Melvin Leok: Research Summary

My research has focused on developing the mathematical foundations of discrete 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 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.

Discrete Geometry. 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 discretizations of field and gauge theories is the development of discrete exterior calculus [19; 20] and discrete connections on principal bundles [67]. This yields compatible discretizations of differential operators on unstructured meshes, and discrete analogues of Hodge–de Rham theory, the Poincaré lemma, Levi-Civita connections and their associated curvatures, as well as an explicit semi-global characterization of discrete reduced spaces arising in discrete reduction by symmetry.

Discrete Mechanics. While Lagrangian systems are endowed with 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 of these structural properties as possible, and towards this end we developed a discrete theory of abelian Routh reduction [31] for systems with symmetry, as well as a generalization of variational integrators to flows on Lie groups and homogeneous spaces [22; 34; 39; 40; 50]. More generally, generalized Galerkin variational integrators [60] 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. It is also possible to handle degenerate Hamiltonian systems without the need to transform into the Lagrangian framework [66].

Computational Geometric Control Theory. By developing a theory of geometric control that is predicated on the discrete-time dynamics associated with variational integrators, and does not introduce any additional approximations, one obtains numerical control algorithms which are geometric structure-preserving and exhibit good long-time behavior. This approach allows us to develop a discrete method of controlled Lagrangians [7–9; 11] for stabilizing relative equilibria. Motivated by applications in robotics, astrodynamics, and autonomous vehicles, we have also developed discrete optimal control on Lie groups [10; 30; 35; 36; 44; 49] and in that setting, studied geometric phase based control [43], reconfiguration of formations of spacecraft using combinatorial optimization [41], time optimal control [45], articulated multi-body systems in space [47] and in perfect fluids [51; 53], tethered spacecraft [52; 55; 56], and autonomous UAVs [54; 58; 59]. We also studied global state estimation [37; 42; 48] and uncertainty propagation on Lie groups [38; 46].

Immediate Research Plans. We have developed discrete Dirac mechanics and discrete Dirac structures [62; 63], which provide a unified treatment of Lagrangian and Hamiltonian mechanics, and symplectic and Poisson structures, respectively. These results are related by the property that Hamilton–Pontryagin integrators preserve the discrete Dirac structure.

Hierarchical, modular and interconnected models of complicated engineering systems are ubiquitous, and the immediate plan is to generalize discrete Dirac mechanics to the case of interconnected Lagrange–Dirac mechanical systems, which will lead to a unified, and intrinsically modular treatment of interconnected systems in continuous time, discrete time, and in computations. This will provide a Lagrangian alternative to the port-Hamiltonian framework, which will more naturally handling covariant systems, allow more general interconnection constraints, and have both a variational and geometric description of the dynamics.

Discrete Dirac structures are intimately related to the geometry of symplectic maps and generating functions, and this provides a natural framework for developing a discrete Hamilton–Jacobi theory [81; 82] and its nonholonomic generalization, as well as the discrete Hamilton–Jacobi–Bellman equation. A combination of discrete Hamilton–Jacobi theory and discrete Hamiltonian mechanics [66] leads to arbitrarily high order of accuracy generalizations of the Bellman equation.

EXTENDED RESEARCH STATEMENT

MELVIN LEOK

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 [71].

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* [28], 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 partially supported by single investigator grants in applied and computational mathematics and engineering, DMS-0726263, DMS-1001521, CMMI-1029445, a *Faculty Early Career Development (CAREER) Award*, DMS-1010687, and a *Focused Research Group (FRG) Award*, DMS-1065972, from the National Science Foundation.

In recognition of the growing impact of the nascent field of computational geometric mechanics and computational geometric control theory, I received the *SciCADE New Talent Award*, *SIAM Student Paper Prize*, and *Leslie Fox Prize in Numerical Analysis*. In addition, my former graduate student, Dr. Taeyoung Lee, was a finalist at the *BGCE Computational Science and Engineering Student Paper Prize* at the SIAM Conference on Computational Science and Engineering in 2007.

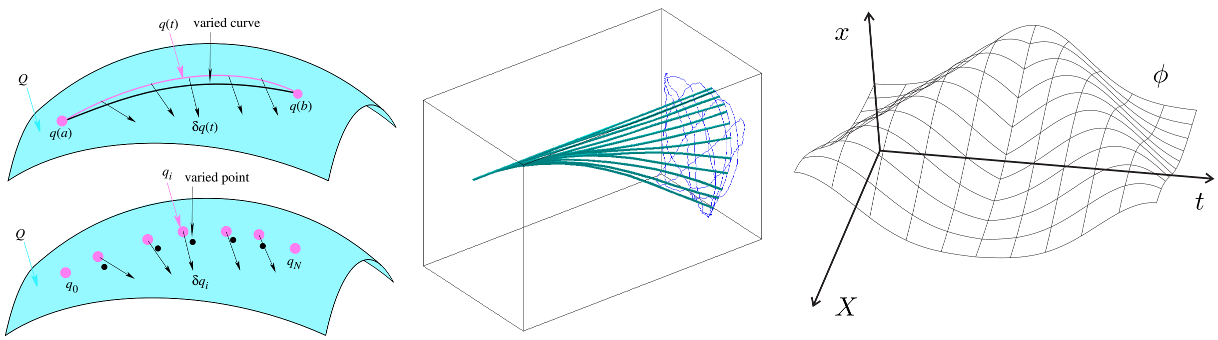
Geometric Integration. Geometric integration aims to construct numerical methods that preserve the geometric structure of a continuous dynamical system. In many problems arising from science and engineering, such as solar system dynamics and molecular dynamics, the underlying geometric structure affects 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 [4]; Smale [86, 87], 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 [17; 21], elasticity [74], field theory, and geometric control theory [13].

