Chapter 1

Introduction

Geometric mechanics (see, for example, Abraham and Marsden [1978]; Arnold [1989]; Marsden and Ratiu [1999]) has motivated the development of new and innovative numerical schemes (see, for example, Kane et al. [1999, 2000]; Marsden and West [2001]; Lew et al. [2003, 2004]) that inherit many of the desirable conservation properties of the original continuous problem. It is the goal of computational geometric mechanics to more directly adopt the approach of geometric mechanics in the construction of computational algorithms, as well as the systematic analysis of their numerical conservation properties. This is part of the broader subject of structure-preserving integrators, and good references for this field include Sanz-Serna and Calvo [1994], Hairer et al. [2002], and Leimkuhler and Reich [2004].

In simulating dynamical systems for a long time, it is often desirable to preserve as many of the physical invariants as possible, since this typically results in a more qualitatively accurate simulation. As an example, symplectic methods have become popular in simulating the solar system, and molecular dynamics, where long-time behavior is of paramount importance. While conditions exist on the coefficients of a Runge–Kutta scheme that ensure that the scheme is symplectic, directly constructing a symplectic method using this approach can be difficult. An alternative approach is to discretize Lagrangian mechanics by considering a discrete Hamilton's principle. The resulting variational integrators (see, for example, Marsden and West [2001]) have the desirable property that they are symplectic and momentum preserving. Forcing and dissipation can also be addressed by considering the discrete Lagrange–d'Alembert principle instead. In either the forced or conservative case, variational integrators exhibit excellent longtime energy behavior that cannot be understood from their local error properties alone. Such discrete conservation laws typically impart longtime numerical stability to computations, since the structure preserving algorithm exactly conserves a discrete quantity that is always close to the continuous quantity of interest. The longtime stability of variational integrators has recently been analyzed using the techniques of Γ-convergence in Müller and Ortiz [2004], which yield insights into the weak$*$ convergence of discrete trajectories, and the convergence of the Fourier transformation of the discrete trajectories.

Classical field theories like electromagnetism and general relativity have a rich underlying geometry, and understanding the role of gauge symmetries in these problems is important for distinguishing between the physically relevant dynamics and the nonphysical gauge modes. One method of eliminating the gauge symmetry is by the process of reduction, where the dynamics is restricted to the constant momentum surface that the flow is on, and the symmetry is further quotiented out. This results in a reduced system of equations that evolve on a lower-dimensional space referred to as the shape space. The shape space is the natural setting for studying relative equilibria, such as rigid-bodies in uniform rotation or translation. Insight is obtained by computing on the shape space that would otherwise remain obscured at the unreduced level.

Staggered mesh schemes like the Yee scheme in computational electromagnetism, and the leapfrog scheme in ordinary differential equations, have good structure-preservation properties due to discretizations that are compatible with the underlying geometry. These geometric relationships are obscured by the use of vector calculus, but when the equations are reformulated in the language of differential forms and exterior calculus, the primal-dual relation reflected in the use of staggered meshes naturally arises. While it is understood how to obtain compatible discretizations for staggered meshes that are logically rectangular, unstructured meshes pose a greater challenge.

In practice, much of the understanding of complex dynamical systems is derived from numerical simulations which, because of their complexity, are typically not fully resolved. Therefore, the behavior of numerical algorithms and discrete geometry for finite discretizations is important. The interaction between numerical methods and the dynamical systems to which they are applied can be non-trivial, and this naturally leads to the question of how to construct canonical discretizations that preserve, at a discrete level, the important properties of the continuous system. Computational geometric mechanics aims, in part, to address this and other questions, but understanding the global behavior of integrators, and their underlying geometry, we are hindered by the absence of the discrete analogues of mathematical tools that geometric mechanics has come to rely on. These include the language of differential forms and exterior calculus, as well as geometric structure encoded in the form of connections on principal bundles. In recent years, there has been increasing interest in the study of numerical schemes as dynamical systems in their own right, and if we are to repeat the success of geometric mechanics in elucidating the underlying geometry of such numerical methods, it is imperative that we develop more of the relevant mathematical infrastructure.

