Foundations of Computational Geometric Mechanics

Thesis by
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"Thought is only a flash between two long nights,
but this flash is everything"

Henri Poincaré, 1854–1912.

Preface

This thesis was submitted at the California Institute of Technology on April 19, 2004, in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Control and Dynamical Systems with a minor in Applied and Computational Mathematics. The thesis was defended on May 6, 2003, in Pasadena, CA, and was approved by the following thesis committee:

- Thomas Y. Hou, Applied and Computational Mathematics,
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- Michael Ortiz, Aeronautics, and Mechanical Engineering,
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This thesis draws upon the following papers that have or will be submitted for publication, but an effort has been made to clarify the manner in which the research relates to each other by incorporating extended introductions and conclusions within each chapter, and through the use of examples that draw upon the various chapters.

- S.M. Jalnapurkar, M. Leok, J.E. Marsden, and M. West, *Discrete Routh Reduction*, J. FoCM, submitted.
- M. Desbrun, A.N. Hirani, M. Leok, and J.E. Marsden, *Discrete Exterior Calculus*, in preparation.
- M. Desbrun, A.N. Hirani, M. Leok, and J.E. Marsden, *Discrete Poincaré Lemma*, Appl. Numer. Math., submitted.

- M. Leok, J.E. Marsden, A.D. Weinstein, *A Discrete Theory of Connections on Principal Bundles*, in preparation.
- M. Leok, *Generalized Galerkin Variational Integrators*, in preparation.

A review article based on preliminary versions of the work on discrete exterior calculus, discrete Poincaré lemma, and discrete connections on principal bundles, received the *SIAM Student Paper Prize*, and the *Leslie Fox Prize in Numerical Analysis* (second prize), both in 2003.

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A special thanks to my parents, Belinda and James, for their unconditional love and support, and for the freedom to pursue my interests. I dedicate this thesis to Lina, who has made my life so much better in countless ways.

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Abstract

Geometric mechanics involves the study of Lagrangian and Hamiltonian mechanics using geometric and symmetry techniques. Computational algorithms obtained from a discrete Hamilton's principle yield a discrete analogue of Lagrangian mechanics, and they exhibit excellent structure-preserving properties that can be ascribed to their variational derivation.

We construct discrete analogues of the geometric and symmetry methods underlying geometric mechanics to enable the systematic development of computational geometric mechanics. In particular, we develop discrete theories of reduction by symmetry, exterior calculus, connections on principal bundles, as well as generalizations of variational integrators.

Discrete Routh reduction is developed for abelian symmetries, and extended to systems with constraints and forcing. Variational Runge–Kutta discretizations are considered in detail, including the extent to which symmetry reduction and discretization commute. In addition, we obtain the Reduced Symplectic Runge–Kutta algorithm, which is a discrete analogue of cotangent bundle reduction.

Discrete exterior calculus is modeled on a primal simplicial complex, and a dual circumcentric cell complex. Discrete notions of differential forms, exterior derivatives, Hodge stars, codifferentials, sharps, flats, wedge products, contraction, Lie derivative, and the Poincaré lemma are introduced, and their discrete properties are analyzed. In examples such as harmonic maps and electromagnetism, discretizations arising from discrete exterior calculus commute with taking variations in Hamilton's principle, which implies that directly discretizing these equations yield numerical schemes that have the structure-preserving properties associated with variational schemes.

Discrete connections on principal bundles are obtained by introducing the discrete Atiyah sequence, and considering splittings of the sequence. Equivalent representations of a discrete connection are considered, and an extension of the pair groupoid composition that takes into account the principal bundle structure is introduced. Discrete connections provide an intrinsic coordinatization of the reduced discrete space, and the necessary discrete geometry to develop more general discrete symmetry reduction techniques.

Generalized Galerkin variational integrators are obtained by discretizing the action integral through appropriate choices of finite-dimensional function space and numerical quadrature. Explicit expressions for Lie group, higher-order Euler–Poincaré, higher-order symplectic-energy-momentum, and pseudospectral variational integrators are presented, and extensions such as spatio-temporally adaptive and multiscale variational integrators are briefly described.

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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 end-point 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.

Chapter 2

Discrete Routh Reduction

In collaboration with Sameer M. Jalnapurkar, Jerrold E. Marsden, and Matthew West.

Abstract

This chapter investigates the relationship between Routh symmetry reduction and time discretization for Lagrangian systems. Within the framework of discrete variational mechanics, a discrete Routh reduction theory is constructed for the case of abelian group actions, and extended to systems with constraints and non-conservative forcing or dissipation. Variational Runge–Kutta discretizations are considered in detail, including the extent to which symmetry reduction and discretization commute. In addition, we obtain the Reduced Symplectic Runge–Kutta algorithm, which can be considered a discrete analogue of cotangent bundle reduction. We demonstrate these techniques numerically for satellite dynamics about the Earth with a non-spherical J_2 correction, and the double spherical pendulum. The J_2 problem is interesting because in the unreduced picture, geometric phases inherent in the model and those due to numerical discretization can be hard to distinguish, but this issue does not appear in the reduced algorithm, and one can directly observe interesting dynamical structures. The main point of the double spherical pendulum is to provide an example with a nontrivial magnetic term in which our method is still efficient, but is challenging to implement using a standard method.

2.1 Introduction

Given a mechanical system with symmetry, we can restrict the flow on the phase space to a level set of the conserved momentum. This restricted flow induces a "reduced" flow on the quotient of this level set by the subgroup of the symmetry group that acts on it. Thus we obtain a reduced dynamical system on a reduced phase space. The process of reduction has been enormously important for many topics in mechanics such as stability and bifurcation of relative equilibria, integrable systems, etc.

The purpose of the present work is to contribute to the development of reduction theory for discrete time mechanical systems, using the variational formulation of discrete mechanics described in Marsden and West [2001]. We also explore the relationship between continuous time reduction and discrete time reduction, and discuss reduction for symplectic Runge–Kutta integration algorithms and its relationship to the theory of discrete reduction.

The discrete time mechanical systems used here are derived from a discrete variational principle on the discrete phase space $Q \times Q$. Properties such as conservation of symplectic structure and conservation of momentum follow in a natural way from the discrete variational principle, and the discrete evolution map can thus be regarded as a symplectic-momentum integrator for a continuous system.

The theory of discrete variational mechanics in the form we shall use it has its roots in the optimal control literature in the 1960's; see, for example, Jordan and Polak [1964], and Hwang and Fan [1967]. It was formulated in the context of mechanics by Maeda [1981], Veselov [1988, 1991] and Moser and Veselov [1991]. It was further developed by Wendlandt and Marsden [1997], and Marsden and Wendlandt [1997], including a constrained formulation, and by Marsden et al. [1998], who extended these ideas to multisymplectic partial differential equations. For a general overview and many more references we refer to Marsden and West [2001].

Although symplectic integrators have typically only been considered for conservative systems, in Kane et al. [2000] it was shown how the discrete variational mechanics can be extended to include forced and dissipative systems. This yields integrators for non-conservative systems which can demonstrate exceptionally good long-time behavior, and which correctly simulate the decay or growth in quantities such as energy and momentum. The discrete mechanics for non-conservative systems is discussed in §2.8.2, and it is shown how the discrete reduction theory can also handle forced and dissipative systems.

The formulation of discrete mechanics in this paper is best suited for constructing structure preserving integrators for mechanical systems that are specified in terms of a regular Lagrangian. Jalnapurkar and Marsden [2003], building on the work of Marsden and West [2001], show how to obtain structure-preserving variational integrators for mechanical systems specified in terms of a Hamiltonian. This method can be applied even if the Hamiltonian is degenerate.