Computational Geometric Mechanics. Computational geometric mechanics is concerned with constructing geometric integrators for Lagrangian and Hamiltonian mechanical systems. Variational integrators [75], 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.

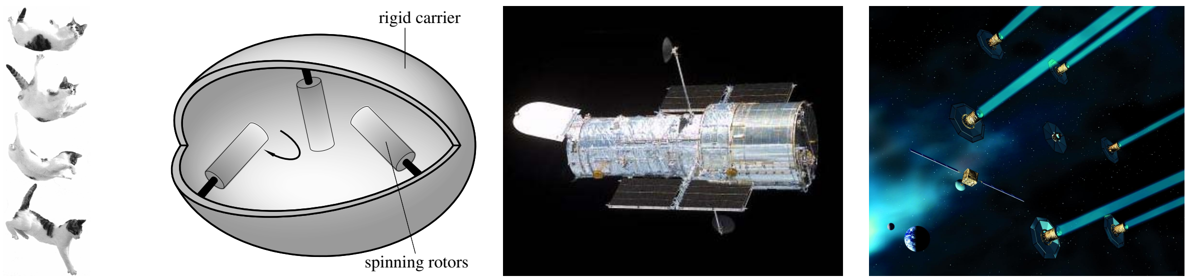
2. Background Material

2.1. **Standard Formulation of Discrete Mechanics.** The standard formulation of discrete variational mechanics [75] is to consider the ***discrete Hamilton's principle*** (see Figure 1(a)), $\delta\mathbb{S}_d = 0$, where the ***discrete action sum***, $\mathbb{S}_d : Q^{n+1} \to \mathbb{R}$, is given by

$$\mathbb{S}_d(q_0, q_1, \dots, q_n) = \sum\nolimits_{i=0}^{n-1} L_d(q_i, q_{i+1}).$$

The ***discrete Lagrangian***, $L_d : Q \times Q \to \mathbb{R}$, is a generating function of the symplectic flow, and is an approximation to the ***exact discrete Lagrangian***,

$$L_d^E(q_0, q_1; h) = \int_0^h L(q_{01}(t), \dot{q}_{01}(t)) dt, \tag{1}$$



(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.

where $q_{01}(0) = q_0$, $q_{01}(h) = q_1$, and q_{01} satisfies the Euler–Lagrange equation in the time interval $(0, h)$. The exact discrete Lagrangian is related to the Jacobi solution of the Hamilton–Jacobi equation. Alternatively, one can characterize the exact discrete Lagrangian in the following way,

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

The exact discrete Lagrangian generates the exact discrete time flow of a Lagrangian system, but cannot be computed explicitly. Instead, these two characterizations of the exact discrete Lagrangian lead to two general approaches for constructing variational integrators.

The discrete variational principle then yields the **discrete Euler–Lagrange (DEL)** equation,

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

where D_i denotes a partial derivative with respect to the i-th argument. This implicitly defines the **discrete Lagrangian map** $F_{L_d} : (q_{k-1}, q_k) \mapsto (q_k, q_{k+1})$ for initial conditions (q_{k-1}, q_k) that are sufficiently close to the diagonal of $Q \times Q$. This is equivalent to the **implicit discrete Euler–Lagrange (IDEL)** equations,

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

which implicitly defines the **discrete Hamiltonian map** $\tilde{F}_{L_d} : (q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$, where the discrete Lagrangian is the Type I generating function of the symplectic transformation. The correspondence between continuous and discrete mechanics is summarized in Figure 3.

2.2. **Multisymplectic Geometry.** The variational principle for Hamiltonian PDEs involve a multisymplectic formulation [76; 77]. The ***base space*** $\mathcal{X}$ 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***, $\pi : Y \to \mathcal{X}$. The configuration of the system is specified by a section of Y over $\mathcal{X}$, which is a continuous map $\phi : \mathcal{X} \to Y$, such that $\pi \circ \phi = 1_{\mathcal{X}}$. This means that for every $(t, x) \in \mathcal{X}$, $\phi((t, x))$ is in the fiber over (t, x), which is $\pi^{-1}((t, x))$.

