing the domain U with U_d, and the third term is the error of the discrete boundary Lagrangian on U_d for projected boundary data.

The multi-Dirac relation is defined by the continuity of the normal momentum (11) across the boundaries of spacetime domains, and it is imposed only weakly or by collocation in multi-Dirac variational integrators. By relying on regularity properties of the boundary-value problem, we aim to relate the convergence properties of the multi-Dirac variational integrator with the three error terms that arise when replacing the boundary Lagrangian with the discrete boundary Lagrangian.

Order-Optimality of Multi-Dirac Integrators. Once the theory of variational error analysis of multi-Dirac integrators is established, it is natural to generalize Theorems 5.1 and 5.2. The first two error terms involve continuous dependence of the boundary-value problem on the domain and the boundary data, and the last error term closely resembles the error term in the ODE analysis.

The analysis of Galerkin multi-Dirac variational integrators will involve a refined Γ-convergence analysis. The sequence of approximation spaces induces a sequence of approximate variational problems, and one needs to relate the rate of convergence of the sequence of minimizers with the best approximation properties of the sequence of approximation spaces. When the Lagrangian density is separable, the requisite coercivity result for the Γ-convergence analysis can be proved.

Reciprocity Theorems. We aim to prove that multi-Dirac variational integrators exhibit discrete reciprocity theorems, such as Lorentz reciprocity in electromagnetism and Betti reciprocity in elasticity. This involves exploring the connection between multisymplecticity and reciprocity. In particular, reciprocity is related to Lagrangian (maximally isotropic) submanifolds (see, §5.6 of [97]), and the multisymplectic form formula (8) is equivalent to $\mathrm{Im}\,\mathbf{d}L_{\partial U}$ being isotropic.

5.2. **Discrete Dirac Mechanics for Interconnected Systems.** Dirac structures [21; 22] provide a natural geometric description of interconnected systems as they can encode the interconnection constraints, and they have been used successfully to model interconnected systems as port-Hamiltonian systems [16]. We aim to construct a discrete Lagrangian formulation of Dirac and multi-Dirac interconnected systems to capitalize on the connection with variational integrators. This will build upon the prior work of me and my collaborators on continuous Dirac interconnection theory [49], discrete Dirac mechanics and geometry [85], and continuous multi-Dirac field theory [124] and geometry [123]. Just as port-Hamiltonian systems provide a framework for interfacing different physical systems—infinite-dimensional, finite-dimensional, electrical, mechanical—and for feedback control design for interconnected systems, interconnected discrete Lagrange–Dirac systems will provide a unified modeling and simulation framework for multiphysics systems with applications to discrete optimal control of interconnected systems.

5.2.1. *Interconnection of Lagrange–Dirac systems [49].* Consider two Lagrange–Dirac systems: (Q_1, L_1, Δ_1) and (Q_2, L_2, Δ_2). Here, Q_i $(i = 1, 2)$ are configuration manifolds, L_i are Lagrangians, and Δ_i are constraint distributions. They have Dirac structures D_{Δ_i}, generalized energies $E_i(q_i, \dot{q}_i, p_i) = \langle p_i, \dot{q}_i\rangle - L(q_i, \dot{q}_i)$, partial vector fields X_i, and they satisfy $(X_i, \mathbf{d}E_i|_{P_i}) \in D_{\Delta_i}$. The ***interconnection*** of these two systems is a system on the product: $Q = Q_1 \times Q_2$, with Lagrangian $L(q_1, q_2, \dot{q}_1, \dot{q}_2) = L_1(q_1, \dot{q}_1) + L_2(q_2, \dot{q}_2)$ and constraint Δ that is a subbundle of $\Delta_1 \times \Delta_2 \subset TQ_1 \oplus TQ_2$. The interaction between the systems is described by an interaction constraint Δ_{int}. Then, the interconnected system satisfies

$$(X_1 \times X_2, \mathbf{d}(E_1 + E_2)|_P) \in D_c,$$

where the interconnection Dirac structure $D_c = (D_{\Delta_1} \oplus D_{\Delta_2}) \bowtie D_{int}$, and the bowtie operator $\bowtie$ is

$$D_A \bowtie D_B \stackrel{\triangle}{=} \{(w, \alpha) \in TT^*Q \oplus T^*T^*Q : w \in \tau_{TT^*Q}(D_A \cap D_B), \alpha - \Omega^\flat_{TT^*Q} w \in (\tau_{TT^*Q}(D_A \cap D_B))^\circ\}.$$

This novel interconnection Dirac structure combines (using the operators in [129]) the Dirac structures on T^*Q_1 and T^*Q_2, and the "Tellegen" structure that encodes the interaction forces.