A complementary approach to the Routh theory of reduction used in this paper is that of Lie–Poisson and Euler–Poincaré reduction, where the dynamics of an equivariant system on a Lie group can be reduced to dynamics on the corresponding Lie algebra. A discrete variational formulation of this was given in Marsden et al. [1999, 2000a], Bobenko et al. [1998], and Bobenko and Suris [1999]. Eventually one will need to merge that theory with the theory in the present paper.

We shall now briefly describe the contents of each section of this paper. In §2.2 we give a summary of some well known results on reduction for continuous-time mechanical systems with symmetry. Specifically, we discuss Routh reduction and its relationship with the theory of cotangent bundle reduction. In §2.3 we develop the theory of discrete reduction, which includes the derivation of a reduced variational principle, and proof of the symplecticity of the reduced flow. We also discuss in this section the relationship between continuous- and discrete-time reduction. In §2.4 we discuss a link between the theory of discrete mechanics and symplectic Runge–Kutta algorithms. In §2.5, we describe how our symplectic Runge–Kutta algorithm for a mechanical system with symmetry can be reduced to obtain a reduced symplectic Runge–Kutta algorithm. In §2.6 we put together in a coherent way the results of the previous sections. We also discuss how the original reduction procedure of Routh [1877, 1884] relates to our results. In §2.8 we extend the theory of discrete reduction to systems with constraints and external forces, and lastly, in §2.9 we present a numerical example of satellite dynamics about an oblate Earth.

2.2 Continuous Reduction

In this section we discuss reduction of continuous mechanical systems, in both the Lagrangian and Hamiltonian settings. Our purpose here is to fix notation and recall some basic results. For a more detailed exposition, see Marsden and Scheurle [1993a,b], Holm et al. [1998], Jalnapurkar and Marsden [2000], Marsden et al. [2000b], and Cendra et al. [2001] for Lagrangian reduction, and for Hamiltonian reduction, see, for example, Abraham and Marsden [1978] as well as Marsden [1992] for cotangent bundle reduction.

Suppose we have a mechanical system with configuration manifold Q, and let $L : TQ \to \mathbb{R}$ be a given Lagrangian. Let $q = (q^1, \ldots, q^n)$ be coordinates on Q. The Euler–Lagrange (EL) equations on TQ are

$$\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} = 0. \tag{2.2.1}$$

These equations define a flow on TQ if L is a regular Lagrangian, which we assume to be the case. Let X_E denote the vector field on TQ that corresponds to the flow. We have a Legendre transformation, $\mathbb{F}L : TQ \to T^*Q$, defined by

$$\mathbb{F}L : (q, \dot{q}) \mapsto \left(q, \frac{\partial L}{\partial \dot{q}}\right).$$

The Hamiltonian H on T^*Q is obtained by pushing forward the energy function E on TQ, which is defined by

$$E(q, \dot{q}) = \langle \mathbb{F}L(q, \dot{q}), \dot{q} \rangle - L(q, \dot{q}).$$

We have a canonical symplectic structure Ω_Q on T^*Q. From Ω_Q and H, we obtain the Hamiltonian vector field X_H on T^*Q. A basic fact is that X_H is the push-forward of X_E using $\mathbb{F}L$. Since the flow of X_H preserves Ω_Q, the flow of X_E, i.e., the flow derived from the EL equations, preserves $\Omega_L := (\mathbb{F}L)^*\Omega_Q$.

Suppose an abelian group G acts freely and properly on Q so that Q is a principal fibre bundle over ***shape space*** $S := Q/G$. Let $\pi_{Q,S} : Q \to S$ be the natural projection. Given $x \in S$, we can find an open set $U \subset S$, such that $\pi_{Q,S}^{-1}(U)$ is diffeomorphic to $G \times U$. Such a diffeomorphism is called a local trivialization. Given a local trivialization, we can use local coordinates on G and on S to obtain a set of local coordinates on Q. If $g = (g^1, \ldots, g^r)$ and $x = (x^1, \ldots, x^s)$ are local coordinates on G and $U \subset S$, respectively, then $q = (g, x) = (g^1, \ldots, g^r, x^1, \ldots, x^s)$ can be taken as local coordinates on Q.

The action of G on Q on be lifted to give actions of G on TQ and T^*Q. We also have a momentum map $J : T^*Q \to \mathfrak{g}^*$, defined by the equation $J(\alpha_q) \cdot \xi = \langle \alpha_q, \xi_Q(q) \rangle$, where $\alpha_q \in T_q^*Q$, $\xi \in \mathfrak{g}$, and $\xi_Q(q)$ is the infinitesimal generator corresponding to the action of G on Q evaluated at q. We can pull-back J to TQ using the Legendre transform $\mathbb{F}L$ to obtain a ***Lagrangian momentum map*** $J_L := \mathbb{F}L^*J : TQ \to \mathfrak{g}^*$.

If the Lagrangian L is invariant under the lifted action of G on TQ, the associated Hamiltonian H will be invariant under the action of G on T^*Q. In this situation, Noether's theorem tells us that the flows on TQ and on T^*Q preserve the momentum maps J_L and J, respectively.

Since locally, $Q \approx G \times S$, we also have the local representation $TQ \approx TG \times TS$. Thus, if $(g, \dot{g})$ are local coordinates on TG, and $(x, \dot{x})$ are local coordinates on TS, $(g, x, \dot{g}, \dot{x})$ are local coordinates on TQ. From the formula for the momentum map and freeness of the action, one sees that $\dot{g}$ is determined from $(g, x, \dot{x})$ and the value of the momentum. Thus, $J_L^{-1}(\mu)$ is locally diffeomorphic to $G \times TS$. If G is abelian (which is what we have assumed), it follows that G acts on $J_L^{-1}(\mu)$, and that $J_L^{-1}(\mu)/G$ is locally diffeomorphic to TS. Let the natural projection $J_L^{-1}(\mu) \to TS$ be denoted by $\pi_{\mu,L}$.

In a local trivialization, let $q \in Q$ correspond to $(g, x) \in G \times S$. Thus T_qQ can be identified with $T_gG \times T_xS$.

Let $\mathfrak{A} : TQ \to \mathfrak{g}$ be a chosen principal connection. Using a local trivialization, the connection can be described by the equation

$$\mathfrak{A}(\dot{g}, \dot{x}) = A(x)\dot{x} + g^{-1} \cdot \dot{g}.$$

Here $A(x) : T_xS \to \mathfrak{g}$ is the restriction of $\mathfrak{A}$ to T_xS. (T_xS is identified with the subspace $T_xS \times \{0\}$ of $T_gG \times T_xS$, which is in turn identified with T_qQ.) Note that the map $A(x)$ depends upon the particular trivialization that we are using.

The connection gives us an intrinsic way of splitting each tangent space to Q into horizontal and vertical subspaces. The vertical space V_q at q is the tangent space to the group orbit through q. If $\mathfrak{A}_q : T_qQ \to \mathfrak{g}$ is the restriction of $\mathfrak{A}$, then the horizontal space H_q is defined as the kernel of $\mathfrak{A}_q$. The maps $\mathrm{hor} : T_qQ \to H_q$ and $\mathrm{ver} : T_qQ \to V_q$ are the horizontal and vertical projections obtained from the split $T_qQ = H_q \oplus V_q$.

If L is of the form kinetic minus potential energy, then $\mathfrak{A}$ can be chosen to be the *mechanical connection*, although we shall not insist on this choice. However, in this case one gets, for example, as in Marsden et al. [2000b], a *global diffeomorphism* $J_L^{-1}(\mu)/G \cong TS$.