For ODEs, the Lagrangian depends on position and its time derivative, which is an element of the tangent bundle TQ, and the action is obtained by integrating the Lagrangian in time. In the multisymplectic case, the Lagrangian density is dependent on the field variables and the partial derivatives of the field variables with respect to the spacetime variables, and the action integral is obtained by integrating the Lagrangian density over a region of spacetime. The multisymplectic analogue of the tangent bundle is the ***first jet bundle*** $J^1 Y$, consisting of the configuration bundle Y, and the first partial derivatives of the field variables with respect to the independent variables. In coordinates, we have $\phi(x^0, \ldots, x^n) = (x^0, \ldots x^n, y^1, \ldots y^m)$, which allows us to denote the partial derivatives by $v^a_\mu = y^a{}_{,\mu} = \partial y^a / \partial x^\mu$. We can think of $J^1 Y$ as a fiber bundle over $\mathcal{X}$. Given a section $\phi : \mathcal{X} \to Y$, we obtain its ***first jet extension***, $j^1\phi : \mathcal{X} \to J^1 Y$, that is given

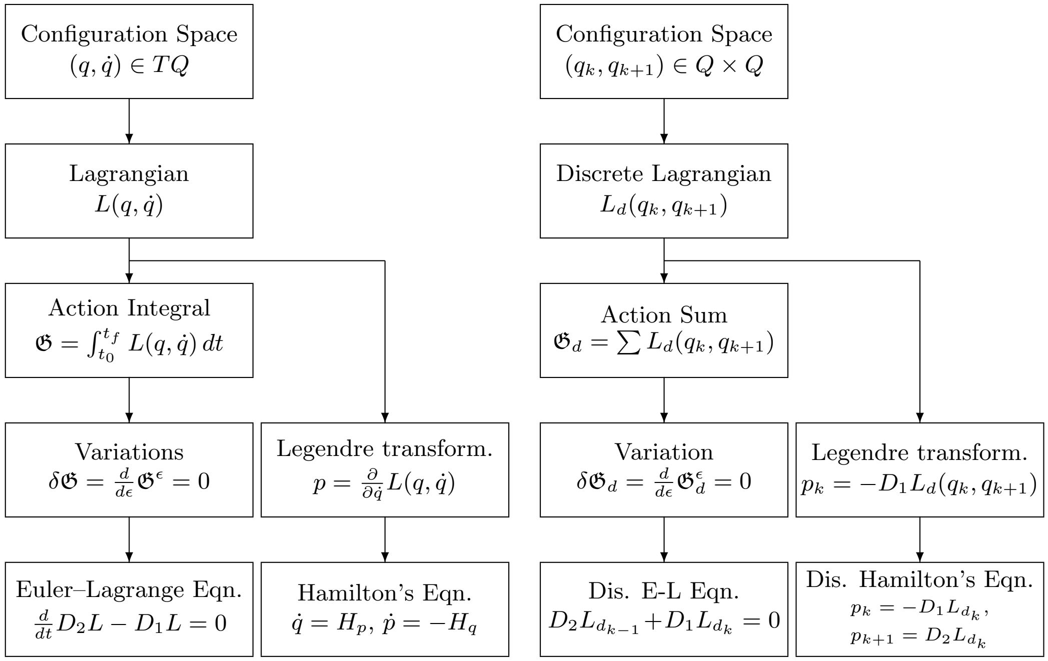


Figure 3: Correspondence between continuous and discrete mechanics

by

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

which is a section of the fiber bundle J^1Y over $\mathcal{X}$. The Lagrangian density is a map $L : J^1Y \to \Omega^{n+1}(\mathcal{X})$. Given the action functional, $\mathcal{S}(\phi) = \int_{\mathcal{X}} L(j^1\phi)$, Hamilton's principle states that $\delta\mathcal{S} = 0$. Multisymplectic variational integrators for Hamiltonian PDEs can be obtained by drawing upon approximation theory to choose an appropriate finite-dimensional function space to represent sections of the configuration bundle, and a quadrature method to approximate the action integral.

2.3. **Desirable Properties of Variational Integrators.**

Symplecticity. Given a discrete Lagrangian L_d, one obtains a discrete fiber derivative, $\mathbb{F}L_d : (q_0, q_1) \mapsto (q_0, -D_1 L_d(q_0, q_1))$. 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 [83].

Approximate Energy Conservation. While variational integrators do not exactly preserve energy, backward error analysis [5; 26; 27; 85] 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 [69], nonsmooth collisions [23], stochastic systems [12], nonholonomic systems [18], and constrained systems [70]. 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 [60]. 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 [39; 40] and homogeneous spaces [50], or exhibit multiple timescales [69; 88].

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)

⇓

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 [19; 20].* A theory of discrete exterior calculus on simplicial complexes of arbitrary finite dimension is constructed in [19]. 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 [20], by constructing a homotopy operator for unstructured meshes.