The corresponding variational formulation involves the Lagrange–d'Alembert–Pontryagin variational principle [49], which extends the Hamilton–Pontryagin principle (1) by including the virtual work of the external forces. The interaction constraints manifest themselves as a compatibility condition (described in terms of a constraint codistribution) on the external forces in each subsystem.

5.2.2. *Specific Research Goals.*

Equivalence-Preserving Discretizations of Forced Systems. When an interconnected system is decomposed into subsystems, constraint forces are introduced. Given a Lagrangian force $f_L : TQ \to T^*Q$, the Lagrange–d'Alembert principle $\delta \int L(q,\dot{q})dt + \int f_L(q,\dot{q}) \cdot \delta q = 0$ yields the forced Euler–Lagrange equations. The representation (L, f_L) of a forced Euler–Lagrange system is not unique since the transformation $L \mapsto L - \psi$ and $f_L \mapsto f_L + \frac{\partial \psi}{\partial q}$ leaves the system invariant. We aim to construct equivalence-preserving discretizations of forced Lagrangian systems so that if two forced Lagrangian systems are equivalent, their discretizations are equivalent as well. Since variational integrators perform better for weakly forced Lagrangian systems, the use of equivalence-preserving discretizations will ensure that the discretization performs well independent of the representation.

Discrete Theory of Interconnections for Lagrange–Dirac Systems. The interconnection Dirac structure is defined in terms of the bowtie operator $\bowtie$ that acts on the space of continuous Dirac structures. We constructed a discrete bowtie operator $\bowtie_d$ that is compatible with discretization, i.e., $(D_A \bowtie D_B)^{d+} = D_A^{d+} \bowtie_d D_B^{d+}$ in [106] for the case of linear configuration spaces. This provides a systematic method of discretizing Lagrange–Dirac systems that are modeled as the interconnection of modular subsystems. In order to expand the class of problems for which can be modeled, we wish to generalize our construction to nonlinear configuration spaces, such as Lie groups and homogeneous spaces.

Continuous and Discrete Theory of Interconnections for Multi-Dirac Field Theories. We aim to extend Dirac interconnection theory to multi-Dirac field theories, which will facilitate the systematic analysis of multiphysics models using the framework of interconnected multi-Dirac field theories. Both fluids and elasticity are multi-Dirac field theories, and it would be interesting to analyze fluid-structure interactions as the interconnection of multi-Dirac field theories.

Discrete Optimal Control of Interconnected Systems. My former postdoc, Prof. Ohsawa, and I established a connection between discrete mechanics and discrete optimal control using discrete Hamilton–Jacobi theory in [103; 104]. Using this, we will construct discrete control algorithms for interconnected systems, such as multi-agent robotic networks. The inherently local nature of the control equations that arise from discrete variational principles will yield distributed discrete control algorithms, and stability of the control algorithms can be established using Lyapunov techniques.

5.3. **Discrete Canonical Formulation of Gauge Field Theories.** There are two equivalent methods for describing field theories: (i) the covariant multisymplectic approach, where the solution is a section of the configuration bundle over spacetime; (ii) the canonical (or instantaneous) approach [36], 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***, which can recover some of the equations of motion automatically from the gauge symmetry, and this is particularly important for covariant field theories, such as general relativity.

Electromagnetism as a Gauge 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,

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

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.

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 [32]. Covariance can be built into a field theory by augmenting the configuration bundle with a second copy of the base space [15]. 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. In relativity, the adjoint formulation reduces to the familiar ADM equations of relativity [6]. We aim to develop a discrete treatment of covariant field theories that clarifies the relationship between the covariant and instantaneous approaches. This will build upon the discrete multi-Dirac field theories proposed in Section 5.1. Additionally, it will rely on generalizing the discrete Hamiltonian formulation [89; 125] that was developed by my former visiting Ph.D. student, Dr. Zhang, former postdoc, Dr. Vankerschaver, and I, and which is described below.