Reduction on the Lagrangian Side. From the connection $\mathfrak{A}$ we obtain a 1-form $\mathfrak{A}_\mu$ on Q defined by

$$\mathfrak{A}_\mu(q)\dot{q} := \langle \mu, \mathfrak{A}(\dot{q}) \rangle.$$

The exterior derivative $\mathbf{d}\mathfrak{A}_\mu$ of $\mathfrak{A}_\mu$ is a 2-form on Q. It can be shown (see, for example, Marsden [1992] or Marsden et al. [2000b]) that $\mathbf{d}\mathfrak{A}_\mu$ is G-invariant and is zero on all vertical tangent vectors to Q. Thus, $\mathbf{d}\mathfrak{A}_\mu$ drops to a 2-form on S, which we shall call β_μ. It is often called the ***magnetic* 2*-form***.

If q is a curve that solves the Euler–Lagrange equations, then it is a solution of Hamilton's variational principle, which states that

$$\delta \int_a^b L(q, \dot{q})\, dt = 0,$$

for all variations δq of q that vanish at the endpoints. The curve x obtained by projecting this solution q onto the shape space also solves a variational principle on the shape space. This reduced variational principle has the form

$$\delta \int_a^b \hat{R}^\mu(x, \dot{x})\, dt = \int_a^b \beta_\mu(\dot{x}, \delta x)\, dt, \tag{2.2.2}$$

for all variations δx of x that vanish at the endpoints and for a function $\hat{R}^\mu$ that we shall now define.

To define the ***Routhian*** $\hat{R}^\mu$ on TS, we first define a function R^μ on TQ by

$$R^\mu(q,\dot{q}) = L(q,\dot{q}) - \mathfrak{A}_\mu(q)\dot{q},$$

where μ is the momentum of the solution q. The restriction of R^μ to $J_L^{-1}(\mu)$ is G-invariant and $\hat{R}^\mu$ is obtained by dropping $R^\mu | J_L^{-1}(\mu)$ to $J_L^{-1}(\mu)/G \approx TS$.

It is easy to check that the reduced variational principle above is equivalent to the equations

$$\frac{\partial \hat{R}^\mu}{\partial x} - \frac{d}{dt}\frac{\partial \hat{R}^\mu}{\partial \dot{x}} = \mathbf{i}_{\dot{x}}\beta_\mu(x), \tag{2.2.3}$$

where $\mathbf{i}_{\dot{x}}$ denotes interior product of the 2-form β_μ with the vector $\dot{x}$. We call Equation 2.2.3 the ***Routh equations***.

Reduction on the Hamiltonian Side. If the group G is abelian (which is what we have assumed), then from equivariance of the momentum map, we see that G acts on the momentum level set $J^{-1}(\mu) \subset T^*Q$. The quotient $J^{-1}(\mu)/G$ can be identified with T^*S. The projection $J^{-1}(\mu) \to T^*S$ called π_μ and can be defined as follows: If $\alpha_q \in J^{-1}(\mu)$, then the ***momentum shift*** $\alpha_q - \mathfrak{A}_\mu(q)$ annihilates all vertical tangent vectors at $q \in Q$, as shown by the following calculation:

$$\langle \alpha_q - \mathfrak{A}_\mu(q), \xi_Q(q)\rangle = J(\alpha_q)\cdot\xi - \langle \mu, \xi\rangle = \langle \mu, \xi\rangle - \langle \mu, \xi\rangle = 0.$$

Thus, $\alpha_q - \mathfrak{A}_\mu(q)$ induces an element of T_x^*S and $\pi_\mu(\alpha_q)$ is defined to be this element.

By Noether's theorem, the flow of the Hamiltonian vector field X_H leaves the set $J^{-1}(\mu)$ invariant and is equivariant, and so the restricted flow induces a reduced flow on T^*S. This reduced flow corresponds to a reduced Hamiltonian vector X_{H_μ} on T^*S, which can be obtained from a reduced Hamiltonian H_μ and a reduced symplectic form Ω_μ. The reduced energy at momentum level μ is denoted H_μ and is obtained by restricting H to $J^{-1}(\mu)$ and then, using its invariance, to drop it to a function on T^*S. Similarly, we get the reduced symplectic form Ω_μ by restricting Ω_Q to $J^{-1}(\mu)$ and then dropping to T^*S; namely, the reduced symplectic structure Ω_μ is related to Ω_Q by the equation

$$\pi_\mu^*\Omega_\mu = i_\mu^*\Omega_Q,$$

and is preserved by the reduced flow. An important result for cotangent bundles is that $\Omega_\mu = \Omega_S - \pi_{T^*S,S}^*\beta_\mu$, where Ω_S is the canonical symplectic form on T^*S, and $\pi_{T^*S,S} : T^*S \to S$ is the natural projection. See, for example, Marsden [1992] for the proof.

Relating Lagrangian and Hamiltonian Reduction. The projections $\pi_{\mu,L} : J_L^{-1}(\mu) \to TS$ and $\pi_\mu : J^{-1}(\mu) \to T^*S$ are related by the equation,

$$\pi_\mu \circ \mathbb{F}L = \mathbb{F}\hat{R}^\mu \circ \pi_{\mu,L},$$

where $\mathbb{F}\hat{R}^\mu : TS \to T^*S$ is the reduced Routh-Legendre transform and is defined by

$$\mathbb{F}\hat{R}^\mu : (x, \dot{x}) \mapsto \left(x, \frac{\partial \hat{R}^\mu}{\partial \dot{x}} \right).$$

Notice that the Routhian $\hat{R}^\mu$ has the momentum shift built into it as does the projection π_μ. It readily follows that the reduced dynamics on TS and on T^*S, given by the Routh equations and the vector field X_{H_μ}, respectively, are also related by the reduced Legendre transform $\mathbb{F}\hat{R}^\mu$. Thus, the relationships between the reduced and "unreduced" spaces and the reduced and unreduced dynamics can be depicted in the following commutative diagram:

$$\begin{array}{ccc} (J_L^{-1}(\mu), EL) & \xrightarrow{\mathbb{F}L} & (J^{-1}(\mu), X_H) \\ \downarrow{\scriptstyle \pi_{\mu,L}} & & \downarrow{\scriptstyle \pi_\mu} \\ (TS, R) & \xrightarrow{\mathbb{F}\hat{R}^\mu} & (T^*S, X_{H_\mu}) \end{array}$$

From the commutativity of this diagram, one sees that conservation of the symplectic 2-form $(\mathbb{F}\hat{R}^\mu)^*(\Omega_S - \pi^*_{T^*S,S}\beta_\mu)$ by the flow of the Routh equations follows from the conservation of the 2-form $\Omega_S - \pi^*_{T^*S,S}\beta_\mu$ by the flow of the reduced Hamiltonian vector field. Conservation of $(\mathbb{F}\hat{R}^\mu)^*(\Omega_S - \pi^*_{T^*S,S}\beta_\mu)$ can also be shown directly from the reduced variational principle (Equation 2.2.2).

Reconstruction. There is a general theory of reconstruction for both the Hamiltonian and Lagrangian sides of reduction. The problem is this: given an integral curve in the reduced space TS or T^*S, a value of μ and an initial condition in the μ-level set of the momentum map, how does one reconstruct the integral curve through that initial condition in TQ or T^*Q? This question involves the theory of geometric phases and of course is closely related to the classical constructions of solutions by quadratures given a set of integrals of motion. This is not a trivial procedure, even for abelian symmetry groups, although in this case things are somewhat more explicit. This procedure is discussed at length in, for example, Marsden et al. [1990], Marsden [1992] and Marsden et al. [2000b]. We shall need this theory at a couple of points in what follows.