3.1.2. *Discrete Connections on Principal Bundles [67].* Motivated by applications to discrete Lagrangian reduction, the discrete analogue of the Atiyah sequence is introduced in [67]. 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 [31].* Abelian symmetry reduction for discrete mechanics is considered in [31]. 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 [22; 34; 39; 40; 50].* 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 [34], and applied to a system of extended rigid bodies interacting under their mutual gravitational potential in [39; 40], 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 [22].

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 [50] 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.

3.2.3. *Generalized Variational Integrators [60; 61; 65; 66].* 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 [61; 65].

The exact discrete Lagrangian associated with Jacobi's solution (1) can be interpreted as 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 [65]). 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, and collocation methods applied to either the Euler–Lagrange vector field or its prolongation (see [64]).

The variational characterization of the exact discrete Lagrangian (2) 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 [60], 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 [66], 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.

3.2.4. *Discrete Dirac Mechanics and Geometry [62; 63].* 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 (see §4.1) 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 [10; 30; 35; 36; 41; 43–45; 47; 49; 51–56; 58; 59].* The discrete optimal control problem is derived as a two stage discrete variational problem. First, a forced Lie group variational integrator [34] 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 [10; 30] 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 [35] and solved using sequential quadratic programming. For continuously actuated control problems, this approach is prohibitively expensive. In [44], 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 [36]. An alternative approach is to parametrize the discrete controls using a lower-dimensional function space, and this is adopted in [47] to develop optimal control strategies for articulated rigid bodies. In addition, we have applied these techniques to articulated multi-body systems in perfect fluids [51; 53], tethered spacecraft [52; 55; 56], and autonomous UAVs [54; 58; 59].

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 [43], 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 [41], and study discrete time-optimal control problems in [45].

3.3.2. *Discrete Controlled Lagrangian Systems [7–9; 11].* 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 [7], and the extension to the case of potential shaping is considered in [8]. The general case of one actuated and one uncontrolled direction was addressed in [9; 11].

3.3.3. *Discrete Optimal Attitude Estimation and Filtering [37; 38; 42; 46; 48].* Attitude estimation is formulated as an optimization problem on the rotation group in [37], 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 [48], the degenerate case of single directional measurements is addressed in [42], and a careful comparison of uncertainty propagation methods is conducted in [38]. A global uncertainty propagation method that synthesizes techniques from polynomial chaos, noncommutative harmonic analysis, and Lie group variational integrators is developed in [46], which allows for probability densities with global support.

3.3.4. *Discrete Hamilton–Jacobi Theory and Bellman Equations [81; 82].* 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 [66] 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 [89–91].* In [89], 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 [90], 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 [91].

3.4.2. *Hamilton–Jacobi Theory for Degenerate Lagrangian Systems [68].* In [68], 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 [15; 57].* In [15], 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 [57].

4. Current research

4.1. **Discrete Hamilton–Pontryagin Principle and Dirac Integrators.**

Variational principles. A mechanical system can be described using a Lagrangian, $L : TQ \to \mathbb{R}$, which is the difference between kinetic and potential energies in terms of position and velocity $(q, v) \in TQ$. **Hamilton's principle** states that on the trajectory joining $q(t_1)$ and $q(t_2)$, the action functional is stationary,

$$\delta \int_{t_1}^{t_2} L(q, v) dt = 0,$$

over second-order curves $q(t)$ with fixed endpoints. **Hamilton's phase-space principle** is expressed in terms of position and momentum $(q, p) \in T^*Q$, and the Hamiltonian $H(q, p) = p \cdot v - L(q, v)|_{p=\partial L/\partial v}$,

$$\delta \int_{t_1}^{t_2} p \cdot \dot{q} - H(q, p) dt = 0.$$

The two formulations are related by the **Legendre transformation** $\mathbb{F}L : TQ \to T^*Q$, $\mathbb{F}L(q, v) = (q, \partial L/\partial v)$.

The **Hamilton–Pontryagin** variational principle involves position, velocity, and momentum $(q, v, p) \in TQ \oplus T^*Q$, and uses a Lagrange multiplier p to impose the second-order curve condition $v = \dot{q}$,

$$\delta \int_{t_1}^{t_2} L(q, v) - p(\dot{q} - v) dt = 0. \tag{3}$$

It encapsulates both Hamilton's and Hamilton's phase space variational principles, as well as the Legendre transformation, and gives the **implicit Euler–Lagrange equations**,