5.3.1. *Hamiltonian Variational Integrators [89].* 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 is achieved by considering the Type II analogue of Jacobi's solution, given by

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

A computable Galerkin 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

$$q_{k+1} = D_2 H_d^+(q_k, p_{k+1}), \qquad p_k = D_1 H_d^+(q_k, p_{k+1}). \tag{12}$$

5.3.2. *Type II Generating Functional and Boundary Hamiltonian [125].* 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 first construct a discrete covariant Hamiltonian formulation by discretizing the ***boundary Hamiltonian***, which is the exact Type II generating functional

$$H_{\partial U}(\varphi_A, \pi_B) = \operatorname*{ext}_{\substack{\phi_{|A}=\varphi_A,\\ \pi_{|B}=\pi_B}} \int_B p_a^\mu \phi^a \, d^n x_\mu - \int_U (p_a^\mu \phi^a_{,\mu} - H(\phi^a, p_a^\mu)) \, d^{n+1}x, \tag{13}$$

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 (12), are given by

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

5.3.3. *Specific Research Goals.*

Discrete Noether's Second Theorem. We aim to prove a discrete analogue of Noether's second theorem in the context of multi-Dirac discretizations of gauge field theories. This will allow us to systematically construct discrete gauge field theories in which the discrete analogues of the equations associated with Noether's second theorem arise naturally from the choice of discretization of the dynamic and kinematic fields, and obtain a compatible discretization of the gauge field theory.

Gauge Freedom in Discretizations of Field Theories. When obtaining analytical solutions of a gauge field theory, a gauge condition is imposed to obtain a well-posed evolution problem. A well-chosen gauge condition can dramatically simplify the process of deriving analytical solutions, but it is much more challenging to do this for realistic problems. While the solution of realistic problems in gauge theory is oftentimes beyond the scope of analytical methods, and numerical approximation techniques are adopted instead, the tendency to fix the gauge *a priori* remains.

Gauge invariance plays a fundamental role in gauge theory, so we aim to study discretizations that retain the gauge variables when discretizing the field theory. Discretization tends to break the gauge invariance, but by allowing the discrete gauge to be specified by the discrete variational principle, instead of being fixed, we aim to construct gauge-adaptive variational integrators and prove that the discrete momentum map associated with the gauge symmetry is conserved.

Hamiltonian Variational Integrators for Field Theories. We will construct Hamiltonian variational integrators for PDEs by discretizing the variational characterization of the boundary Hamiltonian (13) to obtain Galerkin discrete boundary Hamiltonians. We will also derive a discrete Hamilton's phase space variational principle and the discrete Hamilton's equations for PDEs.

Relating the Discrete Covariant Approach and the Initial-Value Formulation. The initial-value formulation involves a discrete Lagrangian that approximates the action integral of the instantaneous Lagrangian over a time interval, and in turn the instantaneous Lagrangian is an integral of the Lagrangian density over a Cauchy surface. Thus, the discrete Lagrangian approximates an integral of the Lagrangian density over a spacetime element, as does the discrete boundary Lagrangian used in the discrete covariant approach. It would be interesting to explore the relationship between the discrete boundary Lagrangian and the discrete Lagrangian, and through this, the relationship between the discrete covariant formulation and the initial-value formulation.

The Discrete Energy-Momentum Map. The continuous energy-momentum map Φ can be viewed, in an integrated sense, as the trace onto a Cauchy surface of the covariant momentum map associated with the gauge group. We aim to develop a discrete analogue of the energy-momentum map by integrating the discrete covariant momentum map over a discrete Cauchy surface, and relate it to discrete analogues of the instantaneous Hamiltonian and adjoint equations, by analogy with the continuous case described below.

The Discrete Adjoint Formulation of Gauge Field Theories. By applying the discrete Hamilton–Pontryagin principle to covariant field theories, we will construct a discrete Hamiltonian formulation with respect to a given spacetime slicing and the induced slicing of the configuration bundle. We will explore the

discrete analogue of the instantaneous Hamiltonian given by

$$H = \int_\Sigma \sum_i \alpha_i \Phi^i(\psi, \rho) d\Sigma,$$

where (ψ, ρ) are dynamic fields, Φ is the energy-momentum map, and α_i are ***atlas fields*** related to the gauge freedom. And, from this, we will derive a discrete version of the ***adjoint formulation***,

$$\frac{d}{d\lambda}\begin{pmatrix}\psi\\ \rho\end{pmatrix} = \mathbb{J} \cdot \sum_i \left[D\Phi^i(\psi(\lambda), \rho(\lambda))\right]^* \alpha_i,$$

where λ is a slicing parameter. In a discrete spacetime mesh-adapting simulation, the atlas fields α_i will specify the way in which the physical mesh moves with respect to the fixed computational mesh. A discrete multi-Dirac theory for covariant fields will lead to algorithms for spacetime adaptive integration of systems ranging from elastica and fluids to electromagnetism.