2.3 Discrete Reduction

2.3.1 Discrete Variational Mechanics

In this paper, we will be using the theory of discrete mechanics as described in Marsden and West [2001]. In this subsection, we briefly describe the essential features of this theory and fix our notation.

Discrete Lagrangians. Given a configuration manifold Q, a discrete Lagrangian system consists of the ***discrete phase space*** $Q \times Q$ and a ***discrete Lagrangian*** $L_d : Q \times Q \to \mathbb{R}$. As we are interested in discrete systems which approximate a given continuous system, we will take discrete Lagrangians which depend on a ***timestep*** h, so that $L_d : Q \times Q \times \mathbb{R} \to \mathbb{R}$ should be thought of as approximating the action for time h,

$$L_d(q_0, q_1, h) \approx \int_0^h L(q(t), \dot{q}(t))\, dt, \tag{2.3.1}$$

where $q : [0, h] \to Q$ is a continuous trajectory solving the Euler–Lagrange equations for L with boundary conditions $q(0) = q_0$ and $q(h) = q_1$. When the timestep is fixed in a discussion, we often neglect the timestep dependence in L_d and write $L_d(q_0, q_1)$ for simplicity.

Discrete Euler–Lagrange Equations. Just as continuous trajectories are maps from $[0, T]$ to Q, we consider ***discrete trajectories***, which are maps from $\{0, h, 2h, \ldots, Nh = T\}$ to Q. This gives a set of points in Q which we denote $\mathbf{q} = \{q_k\}_{k=0}^N$.

Having defined a discrete Lagrangian, we define the ***discrete action*** to be a function mapping discrete trajectories $\mathbf{q} = \{q_k\}_{k=0}^N$ to the reals, given by

$$\mathfrak{G}_d(\mathbf{q}) = \sum_{k=0}^{N-1} L_d(q_k, q_{k+1}). \tag{2.3.2}$$

Hamilton's principle requires that the discrete action be stationary with respect to variations vanishing at $k = 0$ and $k = N$. Computing the variations gives

$$\begin{aligned}
\mathbf{d}\mathfrak{G}_d(\mathbf{q}) \cdot \delta\mathbf{q} &= \sum_{k=0}^{N-1} \left[D_1 L_d(q_k, q_{k+1}) \cdot \delta q_k + D_2 L_d(q_k, q_{k+1}) \cdot \delta q_{k+1} \right] \\
&= \sum_{k=1}^{N-1} \left[D_2 L_d(q_{k-1}, q_k) + D_1 L_d(q_k, q_{k+1}) \right] \cdot \delta q_k \\
&\qquad + D_1 L_d(q_0, q_1) \cdot \delta q_0 + D_2 L_d(q_{N-1}, q_N) \cdot \delta q_N.
\end{aligned}$$

The requirement that this be zero for all variations satisfying $\delta q_0 = \delta q_N = 0$ gives the ***discrete***

Euler–Lagrange (DEL) equations,

$$D_2 L_d(q_{k-1}, q_k) + D_1 L_d(q_k, q_{k+1}) = 0, \tag{2.3.3}$$

for each $k = 1, \ldots, N-1$. These implicitly define the ***discrete Lagrange map***, $F_{L_d} : Q \times Q \to Q \times Q$; $(q_{k-1}, q_k) \mapsto (q_k, q_{k+1})$. We also refer to this map as the ***discrete Lagrangian evolution operator***.

Discrete Lagrange Forms. The boundary terms in the expression for $\mathbf{d}\mathfrak{G}_d$ can be identified as the two ***discrete Lagrange*** 1***-forms*** on $Q \times Q$, which are

$$\Theta^+_{L_d}(q_0, q_1) = D_2 L_d(q_0, q_1)\mathbf{d}q_1, \tag{2.3.4a}$$

$$\Theta^-_{L_d}(q_0, q_1) = -D_1 L_d(q_0, q_1)\mathbf{d}q_0. \tag{2.3.4b}$$

In coordinates, note that

$$\Theta^+_{L_d} = \frac{\partial L_d}{\partial q_1^i} dq_1^i. \tag{2.3.5}$$

We define the ***discrete Lagrange*** 2***-form*** on $Q \times Q$ to be

$$\Omega_{L_d} = -\mathbf{d}\Theta^+_{L_d}, \tag{2.3.6}$$

which in coordinates is

$$\Omega_{L_d} = -\mathbf{d}\left(\frac{\partial L_d}{\partial q_1^i} dq_1^i\right) = \frac{\partial^2 L_d}{\partial q_1^i \partial q_2^j} dq_1^i \wedge dq_2^j. \tag{2.3.7}$$

A straightforward calculation shows that

$$\Omega_{L_d} = -\mathbf{d}\Theta^-_{L_d}. \tag{2.3.8}$$

The space of solutions of the discrete Euler–Lagrange equations can be identified with the space $Q \times Q$ of initial conditions (q_0, q_1). Restricting the free variations of the discrete action to this space shows that we have

$$\mathbf{d}\mathfrak{G}_d|_{Q \times Q} = -\Theta^-_{L_d} + (F^{N-1}_{L_d})^*(\Theta^+_{L_d}),$$

and so taking a second derivative and using the fact that $\mathbf{d}^2 = 0$ shows that

$$(F^{N-1}_{L_d})^*\Omega_{L_d} = \Omega_{L_d}.$$

In particular, taking $N = 2$, we see that *the discrete Lagrange evolution operator is symplectic*; that is,

$$(F_{L_d})^* \Omega_{L_d} = \Omega_{L_d}. \tag{2.3.9}$$

Discrete Legendre Transforms. Given a discrete Lagrangian we define the ***discrete Legendre transforms***, $\mathbb{F}^+ L_d, \mathbb{F}^- L_d : Q \times Q \to T^*Q$, by

$$\mathbb{F}^- L_d(q_0, q_1) = (q_0, -D_1 L_d(q_0, q_1)), \tag{2.3.10a}$$

$$\mathbb{F}^+ L_d(q_0, q_1) = (q_1, D_2 L_d(q_0, q_1)), \tag{2.3.10b}$$

and we observe that the discrete Lagrange 1- and 2-forms are related to the canonical 1- and 2-forms on T^*Q by pull-back under the discrete Legendre transforms; that is, $\Theta^{\pm}_{L_d} = (\mathbb{F}^{\pm} L_d)^*(\Theta)$ and $\Omega_{L_d} = (\mathbb{F}^{\pm} L_d)^*(\Omega)$.

Pushing the discrete Lagrange map forward to T^*Q with the discrete Legendre transform gives the ***push-forward discrete Lagrange map***, $\tilde{F}_{L_d} : T^*Q \to T^*Q$ by $\tilde{F}_{L_d} = \mathbb{F}^{\pm} L_d \circ F_{L_d} \circ (\mathbb{F}^{\pm} L_d)^{-1}$. One checks that one has the same map for the $+$ case and the $-$ case. In fact, the expression for the push-forward discrete Lagrange map can be seen to be determined as follows: $\tilde{F}_{L_d} : (q_0, p_0) \mapsto (q_1, p_1)$, where

$$p_0 = -D_1 L_d(q_0, q_1), \tag{2.3.11a}$$

$$p_1 = D_2 L_d(q_0, q_1). \tag{2.3.11b}$$

Note that by construction, the push-forward discrete Lagrange map preserves the canonical 2-form. The push-forward discrete Lagrange map is thus symplectic; that is, $(\tilde{F}_{L_d})^*(\Omega) = \Omega$.