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

Geometric structure. The Euler–Lagrange equations are symplectic and Hamilton's equations are Poisson. The corresponding geometric structure that is preserved by the Hamilton–Pontryagin flow is the **Dirac structure**, which is a $2n$-dimensional subbundle $D \subset TT^*Q \oplus T^*T^*Q$, with the property that,

$$\langle v_1, p_2 \rangle + \langle v_2, p_1 \rangle = 0,$$

for all $(q, v_1, p_1), (q, v_2, p_2) \in D$, and

$$\langle \pounds_{X_1} \alpha_2, X_3 \rangle + \langle \pounds_{X_2} \alpha_3, X_1 \rangle + \langle \pounds_{X_3} \alpha_1, X_2 \rangle = 0,$$

for all pairs of vector fields and one-forms $(X_1, \alpha_1), (X_2, \alpha_2), (X_3, \alpha_3) \in D$, and where $\pounds_X$ is the Lie derivative along the vector field X. This generalizes the requirement 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 $\Omega : TT^*Q \times TT^*Q \to \mathbb{R}$ and Poisson structure $B : T^*T^*Q \times T^*T^*Q \to \mathbb{R}$, viewed as maps TT^*Q to T^*T^*Q, $v_q \mapsto \Omega(v_q, \cdot)$ and T^*T^*Q to $T^{**}T^*Q \cong TT^*Q$, $\alpha_q \mapsto B(\alpha_q, \cdot)$, are Dirac structures.

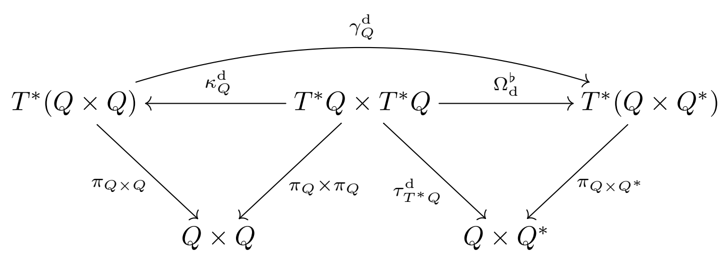
Discrete Hamilton–Pontryagin Principle and Implicit Discrete Lagrangian Systems. The discrete Hamilton–Pontryagin principle imposes the discrete second-order condition $q_k^1 = q_{k+1}^0$ using Lagrange multipliers, which yields a variational principle on $(Q \times Q) \oplus T^*Q$,

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

and the ***implicit discrete Euler–Lagrange equations***,

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

Discrete Dirac Structures. In addition to the discrete variational formulation of Dirac mechanics, the implicit discrete Euler–Lagrange equations can be expressed in terms of discrete Dirac structures [63]. By considering the geometric properties of generating functions of symplectic maps, we construct a discrete Tulczyjew's triple,



which yields a discrete Dirac structure,

$$D_{\Delta_Q}^{\mathrm{d}+} := \left\{ ((z, z^+), \alpha_{\hat{z}}) \in (T^*Q \times T^*Q) \times T^*(Q \times Q^*) \;\middle|\; \left(z, z^+\right) \in \Delta_{T^*Q}^{\mathrm{d}+},\ \alpha_{\hat{z}} - \Omega_{\mathrm{d}+}^\flat \left(z, z^+\right) \in \Delta_{Q\times Q^*}^\circ \right\},$$

Then, an ***implicit discrete Lagrangian system*** satisfies $\left(X_d^k, \mathfrak{D}^+ L_d(q_k^0, q_k^1)\right) \in D_{\Delta_Q}^{d+}$.

Interconnection of Lagrange–Dirac systems. Given two Lagrange–Dirac systems (Q_1, L_1, Δ_1) and (Q_2, L_2, Δ_2), and an interaction constraint Δ_{int}, one can describe the interconnected system in terms of an interconnection Dirac structure D_c,

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

where $D_c = (D_{\Delta_1} \oplus D_{\Delta_2}) \bowtie D_{int}$, and the bowtie construction $\bowtie$ is given by

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

This novel interconnection Dirac structure combines three standard Dirac structures (essentially the graph of the canonical symplectic forms), namely the one on T^*Q_1, the one on T^*Q_2 and the "Tellegen" structure that encodes the forces. One goal would be to generalize this continuous construction to the case of discrete Lagrange–Dirac systems by using discrete Dirac structures.

Specific Objectives:

(1) Develop a discrete Lagrange–Dirac theory of interconnected systems, by considering compositions of discrete Dirac structures. This will provide a discrete port-Lagrangian approach to interconnected systems, that naturally leads to distributed numerical methods.
(2) Generalize the interconnection theorem, for variational principles and Dirac structures, that would allow the interconnection of an arbitrary number of Dirac–Lagrange subsystems simultaneously, with an arbitrary interconnection topology.
(3) Develop a geometric discretization of interconnected systems using the discrete Dirac framework, that preserves the underlying Dirac geometry and connection topology.
(4) Determine how one discretizes the Lagrangian, and the constraints, so that the modified Lagrangian preserves the interconnection topology.
(5) Extend Dirac variational integrators to Lie groupoids and algebroids, nonholonomic problems, interconnected systems, and multi-Dirac integrators for PDEs.