Gauge Symmetry Preserving Discretizations. In order to apply discrete gauge theory, it is necessary to construct finite-element spaces that preserve the gauge symmetry at the discrete level. Motivated by our two applications, electromagnetism and general relativity, we will develop spacetime finite-element exterior calculus, and Lorentzian metric-valued geodesic finite-elements.

Spacetime Finite-Element Exterior Calculus. Finite-element exterior calculus [3; 4] provides a systematic framework for discretizing the de Rham complex of differential forms, and provides a theoretical framework for the construction of stable, compatible mixed finite-element discretizations. They can be systematically constructed from the Whitney forms. Whitney forms are expressed in terms of barycentric coordinates, but this is a suboptimal representation when the explicit computation of the Hodge star of a differential form is necessary, particularly when the Hodge star is taken with respect to a variety of metrics that arise as material properties in a field theory. For example, in electromagnetism, the electric field E and the electric displacement are related by a Hodge star operation associated with the permittivity of the medium, and the magnetic flux density B and the magnetic field intensity H are also related by a Hodge star associated with the magnetic permeability. In order to avoid this issue, we introduced a characterization of a Whitney form and its Hodge dual that is valid for any choice of coordinates, which allows one to choose a coordinate representation that is most suitable for the metric which the Hodge star is taken with respect to.

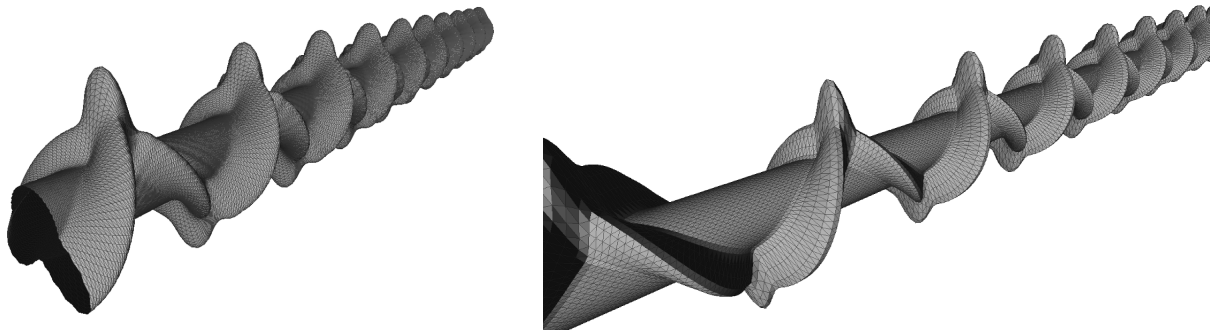
Recently, my former Ph.D. student, Prof. Salamon, and I derived in [110] a characterization of Whitney forms that allows one to explicitly characterize the Hodge dual of the space of Whitney forms. Let ${}^j w_\theta$ represent a Whitney j-form defined over a j-subsimplex θ of an n-simplex σ, let $\tau = \sigma \smallsetminus \theta$ and x represent the position vector. Then, in any flat manifold:

$${}^j w_\theta = \frac{sgn(\theta \cup \tau)}{\star vol(\sigma)} \frac{j!}{n!} \star \bigwedge_{v_k \in \tau} (v_k - x)^\flat,$$

where $vol(\sigma) = \frac{1}{n!}\bigwedge_{i=1}^n (v_i - v_0)^\flat$. By generalizing this using the approach in [108], we will construct higher-order spacetime Whitney forms, and discretize the gauge group for electromagnetism.

The coordinate-independent expressions for Whitney forms that were described above allows us to construct numerical approximations of the wave equation. More than being coordinate-independent, the algorithm is coordinate-free: it uses an abstract spacetime simplicial mesh endowed with Lorentzian distance information on the edges. In particular, the mesh on spacetime is not a tensor-product mesh, and the method does not rely on either a local or global embedding of the simplicial mesh. The simulation indicates that the numerical method performs dramatically better if the spacetime mesh is aligned with the characteristics, which suggests that the use of adaptive spacetime meshing may significantly improve the quality of the numerical results.