Exact Discrete Lagrangians. The relationship between a discrete Lagrangian and the corresponding push-forward discrete Lagrange map is that of ***generating functions*** of the first kind. Generating function theory shows that for any symplectic map $T^*Q \to T^*Q$ (at least those near the identity), there is a corresponding generating function $Q \times Q \to \mathbb{R}$ which generates the map in the sense of Equation 2.3.11.

It is thus clear that there is a discrete Lagrangian for every symplectic map, including the exact flow $F^t_H : T^*Q \to T^*Q$ of the Hamiltonian system corresponding to the Lagrangian L. This is referred to as the ***exact discrete Lagrangian*** and Hamilton–Jacobi theory shows that it is equal to the action,

$$L^E_d(q_0, q_1, h) = \int_0^h L(q(t), \dot{q}(t))\, dt, \tag{2.3.12}$$

where $q : [0, h] \to Q$ solves the Euler–Lagrange equations for L with $q(0) = q_0$ and $q(h) = q_1$. This classical theorem of Jacobi is proved in, for example, Marsden and Ratiu [1999].

Using this exact discrete Lagrangian, the push-forward discrete Lagrange map will be exactly the Hamiltonian flow map for time h, so that $\tilde{F}_{L_d^E} = F_H^h$. That is, discrete trajectories $\mathbf{q} = \{q_k\}_{k=0}^N$ will exactly sample continuous trajectories $q(t)$, namely $q_k = q(kh)$.

Approximate Discrete Lagrangians. If we choose a discrete Lagrangian which only approximates the action, then the resulting push-forward discrete Lagrange map will only approximate the true flow. The orders of approximation are related, so that if the discrete Lagrangian is of order r,

$$L_d = \int_0^h L(q, \dot{q})\, dt, + \mathcal{O}(h^{r+1}), \tag{2.3.13}$$

then the push-forward discrete Lagrange map will also be of order r; that is,

$$\tilde{F}_{L_d}^h = F_H^h + \mathcal{O}(h^{r+1}). \tag{2.3.14}$$

By choosing discrete Lagrangians which are at least consistent ($r \geq 1$) we can regard the discrete Lagrange map as an ***integrator*** for the continuous system.

2.3.2 Discrete Mechanical Systems with Symmetry

Let G be an abelian Lie group that acts freely and properly on the configuration manifold Q. We will assume that our discrete Lagrangian L_d is invariant under the diagonal action of G on $Q \times Q$. Such a discrete Lagrangian could have been obtained by discretizing a continuous Lagrangian L that is invariant under the lifted action of G on TQ. For a discussion of how to construct G-invariant discrete Lagrangians from G-invariant Lagrangians using natural charts, please see §5.3.2.

Note that Q is a bundle over the shape space $S = Q/G$. Using a local trivialization, Q can be locally identified with $G \times S$. Thus $Q \times Q \approx G \times S \times G \times S$. With this identification, $(q_k, q_{k+1}) = (h_k, x_k, h_{k+1}, x_{k+1})$. We will use $\partial/\partial g_i$, $i = 1, 2$, to denote partial derivatives with respect to the first and second group variables, and $\partial/\partial s_i$, $i = 1, 2$, to denote partial derivatives with respect to the first and second shape space variables.

Given a discrete Lagrangian, the ***discrete momentum map***, $J_d : Q \times Q \to \mathfrak{g}^*$, is defined by

$$J_d(q_0, q_1) \cdot \xi = D_2 L_d(q_0, q_1) \cdot \xi_Q(q_1). \tag{2.3.15}$$

Since L_d is invariant under the action of G, we have

$$D_1 L_d(q_0, q_1) \cdot \xi_Q(q_0) + D_2 L_d(q_0, q_1) \cdot \xi_Q(q_1) = 0.$$

Thus,

$$\begin{aligned} J_d(q_0, q_1) \cdot \xi &= D_2 L_d(q_0, q_1) \cdot \xi_Q(q_1) = -D_1 L_d(q_0, q_1) \cdot \xi_Q(q_0) \\ &= \xi_Q(q_1) \lrcorner \Theta^+_{L_d}(q_0, q_1) = \xi_Q(q_0) \lrcorner \Theta^-_{L_d}(q_0, q_1), \end{aligned}$$

where $X \lrcorner \omega$ denotes the interior product of a vector X with a 1-form ω. Thus, if $\{q_0, q_1, q_2, \ldots\}$ solves the DEL equations, then

$$\begin{aligned} J_d(q_1, q_2) \cdot \xi &= D_2 L_d(q_1, q_2) \cdot \xi_Q(q_2) = -D_1 L_d(q_1, q_2) \cdot \xi_Q(q_1) \\ &= D_2 L_d(q_0, q_1) \cdot \xi_Q(q_1) = J_d(q_0, q_1) \cdot \xi. \end{aligned}$$

Thus, the discrete momentum is conserved by the discrete Lagrange map, $F_{L_d} : Q \times Q \to Q \times Q$, $F_{L_d} : (q_0, q_1) \mapsto (q_1, q_2)$. In other words, the discrete momentum is conserved along solutions of the DEL equations, which is referred to as the ***discrete Noether theorem***.

By definition of J_d,

$$J_d(q_0, q_1) \cdot \xi = J(D_2 L_d(q_0, q_1)) \cdot \xi,$$

where $J : T^*Q \to \mathfrak{g}^*$ is the momentum map on T^*Q. Thus,

$$J_d = J \circ \mathbb{F}L_d,$$

where $\mathbb{F}L_d = D_2 L_d : Q \times Q \to T^*Q$ is the discrete Legendre transform. (Note that in §2.3.1 we had two discrete Legendre transforms, $\mathbb{F}^+ L_d$ and $\mathbb{F}^- L_d$. For the remainder of this paper, we use the term discrete Legendre transform and the symbol $\mathbb{F}L_d$ to denote $\mathbb{F}^+ L_d$ to make a specific choice.) Thus, $\mathbb{F}L_d$ maps $J_d^{-1}(\mu)$, which is the μ-level set of the discrete momentum to $J^{-1}(\mu)$. Also, since J_d is conserved by the discrete evolution operator F_{L_d}, it follows that the push-forward discrete Lagrange map $\tilde{F}_{L_d} : T^*Q \to T^*Q$ preserves J.

In a local trivialization, where $q_1 = (\theta_1, x_1)$,

$$\xi_Q(q_1) = \frac{d}{dt}\Big|_{t=0} (\exp(t\xi) \cdot \theta_1, x_1) = (TR_{\theta_1} \cdot \xi, 0),$$

where R_{θ_1} denotes right multiplication on G by θ_1. Thus,

$$J_d(q_0, q_1) \cdot \xi = \begin{bmatrix} \dfrac{\partial L_d}{\partial g_2} & \dfrac{\partial L_d}{\partial s_2} \end{bmatrix} \cdot \begin{bmatrix} TR_{\theta_1} \cdot \xi \\ \\ 0 \end{bmatrix} = \frac{\partial L_d}{\partial g_2} \circ TR_{\theta_1} \cdot \xi.$$

Hence,

$$J_d(q_0, q_1) = \frac{\partial L_d}{\partial g_2}(\theta_0, x_0, \theta_1, x_1) \circ TR_{\theta_1}.$$

The momentum map, $J_d : Q \times Q \to \mathfrak{g}^*$, is ***equivariant*** as the following calculation shows:

$$\begin{aligned} J_d(\theta \cdot q_0, \theta \cdot q_1) \cdot \xi &= D_1 L_d(\theta \cdot q_0, \theta \cdot q_1) \cdot \xi_Q(\theta \cdot q_0) \\ &= D_1 L_d(\theta \cdot q_0, \theta \cdot q_1) \cdot \theta \cdot (\mathrm{Ad}_{\theta^{-1}} \xi)_Q(q_0) \\ &= D_1 L_d(q_0, q_1) \cdot (\mathrm{Ad}_{\theta^{-1}} \xi)_Q(q_0) \\ &= J_d(q_0, q_1) \circ \mathrm{Ad}_{\theta^{-1}} \cdot \xi \\ &= (\mathrm{Ad}^*_{\theta^{-1}} J_d(q_0, q_1)) \cdot \xi. \end{aligned}$$

Thus, the coadjoint isotropy subgroup G_μ of G acts on $J_d^{-1}(\mu)$. Since G is abelian, $G_\mu = G$, and thus G acts on $J_d^{-1}(\mu)$.