4.2. **Dirac Mechanics for Covariant Field Theories.** While the theory of Dirac geometry and mechanics has been developed in the case of ODEs, the corresponding generalization to the PDE setting is less established. We propose to develop the corresponding Dirac variational treatment of covariant field theories, which will clarify the role of gauge degrees of freedom in field theories. Recent attempts at constructing covariant formulations of Lagrangian field theories in the multisymplectic setting naturally leads to two copies of the base space, which is typically spacetime. In the discrete setting, this is related to the use of distinct computational and physical spacetime meshes, which allows for the introduction of mesh adaptivity. In particular, the moving mesh can be viewed as a discrete diffeomorphism which maps a regular mesh on the computational domain to an irregular mesh on the physical domain. This covariant formulation of Dirac field theories provides an appropriate theoretical setting for the development of mesh adaptive algorithms in the context of geometric numerical integration.

Boundary Lagrangians. We introduced the natural analogue of Jacobi's solution of the Hamilton–Jacobi equation in the context of field theories, which we refer to as the ***boundary Lagrangian***,

$$L_{\partial\Omega}(\psi) = \operatorname*{ext}_{\phi|_{\partial\Omega}=\psi} \int_\Omega \mathcal{L}(j^1\phi).$$

This can be considered a generating functional, which encodes a functional relationship between the field values and the normal momenta on the boundary $\partial\Omega$. In particular, one can show that the normal momenta π on the boundary is given by,

$$\pi = \frac{\delta L_{\partial\Omega}}{\delta\psi},$$

which is the field theoretic analogue of a symplectic map $(q_0, p_0) \mapsto (q_1, p_1)$ being defined implicitly in terms of a Type I generating function $L_d : Q \times Q \to \mathbb{R}$ by,

$$p_0 = -\frac{\partial L_d}{\partial q_0}, \qquad p_1 = \frac{\partial L_d}{\partial q_1},$$

where the sign in the first equation is due to the orientation of the boundary. A Legendre transform at the level of the generating functional yields a Type II generating functional $H_{\partial\Omega}$ that provides the natural framework for Hamiltonian field theories. Both $L_{\partial\Omega}$ and $H_{\partial\Omega}$ can be viewed as exact generating functionals for the solution of the Lagrangian and Hamiltonian field equations, and they are the natural objects to develop a variational error order theory for discrete variational integrators for field theories that preserve the multisymplectic and multi-Dirac structures.

Covariant Field Theories. A field theory is said to be ***covariant*** if its Lagrangian is invariant under arbitrary coordinate transformations (equivalently, when the Lagrangian is invariant under the action of the group of diffeomorphisms of $\mathcal{X}$ on the bundle). The concept of 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; see [24].

Covariance can be built into a field theory by augmenting the fiber bundle with a second copy of the base space as in [14]. As a result, the spacetime variables appear as new fields on the same footing as the original fields. From a computational point of view, this corresponds to using distinct computational and physical meshes, and hence opens the door for mesh-adapting algorithms.

The Hamilton–Pontryagin Principle. The Hamilton–Pontryagin principle for mechanics given in (3) can be extended to field theories. Let $\phi : \mathcal{X} \to Y$ be a field, then the Hamilton–Pontryagin principle is given by

$$\delta \int_{\mathcal{X}} L(x^\mu, y^a, v^a_\mu) + p^\mu_a \left(\frac{\partial \phi^a}{\partial x^\mu} - v^a_\mu \right) d^{n+1}x = 0,$$

where L is a Lagrangian density, x^μ are spacetime variables, y^a are fields, and v^a_μ are derivatives of the fields with respect to spacetime. An associated variational principle for covariant field theories was used to obtain a first-order Hamiltonian description for gauge field theories,

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

Here, (ψ, ρ) represent the dynamical degrees of freedom, while the ***atlas fields*** α_i can be specified arbitrarily and represent the gauge redundancy. In a discrete, spacetime mesh-adapting simulation, the fields α_i specify the way in which the physical mesh moves with respect to the fixed, computational mesh. A practical result of the development of continuous and discrete Dirac geometry for covariant fields will be an algorithm for spacetime adaptive integration of interconnected PDE-governed systems spanning elastica, fluids, and electromagnetism. To achieve this goal, we require additional multiphysics simulation technologies that we will describe next.

Specific Objectives:

(1) Develop a variational order theory for multi-Dirac variational integrators based on comparisons with discrete Type I and II generating functionals, and the rate at which they approximate the boundary Lagrangian and boundary Hamiltonian.
(2) Use the concept of the boundary Lagrangian to systematically derive the field-theoretic analogue of Hamilton–Jacobi theory, with a view towards developing a discrete Hamilton–Jacobi theory for Hamiltonian PDEs, and deriving a discrete Hamilton–Jacobi–Bellman equation describing the optimal control problem for Hamiltonian PDEs (this would generalize the results of §3.3.4 to field theories).
(3) Develop the Hamilton–Pontryagin principle for covariant field theories, with a view towards developing multi-Dirac variational integrators with spacetime adaptivity. This will yield more efficient methods for field theories that fit into the Dirac interconnection framework.