Geodesic Finite-Elements on Symmetric Spaces. We will develop a discretization for general relativity using geodesic finite-elements [38; 111; 112] applied to the space of Lorentzian metrics. We will endow the space of Lorentzian metrics with a Riemannian metric, which is achieved by realizing the space of Lorentzian metrics as a symmetric space $GL_4(\mathbb{R})/O_{1,3}$, where $O_{1,3}$ acts on $GL_4(\mathbb{R})$ by conjugation, and the involution $s : \mathfrak{gl}_4 \to \mathfrak{gl}_4$ is given by $s(v) = -bv^T b$, where $b = \mathrm{diag}(-1, 1, 1, 1)$. The Riemannian metric on $GL_4(\mathbb{R})$ induces a well-defined Riemannian metric on the space of Lorentzian metrics, since it is a symmetric space.



(a) Unadapted spacetime mesh exhibits the effect of numerical dispersion, but this effect is reduced on meshes with higher spatio-temporal resolution.

(b) An adapted spacetime mesh that is aligned along the integral lines, i.e., the light-cone, yields the exact solution, even at low resolution (40 nodes per space-like slice).

Figure 9: The $\mathbb{R}^{1+1}$ wave equation with a spatial periodic boundary condition discretized using spacetime Whitney forms and a multisymplectic variational integrator. The cylinder's axis is the time direction; taking slices perpendicular to the time direction yields snapshots of the wave on the circle.

Given a Riemannian manifold (M, g), the geodesic finite-element $\varphi : \Delta^n \to M$ associated with a set of linear space finite-elements $\{v_i : \Delta^n \to \mathbb{R}\}_{i=0}^n$ is given by the Fréchet (or Karcher) mean,

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

where the optimization problem involved can be solved using optimization algorithms developed for matrix manifolds [2]. The spatial derivatives of the geodesic finite-element can be computed in terms of an associated optimization problem [113]. The advantage of the geodesic finite-element approach is that it inherits the approximation properties of the underlying linear space finite-element [39].

Group-Equivariant Interpolation on Symmetric Spaces via the Generalized Polar Decomposition. As an alternative to the approach based on geodesic finite-elements, which requires one to perform numerical optimization on the symmetric space in order to evaluate the geodesic finite-element, we developed an alternative but related approach that is more computationally efficient based on the Cartan decomposition,

$$\mathfrak{g} = \mathfrak{p} \oplus \mathfrak{k}, \tag{14}$$

which can be viewed as a generalization of the polar decomposition or the singular value decomposition. This leads to the following commutative diagram,

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

In particular, the last line of the diagram yields a local diffeomorphism between the symmetric space $\mathcal{S}$ and its associated Lie triple system $\mathfrak{p}$, which is a linear space. This can then be used to construct a group-equivariant interpolant, and in particular, the interpolant [30] and its associated Fréchet derivatives [31] can be efficiently computed using iterative methods for computing the generalized polar decomposition.

5.4. **Discrete Hamilton–Jacobi Theory for Lagrangian PDEs and Control Theory.** In classical mechanics, the Hamilton–Jacobi equation arises as a PDE that is satisfied by the action integral. Conversely, a solution of the Hamilton–Jacobi equation yields a generating function for the family of canonical transformations that correspond to solutions of Hamilton's equations. This relationship provides the theoretical basis

for exactly integrating Hamilton's equations using the method of separation of variables. By considering the control Hamiltonian of an optimal control problem, one can obtain the Hamilton–Jacobi–Bellman equation that plays a critical role in optimal control theory. Recent advances in discrete Hamiltonian mechanics [89], continuous [88; 91] and discrete Hamilton–Jacobi theory [104], and generating functionals for multisymplectic PDEs [125] will allow us to develop a discrete Hamilton–Jacobi theory for multisymplectic PDEs, and the Bellman equations for discrete PDE optimal control problems.

5.4.1. *Discrete Hamilton–Jacobi and the Bellman Equations [103; 104].* In the context of discrete variational mechanics, a discrete Hamilton–Jacobi theory was developed by my postdoctoral fellow, Prof. Ohsawa, and I in [104]. The ***discrete Hamilton–Jacobi equation***,

$$S_{\mathrm{d}}^{k+1}(q_{k+1}) - S_{\mathrm{d}}^{k}(q_k) - DS_{\mathrm{d}}^{k+1}(q_{k+1}) \cdot q_{k+1} + H_{\mathrm{d}}^{+}\left(q_k, DS_{\mathrm{d}}^{k+1}(q_{k+1})\right) = 0,$$

can be derived from a discrete analogue of Jacobi's solution, i.e., the discrete action sum evaluated on a solution of the discrete Hamilton's equations, and computing how the discrete action sum changes in discrete time. Discrete optimal control problems involve minimizing a discrete cost functional, $\min_{u_{\mathrm{d}}} J_{\mathrm{d}} = \min_{u_{\mathrm{d}}} \sum_{k=0}^{N-1} C_{\mathrm{d}}(q_k, u_k)$, subject to the constraint $q_{k+1} = f_{\mathrm{d}}(q_k, u_k)$. This gives a discrete control Hamiltonian,

$$H_d^{+}(q_k, p_{k+1}) = \operatorname*{ext}_{u_k} \left[p_{k+1} \cdot f_{\mathrm{d}}(q_k, u_k) - C_{\mathrm{d}}(q_k, u_k)\right].$$