In particular, there has been interest in developing a theory of symmetry reduction at the discrete level, including work on the Discrete Euler–Poincaré equations (see Marsden et al. [1999, 2000a]), and the Discrete Routh equations (see Jalnapurkar et al. [2003]). The discrete analogues of exterior calculus and curvature that arose in the development of discrete reduction (see Leok [2002]) motivated us to systematically develop a discrete theory of exterior calculus (see Desbrun et al. [2003a]). Similarly, attempts to develop a discrete analogue of the continuous theory of Lagrangian reduction (see, for example, Cendra et al. [2001]) lead to the construction of discrete connections on principal bundles (see Leok et al. [2003]). In addition, the construction of G-invariant discrete Lagrangians suitable for discrete reduction motivated the work on generalized Galerkin variational integrators (see Leok [2004]).

In the rest of this chapter, we will provide an overview of the material presented in this thesis.

Discrete Routh Reduction. We consider the problem of a discrete Lagrangian system with an abelian symmetry group. By the discrete Noether's theorem, the dynamics is restricted to a constant discrete momentum surface $J_d^{-1}(\mu)$. By symmetry considerations, the dynamics can be further restricted to $J^{-1}(\mu)/G$. We first construct a semi-global isomorphism between $J_d^{-1}(\mu)$ and $S \times S$ using a discrete mechanical connection. This choice of discrete connection allows the reconstruction of the reduced trajectory on $S \times S$ to the full trajectory on $Q \times Q$ to be interpreted as a discrete horizontal lift.

By using the connection to split the variations in the discrete Hamilton's principle into horizontal and vertical variations, we drop the variational principle on $Q \times Q$ to the reduced variational principle on $S \times S$. The discrete equations corresponding to the reduced variational principle are the discrete Routh equations, which are symplectic with respect to a reduced symplectic form that includes a magnetic term arising from the curvature of the connection. This is particularly significant, since standard symplectic methods can only preserve the canonical symplectic form, and discrete Routh equations are the first numerical scheme that have the correct conservation properties in the presence of a non-canonical symplectic form.

On the Hamiltonian side, the analogue of cotangent bundle reduction yields the Reduced Symplectic Partitioned Runge–Kutta (RSPRK) algorithm. This algorithm is also symplectic with respect to the non-canonical symplectic form on the reduced space, and includes corrections to Symplectic Runge–Kutta that involve the curvature of the connection. Both the RSPRK algorithm and the discrete Routh equations are consistent with the continuous theory of Lagrangian and Hamiltonian reduction, and they form a commutative cube of equations that are related by maps between the discrete and continuous theory, projections from the unreduced to the reduced spaces, and the fiber derivatives that go between the Lagrangian and Hamiltonian formulation.

Forced or dissipative systems can be addressed in the reduced framework by reducing the discrete Lagrange–d'Alembert principle, and the resulting methods exhibit superior tracking of the energy decay, as compared to traditional methods. Constraints are handled through the use of Lagrange multipliers, and allow computations on manifolds to be realized using constraint surfaces in a linear space, thereby resulting in additional computational efficiency.

These reduced algorithms are particularly relevant when studying phenomena, such as relative equilibria and relative periodic orbits, that are associated with dynamical structures on the reduced space.

Discrete Exterior Calculus. A theory of discrete exterior calculus on simplicial complexes of arbitrary finite dimension is constructed. In addition to dealing with discrete differential forms as cochains, discrete vector fields and the operators acting on these objects are introduced. The various interactions between forms and vector fields (such as Lie derivatives) which are important in many applications, including fluid dynamics, can be addressed. Previous attempts at discrete exterior calculus have addressed only differential forms. The notion of a circumcentric dual of a simplicial complex is also introduced. The importance of dual complexes in this field has been well understood, but previous researchers have used barycentric subdivision or barycentric duals. It is shown that the use of circumcentric duals is crucial in arriving at a theory of discrete exterior calculus that admits both vector fields and forms.

In this framework, one can systematically recover discrete vector differential operators like the divergence, gradient, curl and the Laplace–Beltrami operator. These can be thought of as generalizations of mimetic difference operators (see, for example, Shashkov [1996]; Hyman and Shashkov [1997b,a]) to unstructured meshes, without the need for interpolation. Instead, these discrete differential operators are realized as combinatorial operations on the mesh. Methods based on interpolation through the use of Whitney forms can be found in Bossavit [1998] and Hiptmair [1999].