If the value of the momentum is μ, the equation

$$\frac{\partial L_d}{\partial g_2}(\theta_0, x_0, \theta_1, x_1) \circ TR_{\theta_1} = \mu,$$

determines θ_1 implicitly as a function of θ_0, x_0, x_1 and μ. Thus the level set $J_d^{-1}(\mu)$ can be (locally) identified with $G \times S \times S$. The quotient $J_d^{-1}(\mu)/G$ is thus locally diffeomorphic to $S \times S$.

If we choose a momentum μ, it follows from the above discussion that there is a unique map $\psi_\mu : S \times S \to G$, such that,

$$J_d(e, x_k, \psi_\mu(x_k, x_{k+1}), x_{k+1}) = \mu.$$

Further, if $\theta_k \in G$, $\theta_k \cdot (e, x_k, \psi_\mu(x_k, x_{k+1}), x_{k+1}) = (\theta_k, x_k, \theta_k \cdot \psi_\mu(x_k, x_{k+1}), x_{k+1})$ is also in $J_d^{-1}(\mu)$. Thus for a given μ, the function giving θ_{k+1} in terms of θ_k, x_k and x_{k+1} is

$$\theta_{k+1} = \theta_k \cdot \psi_\mu(x_k, x_{k+1}). \tag{2.3.16}$$

Reconstruction. The following lemma gives a basic result on the reconstruction of discrete curves in the configuration manifold Q from those in the shape space S. The lemma is similar to its continuous counterpart, as in Lemma 2.2 of Jalnapurkar and Marsden [2000]. Recall that V_q denotes the vertical space at q, which is the space of all vectors at q that are infinitesimal generators $\xi_Q(q) \in T_qQ$. We say that the discrete Lagrangian L_d is ***group-regular*** if the bilinear map $D_2D_1L_d(q,q) : T_qQ \times T_qQ \to \mathbb{R}$ restricted to the subspace $V_q \times V_q$ is nondegenerate. Besides regularity, we shall make group-regularity a standing assumption in this chapter as well.

Lemma 2.1 (Reconstruction Lemma). *Let $\mu \in \mathfrak{g}^*$ be given, and $\mathbf{x} = \{x_0, \ldots, x_n\}$ be a sufficiently closely spaced discrete curve in S. Let $q_0 \in Q$ be such that $\pi_{Q,S}(q_0) = x_0$. Then, there is a unique closely spaced discrete curve $\mathbf{q} = \{q_0, \ldots, q_n\}$ such that $\pi_{Q,S}(q_k) = x_k$ and $J_d(q_k, q_{k+1}) = \mu$, for $k = 0, \ldots, n-1$.*

Proof. We must construct a point q_1 close to q_0 such that $\pi_{Q,S}(q_1) = x_1$ and $J_d(q_0, q_1) = \mu$. The construction of the subsequent points $q_2, \ldots, q_n$ will follow in an inductive fashion.

To do this, pick a local trivialization of the bundle $\pi_{Q,S} : Q \to Q/G$, where $Q \approx G \times S$ locally, and write points in this trivialization as $q_k = (\theta_k, x_k)$.

Given the point $q_0 = (\theta_0, x_0)$, we seek a near identity group element g, such that $q_1 := (g\theta_0, x_1)$ satisfies $J_d(q_0, q_1) = \mu$. By the definition of the discrete momentum map (Equation 2.3.15), this means that we must satisfy the condition

$$D_2L_d(q_0, q_1) \cdot \xi_Q(q_1) = \langle \mu, \xi \rangle$$

for all $\xi \in \mathfrak{g}$. In the local trivialization, this means that

$$D_2L_d((\theta_0, x_0), (g\theta_0, x_1)) \cdot (TR_{g\theta_0}\xi, 0) = \langle \mu, \xi \rangle ,$$

where R_g denotes right translation on the group by the element g.

Consider solving the above equation for $\theta_1 = g\theta_0$ as a function of θ_0, x_0, x_1, with μ fixed. We know the base solution corresponding to the case $x_1 = x_0$, namely $g = e$. The implicit function theorem tells us that when x_1 is moved away from x_0, there will be a unique solution for g near the identity, provided that the derivative of the defining relation with respect to g at the identity is invertible. But this condition is a consequence of group-regularity, so the result follows. □

Note that the above lemma makes no hypotheses about the sequence satisfying the discrete Euler–Lagrange equations.

To obtain the reconstruction equation in the continuous case, we require that the lifted curve is second-order, on the momentum surface, and that it projects down to the reduced curve. It is appropriate to consider the discrete analogue of the second-order curve condition, since it may not be apparent where we imposed such a condition.

We consider a discrete curve $\mathbf{x}$ as a sequence of points, $(x_0, x_1), (x_1, x_2), \ldots, (x_{n-1}, x_n)$ in $S \times S$. Lift each of the points in $S \times S$ to the momentum surface $J_d^{-1}(\mu) \subset Q \times Q$. This yields the sequence, $(q_0^0, q_1^0), (q_0^1, q_1^1), \ldots, (q_0^{n-1}, q_1^{n-1})$, which is unique up to a diagonal group action on $Q \times Q$. The discrete analogue of the second-order curve condition is that this sequence in $Q \times Q$ defines a discrete curve in Q, which corresponds to requiring that $q_1^k = q_0^{k+1}$, for $k = 0, \ldots, n-1$, which is clearly possible in the context of the reconstruction lemma.

This discussion of the discrete reconstruction equation naturally leads to issues of geometric phases, and it would be interesting to obtain an expression for the discrete geometric phase in terms of the discrete curve on shape space.

Reconstruction of Tangent Vectors. Let (q_0, q_1) be a lift of (x_0, x_1) to $J_d^{-1}(\mu)$, and $(\delta x_0, \delta x_1)$ be a tangent vector to $S \times S$ at (x_0, x_1). Given $\delta q_0 \in T_{q_0} Q$, with $T\pi_{Q,S} \cdot \delta q_0 = \delta x_0$, it is possible to find a $\delta q_1 \in T_{q_1} Q$, with $T\pi_{Q,S} \cdot \delta q_1 = \delta x_1$, such that $(\delta q_0, \delta q_1)$ is a tangent vector to $J_d^{-1}(\mu)$ at (q_0, q_1). Indeed, if in a local trivialization, $\delta q_0 = (\delta\theta_0, \delta x_0)$, then the required δq_1 is $(\delta\theta_1, \delta x_1)$, where $\delta\theta_1$ is obtained by differentiating Equation 2.3.16 as follows:

$$\delta\theta_1 = \delta\theta_0 \cdot \psi_\mu(x_0, x_1) + \theta_0 \cdot D_1\psi_\mu(x_0, x_1)\delta x_0 + \theta_0 \cdot D_2\psi_\mu(x_0, x_1)\delta x_1.$$

Discrete Connection. It should be noted that although our discussion of reconstruction is cast in terms of local trivializations, it is in fact intrinsic and can be thought of as a discrete horizontal lift in the sense of discrete connections developed in Chapter 4. The discrete connection associated with the reconstruction to the discrete μ-momentum surface is represented by the discrete connection 1-form $\mathcal{A}_d : Q \times Q \to G$, defined on a G-invariant neighborhood of the diagonal by $\mathcal{A}_d(q_0, q_1) = e$ iff $J_d(q_0, q_1) = \mu$, and extended to other points by

$$\mathcal{A}_d(g_0 q_0, g_1 q_1) = g_1 g_0^{-1}.$$

The reconstruction lemma (Lemma 2.1) may be viewed as providing the horizontal lift of this discrete connection.