The discrete action sum in terms of the discrete control Hamiltonian is the ***optimal discrete cost-to-go function***, and the discrete Hamilton–Jacobi equation yields the Bellman equations of discrete optimal control,

$$\min_{u_k} \left(J_{\mathrm{d}}^{k+1}(f_{\mathrm{d}}(q_k, u_k)) + C_{\mathrm{d}}(q_k, u_k)\right) = J_{\mathrm{d}}^{k}(q_k).$$

The significance of deriving the discrete Hamilton–Jacobi equations and Bellman equations in this way is that it allows one to tap into the Galerkin variational integrator methods developed for discrete Hamiltonian problems in [89], that are valid even if the Hamiltonian is degenerate. Furthermore, it allows us to extend the construction to the case of Lagrangian and Hamiltonian PDEs in a natural way by considering the PDE analogue of Jacobi's solution that is given by the boundary Lagrangian.

5.4.2. *Specific Research Goals.*

Hamilton–Jacobi–Bellman for Optimal Control of Interconnected Systems. We will obtain a continuous and discrete geometric formulation of optimal control for interconnected systems by combining Dirac interconnection theory with Hamilton–Jacobi theory. The mechanical nature of the resulting controlled system makes it particularly amenable to the use of Lyapunov techniques to prove stability. Modeling robotic networks as an interconnected system will allow us to construct distributed discrete control algorithms, due to the inherently local nature of the control equations that arise from discrete variational principles.

Hamilton–Jacobi–Bellman for PDE Optimal Control Problems. We will derive the De Donder–Weyl Hamilton–Jacobi theory for fields using the boundary Lagrangian and boundary Hamiltonian, and relate it to optimal control by considering the control boundary Hamiltonian. This will yield a Hamilton–Jacobi–Bellman equation for PDE optimal control problems. A similar discrete analysis using a discrete boundary Lagrangian will yield discrete PDE optimal control that is related to multisymplectic variational integrators.

5.5. **Variational Integrators for Adjoint Sensitivity and Optimization.** In addition to expanding the applicability of variational integrators to noncanonical and degenerate Lagrangian systems, we propose to apply them to systems which have no apparent geometric or variational structure. Sanz-Serna [114] observed that symplectic Runge–Kutta methods have desirable properties when applied to nonvariational problems, such as arbitrary systems of differential equations and their adjoint equations. In particular, the adjoint of a Runge–Kutta discretization of a system of differential equations is equivalent to a Runge–Kutta discretization of the continuous adjoint equations if and only if the method is symplectic. This manifested itself in the discretization of two-point optimal control problems, where variational discretizations were able to converge using single-shooting [63], whereas non-symplectic discretizations required the use of multiple-shooting.

We propose to combine the method of formal Lagrangians with Dirac variational integrators for Lagrangian field theories and systematic discretizations of generating functionals. This will allow us to apply variational integrators to the computation of adjoint equations for nonvariational differential equations, which is broadly

applicable and of fundamental importance in optimal control, uncertainty quantification, optimal design, and adaptivity based on adjoint sensitivity analysis.

Formal Lagrangians and Adjoint Equations. Ibragimov [48] shows that a system of differential equations and its adjoint arise as the Euler–Lagrange equations of a formal Lagrangian. Variational integrators based on formal Lagrangians for nonvariational PDEs were constructed in [51], which yielded numerical integrators that respect the conservation laws of the original system of equations. Here, we recall the definition of the adjoint operator from Ibragimov [47], which provides a simple way of computing the adjoint of nonlinear differential equations.