The exactness property of the discrete variational complex is critical in many applications. Along these lines, a discrete Poincaré lemma is proved in the context of discrete exterior calculus. Here, a homotopy operator that is valid for a large class of unstructured meshes is constructed, and the lemma holds globally for specific examples of regular triangulations and tetrahedralizations of $\mathbb{R}^2$ and $\mathbb{R}^3$.

Discrete exterior calculus (DEC) and discrete variational mechanics have an interesting relationship. In particular, discretizing the equations describing harmonic maps and electromagnetism using DEC yield the same numerical scheme as that obtained from the discrete variational principle corresponding to an action integral that is discretized using DEC. This implies that directly discretizing the equations for harmonic maps and electromagnetism yield numerical schemes that have the structure-preservation properties of variational schemes.

We also consider extensions to dynamic problems by using the groupoid formulation of discrete diffeomorphisms and flows, and introduce the push-forward and pull-back of discrete vector fields and forms. A method for remeshing cochains is also introduced, and this provides the restriction and prolongation operators necessary to apply DEC operators in multigrid computations.

Discrete Connections on Principal Bundles. We were motivated by applications to discrete Lagrangian reduction to introduce the notion of a discrete connection as a splitting of $Q \times Q$ into horizontal and vertical subspaces. The sense in which these horizontal and vertical subspaces are complementary, and combine to recover $Q \times Q$ requires introducing a composition of horizontal and vertical elements that extends the pair groupoid composition on $Q \times Q$.

This choice of discrete horizontal and vertical subspaces is equivalent to the choice of a splitting of the discrete Atiyah sequence. Equivalent representations of a discrete connection, such as the discrete connection 1-form, and the discrete horizontal lift, are also considered. Computational issues such as the order of approximation to a continuous connection are addressed.

The composition on $Q \times Q$ to compose horizontal and vertical elements can be further extended by using the discrete connection. This is significant, since it extends the pair groupoid composition on $Q \times Q$ in a manner that is consistent with the principal bundle structure of $\pi : Q \to S$, and allows (q_0, q_1) to be composed with $(\tilde{q}_0, \tilde{q}_1)$ provided $\pi q_1 = \pi \tilde{q}_0$. In the case when $q_1 = \tilde{q}_0$, this extended composition reduces to the standard pair groupoid composition.

Given a discrete G-invariant Lagrangian in discrete mechanics, one can introduce a discrete momentum map. From this, a discrete mechanical connection is constructed by requiring that a pair of points are in the horizontal distribution if their discrete momentum is zero. By using the theory of equivalent representations of the discrete connection, the discrete mechanical connection can be represented as a discrete connection 1-form.

The applications of discrete connections include discrete Lagrangian reduction, geometric control theory, and a discrete notion of a Riemannian manifold, and the associated Levi-Civita connection and its curvature.

Generalized Variational Integrators. We consider a generalization of variational integrators by recognizing that the fundamental object that is being discretized is the action integral, and this is achieved by discretizing sections of the configuration bundle over a base space through the choice of a finite-dimensional function space, and the choice of a numerical quadrature in approximating the action integral.

By expanding the interpolatory spaces to include those that are not parameterized by their endpoint values, we obtain a general class of variational integrators that impose continuity at endpoints through the use of Lagrange multipliers. When the degrees of freedom chosen include the endpoint values, the Lagrange multipliers can be eliminated to recover the standard discrete Euler–Lagrange equations, and recovers the theory of high-order variational integrators as a special case.

Nonlinear approximation techniques, which allow space-time mesh points to vary, are the natural method of incorporating spatio-temporal adaptivity in variational integrators and naturally generalize Symplectic-Energy-Momentum integrators. In multiscale problems, the function space is chosen to include solutions of the cell problem, corresponding to solving for the fast dynamics while keeping the slow variables fixed. The highly oscillatory integral is then evaluated using Filon–Lobatto techniques that are a class of exponentially fitted numerical quadrature schemes with many desirable properties. The combination of these two choices allows the multiscale variational integrator to exactly solve for the fast dynamics, and thereby achieve convergence rates that are independent of the ratio of the fast and slow timescales.

In expanding the function spaces that can be handled using the variational framework, Lie group variational methods, and pseudospectral variational methods can be constructed as well, which are of particular relevance to quantum mechanical simulations.