The discrete connection given above is the natural choice of connection on $Q \times Q$ for the purpose of constructing a unified formulation of discrete, Lagrangian, and Hamiltonian reduction. Recall the following diagram,

$$\begin{array}{ccc} (TQ, J_L) & \xrightarrow{\mathbb{F}L} & (T^*Q, J) \\ & & \uparrow {\scriptstyle \mathbb{F}L_d} \\ & & (Q \times Q, J_d) \end{array}$$

and consider the horizontal space on TQ given by the μ-momentum surface, $J_L^{-1}(\mu)$. Since $J_L = (\mathbb{F}L)^* J$, and $J_d = (\mathbb{F}L_d)^* J$, it follows that $(\mathbb{F}L)_* J_L^{-1}(\mu) = (\mathbb{F}L_d)_* J_d^{-1}(\mu)$, and as a consequence, $(\mathbb{F}L_d)^*(\mathbb{F}L)_* J_L^{-1}(\mu) = J_d^{-1}(\mu)$. This implies that the discrete reconstruction equation is simply the horizontal lift with respect to the discrete connection on $Q\times Q$ that is consistent with the connection on TQ with respect to the fiber derivatives $\mathbb{F}L$ and $\mathbb{F}L_d$, and is therefore an intrinsic operation. The discrete connection obtained in this way is related to the discrete mechanical connection, and is given by the discrete connection 1-form introduced above.

Discrete connections also yield a semi-global isomorphism $(Q \times Q)/G \cong (S \times S) \oplus \tilde{G}$ (see §4.4.8) for neighborhoods of the diagonal, and this induces a semi-global isomorphism $J_d^{-1}(\mu)/G \cong S \times S$, which is a discrete analogue of the global diffeomorphism, $J_L^{-1}(\mu)/G \cong TS$, that was obtained in Marsden et al. [2000b] with the use of the mechanical connection.

2.3.3 Discrete Reduction

In this section, we start by assuming that we have been given a discrete Lagrangian, $L_d : Q\times Q \to \mathbb{R}$, that is invariant under the action of an abelian Lie group G on $Q \times Q$.

Let $\mathbf{q} := \{q_0, \ldots, q_n\}$ be a solution of the discrete Euler–Lagrange (DEL) equations. Let the value of the discrete momentum along this trajectory be μ. Let $x_i = \pi_{Q,S}(q_i)$, so that $\mathbf{x} := \{x_0, \ldots, x_n\}$ is a discrete trajectory on shape space. Since $\mathbf{q}$ satisfies the discrete variational principle, it is appropriate to ask if there is a reduced variational principle satisfied by $\mathbf{x}$.

An important issue in dropping the discrete variational principle to the shape space is whether we require that the varied curves are constrained to lie on the level set of the momentum map. The constrained approach is adopted in Jalnapurkar and Marsden [2000], and the unconstrained approach is used in Marsden et al. [2000b]. In the rest of this section, we will adopt the unconstrained approach of Marsden et al. [2000b], and will show that the variations in the discrete action sum evaluated at a solution of the discrete Euler–Lagrange equation depends only on the quotient variations, and therefore drops to the shape space without constraints on the variations.

By G-invariance of L_d, the restriction of L_d to $J_d^{-1}(\mu)$ drops to the quotient $J_d^{-1}(\mu)/G \approx S \times S$. The function obtained on the quotient is called the reduced Lagrangian and is denoted $\hat{L}_d$. Let $\pi_{\mu,d} : J_d^{-1}(\mu) \to S \times S$ be the projection. Let $(q_0, q_1) \in J_d^{-1}(\mu)$, and $(\delta q_0, \delta q_1) \in T_{(q_0,q_1)} J_d^{-1}(\mu)$. If $\pi_{Q,S} \cdot q_i = x_i$ and $T\pi_{Q,S} \cdot \delta q_i = \delta x_i$, $i = 0, 1$, then $\pi_{\mu,d}(q_0, q_1) = (x_0, x_1)$ and $T\pi_{\mu,d} \cdot (\delta q_0, \delta q_1) = (\delta x_0, \delta x_1)$. In this situation, we get $L_d(q_0, q_1) = \hat{L}_d(x_0, x_1)$, and so

$$DL_d(q_0, q_1) \cdot (\delta q_0, \delta q_1) = D\hat{L}_d(x_0, x_1) \cdot (\delta x_0, \delta x_1). \tag{2.3.17}$$

For $\mathbf{q}$ a solution of the DEL equations, and $\mathbf{x}$ the corresponding curve on the shape space

S, let $\delta\mathbf{x} = \frac{d}{d\varepsilon}\big|_{\varepsilon=0}\mathbf{x}_\varepsilon$ be a variation of $\mathbf{x}$. Let $\delta\mathbf{q} = \frac{d}{d\varepsilon}\big|_{\varepsilon=0}\mathbf{q}_\varepsilon$ be any variation of $\mathbf{q}$ such that $T\pi_{Q,S} \cdot \delta q_i = \delta x_i$. Then,

$$\begin{aligned}
\delta \sum_{k=0}^{n-1} L_d(q_k, q_{k+1}) &= \frac{d}{d\varepsilon}\Big|_{\varepsilon=0} \sum_k L_d(q_{k\varepsilon}, q_{k+1\varepsilon}) \\
&= \sum_k DL_d(q_k, q_{k+1}) \cdot (\delta q_k, \delta q_{k+1}) \\
&= D_1 L_d(q_0, q_1) \cdot \delta q_0 \\
&\quad + \sum_{k=1}^{n-1} (D_2 L_d(q_{k-1}, q_k) + D_1 L_d(q_k, q_{k+1})) \cdot \delta q_k \\
&\quad + D_2 L_d(q_{n-1}, q_n) \cdot \delta q_n \\
&= D_1 L_d(q_0, q_1) \cdot \delta q_0 + D_2 L_d(q_{n-1}, q_n) \cdot \delta q_n, \qquad (2.3.18)
\end{aligned}$$

where we have used the fact that $\mathbf{q}$ satisfies the discrete Euler–Lagrange equations.