Definition 5.3 (Definition 2.2 of [47])**.** *Given a system of s-th order differential equations,*

$$F_\alpha(x, u, \dots, u_{(s)}) = 0, \qquad \alpha = 1, \dots, m,$$

with independent variables x, and dependent variables u, the adjoint equations are defined by,

$$F^*_\alpha(x, u, v, \dots, u_{(s)}, v_{(s)}) \equiv \frac{\delta(v^\beta F_\beta)}{\delta u^\alpha} = 0, \qquad \alpha = 1, \dots m,$$

where $\frac{\delta}{\delta u^\alpha} = \frac{\partial}{\partial u^\alpha} + \sum_{s=1}^{\infty}(-1)^s D_{i_1} \dots D_{i_s} \frac{\partial}{\partial u^\alpha_{i_1 \dots i_s}}$ is the variational derivative.

The following theorem states that a system of differential equations and its adjoint has a variational formulation, even if the original system of equations is nonvariational.

Theorem 5.4 (Theorem 2.3 of [47])**.** *The Euler–Lagrange equations for the Lagrangian $\mathcal{L} = v^\beta F_\beta$ recover any system of s-th order differential equations together with its adjoint equations.*

In retrospect, the variational characterization of differential equations and their adjoints can be obtained by applying the Pontryagin Maximum Principle [107] to an unforced system. Alternatively, the equations and its adjoint describe the cotangent lifted trajectory, which is always symplectic and hence locally Hamiltonian. The differential equations, linearized equations, and adjoint equations are naturally described by Dirac and multi-Dirac mechanics on the Pontryagin bundle $TT^*Q \oplus T^*T^*Q$ or the Pontryagin jet bundle $J^1Y \times_Y J^1Y^\star$, and can be discretized by applying the Dirac variational integrators [85] and discrete Hamilton–Jacobi theory [104] that we have developed.

Bregman Lagrangians and Hamiltonians. Consider the optimization problem,

$$\min_{x \in X} f(x),$$

where $X \subset \mathbb{R}^n$ is a convex domain and $f : X \to \mathbb{R}$ is a continuously differentiable convex function, with a unique minimizer $x^* \in X$. Given a convex function $h : X \to \mathbb{R}$, an alternative (asymmetric) notion of distance between two points can be obtained by considering the *Bregman divergence*,

$$D_h(y, x) = h(y) - h(x) - \langle \nabla h(x), y - x \rangle,$$

which is nonnegative as h is convex. When x is close to y, this approximates the *Hessian metric*,

$$D_h(y, x) \approx \frac{1}{2}\langle y - x, \nabla^2 h(x)(y - x)\rangle \equiv \frac{1}{2}\|y - x\|^2_{\nabla^2 h(x)}.$$

The *Bregman Lagrangian* was introduced in [126], and is given by,

$$L(x, v, t) = e^{\alpha(t)+\gamma(t)}(D_h(x + e^{-\alpha(t)}v, x) - e^{\beta(t)} f(x)),$$

and the *Bregman Hamiltonian* is given by

$$H(x, p, t) = e^{\alpha(t)+\gamma(t)}(D_{h^*}(\nabla h(x) + e^{-\gamma(t)}p, \nabla h(x)) + e^{\beta(t)} f(x)),$$

where h^* is the convex dual of h. Under the growth conditions $\dot\beta \le e^\alpha$, $\dot\gamma = e^\alpha$, the solutions of the associated Euler–Lagrange equations exhibit the following convergence property [126],

$$f(x(t)) - f(x^*) \le \mathcal{O}(e^{-\beta(t)}),$$

which was shown using a Lyapunov function approach. In particular, for $p > 0$, if we choose $\alpha(t) = \log p - \log t$, $\beta(t) = p \log t + \log C$, $\gamma(t) = p \log t$, where $C > 0$, then the growth condition above is satisfied, and the Euler–Lagrange flow converges to the optimal value in $\mathcal{O}(1/t^p)$.

5.5.1. *Specific Research Goals.*

Dirac and Multi-Dirac Variational Integrators for Formal Lagrangian Systems. Formal Lagrangians provides a variational characterization of a system of differential equations and its adjoints. Since the formal Lagrangian is degenerate, we propose to explore this intriguing connection using Dirac and multi-Dirac variational integrators, which are well-suited for degenerate systems.

Hamiltonian Variational Integrators for Formal Lagrangian Systems. Observe that for equations of the form $\dot{q} = f(q)$, the formal Lagrangian $L = p^T(\dot{q} - f(q))$ is related by the Legendre transform to a formal Hamiltonian $H(q,p) = p^T f(q)$, which is precisely what we obtain by applying the Pontryagin Maximum Principle to an unforced system. Then, the formal Hamiltonian can be discretized by using the Hamiltonian variational integrators we introduced in [89].