4.3. **Noncommutative Harmonic Analysis and Multisymplectic Variational Integrators on Lie Groups and Homogeneous Spaces.** Many Hamiltonian PDEs on Lie groups and homogeneous spaces are invariant under the action of an appropriate symmetry group, and by Noether's theorem conserve the corresponding momentum map. For example, an ideal incompressible fluid evolves under the L^2 geodesic flow on the space of volume-preserving diffeomorphisms $\mathcal{D}_{\text{vol}}$ [3; 21]. This Lagrangian formulation of fluids is invariant under the lifted right action of $\mathcal{D}_{\text{vol}}$ on itself, which corresponds to the symmetry of the total kinetic energy of the fluid under a relabeling of the fluid particles. The associated conservation law is the

Kelvin's Circulation Theorem, which states that the circulation around a material loop is conserved. The Euler–Poincaré reduction of this formulation of fluids under the symmetry action of $\mathcal{D}_{\mathrm{vol}}$ recovers the familiar Euler equations of fluid dynamics.

When constructing a multisymplectic discretization of a Hamiltonian PDE, it is desirable for the discrete Lagrangian density to inherit as many of the symmetries of the continuous Lagrangian density as possible. By the discrete Noether's theorem, this ensures that the resulting multisymplectic variational integrator conserves the corresponding discrete momentum map. In discretizing a PDE, it is often difficult to achieve invariance with respect to the full symmetry group, but even invariance with respect to a subgroup is desirable, since it implies that the corresponding momentum map is approximately conserved [83].

As such, it is natural to consider finite dimensional function spaces on Lie groups and homogeneous spaces that are invariant under a subgroup of the symmetry group. This is addressed by applying noncommutative harmonic analysis techniques based on the Peter-Weyl theorem [84], which provides a complete orthonormal basis for L^2 functions on a compact Lie group G in terms of its irreducible unitary representations.

A group representation is a group homomorphism $\varphi : G \to GL(V)$ where V is a vector space, i.e., $\varphi(g \cdot h) = \varphi(g) \cdot \varphi(h)$. The Peter-Weyl theorem states that for a compact Lie group G and $V = \mathbb{C}^n$,

$$L^2(G) = \bigoplus\nolimits_{\varphi \in \hat{G}} V_\varphi,$$

which is to say that the space of L^2 functions on a compact Lie group G is decomposed into orthogonal subspaces which correspond to the irreducible unitary representations of G. Furthermore, given a basis $\{e_i\}_{i=1}^n$ for $\mathbb{C}^n$, the corresponding dual basis $\{e^j\}_{j=1}^n$, and an irreducible unitary representation $\varphi : G \to GL(\mathbb{C}^n)$, the maps $g \mapsto \langle e^j, \varphi(g) \cdot e_i \rangle$, which are the matrix coefficients of the matrix representation of $\varphi(g) \in GL(\mathbb{C}^n)$ with respect to the given basis, are smooth, and they form a basis for the subspace V_φ.

A discrete Lagrangian that inherits the symmetry properties of the continuous Lagrangian can be obtained using group-equivariant interpolatory schemes, constructed using the matrix components of the irreducible unitary representations [80]. These functions are naturally graded in terms of the dimension of the representation, which is a natural generalization of the notion of degree for finite dimensional subsets of polynomial spaces. By combining noncommutative harmonic analysis with variational integrators, we will obtain spectral multisymplectic integrators for Hamiltonian PDEs on Lie groups and homogeneous spaces.

Much of the tools of classical harmonic analysis, including the Fourier transform and its inverse, the Plancherel theorem, and the Fast Fourier transform generalize to compact Lie groups [2], as well as Lie groups with a bi-invariant Haar measure, such as the special Euclidean group. This provides the theoretical basis for efficient numerical linear algebra methods for the linear systems arising in Lie group spectral variational integrators. As discussed in [16], techniques of noncommutative harmonic analysis have a large variety of engineering applications, including robotic manipulators, tomography, and stochastic estimation.

Specific Objectives:

(1) Construct spectral multisymplectic variational integrators on Lie groups and homogeneous spaces by combining noncommutative harmonic analysis techniques with multisymplectic integrators.
(2) Develop geometrically exact methods for discrete elasticity by using multivariate interpolation on the orthonormal frame bundle, multisymplectic discretization, and a characterization of elastic stress in terms of discrete curvature in the sense of discrete exterior calculus [19; 32].

4.4. **Uncertainty Propagation and Stochastic Variational Integrators.** An increasingly important aspect of scientific computation is the quantification of uncertainty in simulations. Models of complex dynamical systems typically involve coupled subsystems that themselves exhibit approximations, unmodeled physical processes, and parametric uncertainty. Computation is increasingly complementary to experiments in validating and guiding theoretical developments in science, and understanding uncertainty propagation is an essential aspect of computational science and engineering. A synthesis of numerical parametric uncertainty analysis techniques [92; 93], noncommutative harmonic analysis [16], and geometric integration will yield efficient methods for characterizing the evolution of uncertainty on Lie groups and homogeneous spaces. Such tools will serve as a driving force behind robust and reliable computational results that serve to inform and motivate theoretical advances in science and engineering.

Nonlinearities of the flow imply that standard numerical methods for propagating uncertainties using linearization rapidly degrade in performance, unless frequent physical measurements are available [38]. It is therefore desirable to construct efficient numerical methods for solving the Liouville equation that describes the evolution of a probability distribution advected by a prescribed flow. The method of generalized polynomial chaos [92; 93] relies on augmenting the base space of independent variables with additional dimensions to represent uncertain initial conditions and parameters. The flows for different parameters are decoupled, and sample points are evolved under the dynamics and used to reconstruct the distribution at a later time, as opposed to being used to compute statistical properties of the advected distribution.

The Gromov nonsqueezing theorem [25] from symplectic geometry places fundamental limits on how the uncertainty of a Hamiltonian mechanical system evolves [29]. It is therefore essential that symplectic methods, such as variational integrators, be used to propagate individual trajectories when using the method of generalized polynomial chaos to analyze uncertainty propagation in Hamiltonian systems. Since uncertainty propagation is a property of the flow, the geometric integration paradigm of approximating the flow as an operator is particularly appropriate. Interpolatory spaces arising from noncommutative harmonic analysis are well suited to represent uncertainty distributions on Lie groups, such as the rotation group, which are of importance in the attitude dynamics of satellites. In particular, instead of directing advecting the probability distributions, we advect a function ψ such that ψ^2 is the probability distribution. Motivated by analogy to the wave function in the Schrödinger equation, it avoids having to use a complicated constraint on the coefficients of the spectral expansion to ensure positivity [72]. Instead, by the Plancherel theorem, ensuring that the flow is unitary reduces to simply requiring that the l^2 norm of the spectral coefficients is constant.

Unmodeled dynamics is typically characterized as a stochastic perturbation to the deterministic model. As such, another aspect of uncertainty quantification is the extension of geometric integration techniques to stochastic Hamiltonian systems [6]. This has spurred the development of stochastic numerical methods in mathematical physics [78], including symplectic integrators for stochastic Hamiltonian systems [79]. There has also been recent work on Lie group methods for stochastic systems [73]. It would be desirable to extend Lie group variational integrators to stochastic Hamiltonian systems. This will proceed along the lines suggested by the variational formulation of stochastic Hamiltonian systems introduced in [33].

Specific Objectives:

(1) Adapt generalized polynomial chaos methods for uncertainty propagation to Hamiltonian systems on Lie groups by combining Lie group variational integrators and noncommutative harmonic analysis.
(2) Construct a multisymplectic discretization of the variational formulation of stochastic Hamiltonian systems, so as to generalize Lie group variational integrators to stochastic Hamiltonian systems.
(3) Use an operator splitting approach to combine fast methods for anisotropic diffusion based on noncommutative harmonic analysis with deterministic uncertainty propagation methods to obtain a mesh-free method for efficiently solving the Fokker–Planck equation on Lie groups and homogeneous spaces.

4.5. **Computational Geometric Control and Controlled Lagrangian Systems.** A natural extension of the existing work on discrete geometric optimal control (§3.3.1) would be to systems with uncertainty. Since many engineering problems exhibit parametric or model uncertainty, it is desirable to develop control algorithms that are uniformly applicable to an ensemble of physical systems. This can be achieved by generalizing discrete optimal control to the extended base spaces used in generalized polynomial chaos methods, and by considering cost functionals that involve a probability weighted integral over the ensemble trajectory. This would yield optimal control algorithms that are more robust to uncertainty.

The method of controlled Lagrangians provide a systematic means of constructing discrete-time feedback stabilizing controllers (§3.3.2), but it relies on a formulation of discrete mechanics that does not preserve the Lie group and homogeneous space structure that typically arise in configuration and shape spaces. It is therefore natural to generalize the method to Lie group and homogeneous variational integrators (§3.2.2).

Dirac structures and Dirac variational integrators based on the discrete Hamilton–Pontryagin principle (§4.1) provide a unified basis for studying Dirac constraints, and nonholonomic and interconnected systems, and provide the natural setting to study the discrete geometric control of such problems.

Specific Objectives:

(1) Develop the theoretical and numerical framework for optimal control in the presence of uncertainty.
(2) Synthesize the method of controlled Lagrangians with Lie group and homogeneous variational integrators to enable the method to apply to the stabilization of rigid body dynamics.
(3) Extend discrete optimal control and controlled Lagrangians to the setting of Dirac variational integrators, with an emphasis on applications to constrained, nonholonomic, and interconnected systems.

5. 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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