Applications of Formal Lagrangians to Discretizations of Adjoint Systems. We will apply Dirac variational integrators to the geometric numerical integration of adjoint equations. In particular, we will explore the connection between the direct and indirect methods of discrete optimal control in the context of formal Lagrangians and the Pontryagin Maximum Principle. We will also apply Dirac variational integrators to uncertainty quantification and optimal estimation.

Symplectic Discretization of Accelerated Optimization Techniques. We will consider variational discretizations of the Bregman Lagrangian and Hamiltonian, including the recently developed adaptive variational integrators [117] that allow for arbitrary monitor functions, and explore their structure-preservation and convergence properties when applied to optimization problems.

5.6. **Information Geometry and Discrete Mechanics.** A *divergence function* is an asymmetric distance between two probability densities that induces differential geometric structures in the context of information geometry, and yields efficient machine learning algorithms that minimize the duality gap. The divergence function has an interpretation as a discrete Lagrangian. Let the configuration manifold be the statistical manifold, i.e., $Q = \mathbb{M}$, and the discrete Lagrangian be the divergence function $L_d = \mathcal{D}$. With this identification, the symplectic structure on $\mathbb{M} \times \mathbb{M}$ from information geometry agrees with the discrete symplectic structure for discrete mechanics on $Q \times Q$. A divergence function also generates the Riemannian metric and affine connection structures. The following theorem addresses the extent to which we can view the divergence function as corresponding to the exact Lagrangian flow of an associated continuous Lagrangian.

Theorem 5.5. *The exact discrete Lagrangian $L_d^E(q(0), q(h), h)$ can be approximated by a divergence function $\mathcal{D}(q(0), q(h))$ up to third order $\mathcal{O}(h^3)$ accuracy*

$$L_d^E(q(0), q(h), h) = hL(q(0), v(0)) + \mathcal{D}(q(0), q(h)) + \mathcal{O}(h^3)$$

if and only if Q is a Hessian manifold, i.e., $\mathcal{D}$ is the canonical divergence $\mathcal{B}$.

This result relies on backward error analysis [7; 41; 109], which relates a discrete time map to the time-h flow map of a continuous dynamical system. Thus, machine and statistical learning algorithms in the context of information geometry can be realized as dynamical systems on the space of probability distributions, which yields a unified theory of information-mechanical systems. The same way that linear algebra algorithms viewed as flow maps of smooth dynamical systems [19], or optimization algorithms such as Newton's method viewed as the Euler approximation of the continuous Newton flow [45], have lead to novel numerical algorithms by allowing one to systematically apply numerical ODE techniques to the discretization of such problems, the connection between discrete learning algorithms, information geometry, and geometric mechanics promises to yield similar dividends.

6. Conclusion

Computational geometric mechanics and its applications to geometric control theory promises to be a truly multidisciplinary field, drawing upon techniques from differential geometry, numerical analysis, mechanics, and control theory. In particular, there has been a fruitful cross-fertilization of ideas between discrete geometry and computer graphics. More significantly, the resulting discrete differential geometric tools are widely applicable, even to problems that are not explicitly cast in the language of differential geometry.

The unifying framework of discrete Dirac mechanics and discrete Dirac structures allow one to handle Lagrangian and Hamiltonian descriptions of the mechanics, as well as symplectic and Poisson descriptions of the geometry. A critical advantage is that nonholonomic constraints and interconnections between systems

can be encoded in Dirac structures, and as such, discrete Dirac geometry and mechanics provides important insights into the discretization of nonholonomic mechanics and interconnected systems.

There are deep links between discrete mechanics and discrete optimal control, and in turn, the notion of optimal control is closely related to that of optimal design. Indeed, one can view optimal design as a static optimal control problem. The next stage of evolution for numerical computation is not simply to predict model behavior, but rather to enable simulation driven design using adjoint techniques.

This is part of a longer term project to develop theoretical and computational infrastructure to enable rapid prototyping and interactive design space exploration for complex anthropogenic interconnected systems. Novel geometric structure-preserving numerical methods that explicitly incorporate notions of *modularity*, *reusability*, and *interconnection* will enable high-fidelity simulation of the highly-complex multiphysics systems arising from engineering design processes. To achieve this, we will develop scalable and algorithmically transparent methods for robust, accurate, and efficient large-scale simulations through the use of modular and reusable submodels with arbitrary interconnection topology.

This will without a doubt involve a vast interdisciplinary effort, but the broad background I have in mathematics, applied mathematics, physics, and engineering will enable me to bridge traditional boundaries, and facilitate collaboration between fields.

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