Recall that the discrete momentum map is given by

$$J_d(q_k, q_{k+1}) \cdot \xi = D_2 L_d(q_k, q_{k+1}) \cdot \xi_Q(q_{k+1}) = -D_1 L_d(q_k, q_{k+1}) \cdot \xi_Q(q_k).$$

Given any connection $\mathfrak{A}$ on Q, we have a horizontal-vertical split of each tangent space to Q. Thus,

$$D_2 L_d(q_{n-1}, q_n) \cdot \delta q_n = D_2 L_d(q_{n-1}, q_n) \cdot \text{hor } \delta q_n + D_2 L_d(q_{n-1}, q_n) \cdot \text{ver } \delta q_n.$$

Now, ver $\delta q_n = \xi_Q(q_n)$, where $\xi = \mathfrak{A}(\delta q_n)$. Thus, $\mathfrak{A}(\delta q_n) = \mathfrak{A}(\text{ver } \delta q_n) = \mathfrak{A}(\xi_Q(q_n))$. So,

$$\begin{aligned}
D_2 L_d(q_{n-1}, q_n) \cdot \text{ver } \delta q_n &= D_2 L_d(q_{n-1}, q_n) \cdot \xi_Q(q_n) \\
&= J_d(q_{n-1}, q_n) \cdot \xi = \langle \mu, \xi \rangle = \langle \mu, \mathfrak{A}(\xi_Q(q_n)) \rangle \\
&= \langle \mu, \mathfrak{A}(\delta q_n) \rangle = \mathfrak{A}_\mu(q_n) \cdot \delta q_n. \qquad (2.3.19)
\end{aligned}$$

Thus,

$$D_2 L_d(q_{n-1}, q_n) \cdot \delta q_n = D_2 L_d(q_{n-1}, q_n) \cdot \text{hor } \delta q_n + \mathfrak{A}_\mu(q_n) \cdot \delta q_n. \qquad (2.3.20)$$

Similarly,

$$D_1 L_d(q_0, q_1) \cdot \delta q_0 = D_1 L_d(q_0, q_1) \cdot \text{hor } \delta q_0 - \mathfrak{A}_\mu(q_0) \cdot \delta q_0. \qquad (2.3.21)$$

Thus, from Equation 2.3.18,

$$\frac{d}{d\varepsilon}\Big|_{\varepsilon=0}\sum_k L_d(q_{k_\varepsilon}, q_{k+1_\varepsilon}) = D_1 L_d(q_0, q_1)\cdot \text{hor }\delta q_0 + D_2 L_d(q_{n-1}, q_n)\cdot \text{hor }\delta q_n + \mathfrak{A}_\mu(q_n)\cdot\delta q_n - \mathfrak{A}_\mu(q_0)\cdot\delta q_0. \tag{2.3.22}$$

Define a 1-form $\mathcal{A}$ on $Q\times Q$ by

$$\mathcal{A}(q_0, q_1)(\delta q_0, \delta q_1) = \mathfrak{A}_\mu(q_1)\cdot\delta q_1 - \mathfrak{A}_\mu(q_0)\cdot\delta q_0. \tag{2.3.23}$$

If $\pi_1, \pi_2 : Q\times Q \to Q$ are projections onto the first and the second components, respectively. Then,

$$\mathcal{A} = \pi_2^*\mathfrak{A}_\mu - \pi_1^*\mathfrak{A}_\mu.$$

Using G-invariance of $\mathfrak{A}_\mu$, it follows that $\mathcal{A}$ is G-invariant. Also,

$$\mathcal{A}(q_0, q_1)(\xi_Q(q_0), \xi_Q(q_1)) = \mathfrak{A}_\mu(q_1)\cdot\xi_Q(q_1) - \mathfrak{A}_\mu(q_0)\cdot\xi_Q(q_0) = \langle\mu,\xi\rangle - \langle\mu,\xi\rangle = 0.$$

Thus, $\mathcal{A}$ annihilates all vertical tangent vectors to $Q\times Q$. It is easy to check that the 1-form $\mathcal{A}|J_d^{-1}(\mu)$, obtained by restricting $\mathcal{A}$ to $J_d^{-1}(\mu)$ is also G-invariant and annihilates vertical tangent vectors to $J_d^{-1}(\mu)$. Therefore, $\mathcal{A}|J_d^{-1}(\mu)$ drops to a 1-form $\hat{\mathcal{A}}$ on $J_d^{-1}(\mu)/G \approx S\times S$.

If $\pi_{\mu,d} : J_d^{-1}(\mu) \to J_d^{-1}(\mu)/G$ is the projection, and $i_{\mu,d} : J_d^{-1}(\mu) \to Q\times Q$ is the inclusion, then $\hat{\mathcal{A}}$ and $\mathcal{A}$ are related by the equation

$$\pi_{\mu,d}^*\hat{\mathcal{A}} = i_{\mu,d}^*\mathcal{A}.$$

We define the 1-forms $\hat{\mathcal{A}}^+$ and $\hat{\mathcal{A}}^-$ on $S\times S$ and the maps $\hat{\mathcal{A}}_1, \hat{\mathcal{A}}_2 : S\times S \to T^*S$ by the relations

$$\hat{\mathcal{A}}^+(x_0, x_1)\cdot(\delta x_0, \delta x_1) = \hat{\mathcal{A}}_2(x_0, x_1)\cdot\delta x_1 = \hat{\mathcal{A}}(x_0, x_1)\cdot(0, \delta x_1),$$
$$\hat{\mathcal{A}}^-(x_0, x_1)\cdot(\delta x_0, \delta x_1) = \hat{\mathcal{A}}_1(x_0, x_1)\cdot\delta x_0 = \hat{\mathcal{A}}(x_0, x_1)\cdot(\delta x_0, 0).$$

Note that we have the relations $\hat{\mathcal{A}} = \hat{\mathcal{A}}^+ + \hat{\mathcal{A}}^-$, and

$$\hat{\mathcal{A}}(x_0, x_1)\cdot(\delta x_0, \delta x_1) = \hat{\mathcal{A}}_1(x_0, x_1)\cdot\delta x_0 + \hat{\mathcal{A}}_2(x_0, x_1)\cdot\delta x_1.$$

From Equation 2.3.23, it follows that,

$$\mathfrak{A}_\mu(q_n)\cdot\delta q_n - \mathfrak{A}_\mu(q_0)\cdot\delta q_0 = \sum_{k=0}^{n-1}\mathfrak{A}_\mu(q_{k+1})\cdot\delta q_{k+1} - \mathfrak{A}_\mu(q_k)\cdot\delta q_k$$

$$= \sum_{k=0}^{n-1} \mathcal{A}(q_k, q_{k+1}) \cdot (\delta q_k, \delta q_{k+1}). \tag{2.3.24}$$

Thus, Equation 2.3.22 can be rewritten as

$$\begin{aligned} \frac{d}{d\varepsilon}\Big|_{\varepsilon=0} \sum_{k=0}^{n-1} L_d(q_{k_\varepsilon}, q_{k+1_\varepsilon}) =& D_1 L_d(q_0, q_1) \cdot \text{hor } \delta q_0 + D_2 L_d(q_{n-1}, q_n) \cdot \text{hor } \delta q_n \\ &+ \sum_{k=0}^{n-1} \mathcal{A}(q_k, q_{k+1}) \cdot (\delta q_k, \delta q_{k+1}), \end{aligned} \tag{2.3.25}$$

or equivalently,

$$\sum_{k=0}^{n-1} (DL_d - \mathcal{A})(q_k, q_{k+1}) \cdot (\delta q_k, \delta q_{k+1}) = D_1 L_d(q_0, q_1) \cdot \text{hor } \delta q_0 + D_2 L_d(q_{n-1}, q_n) \cdot \text{hor } \delta q_n. \tag{2.3.26}$$

The following lemma shows the sense in which the 1-form $(DL_d - \mathcal{A})$ on $Q \times Q$ drops to the quotient $J_d^{-1}(\mu)/G \approx S \times S$.

Lemma 2.2. *If* $(q_0, q_1) \in J_d^{-1}(\mu)$ *and* $(\delta q_0, \delta q_1) \in T_{(q_0,q_1)} Q \times Q$ *with* $\pi_{Q,S}(q_i) = x_i$ *and* $T\pi_{Q,S} \cdot \delta q_i = \delta x_i$, $i = 0, 1$, *then*

$$(DL_d - \mathcal{A})(q_0, q_1) \cdot (\delta q_0, \delta q_1) = (D\hat{L}_d - \hat{\mathcal{A}})(x_0, x_1) \cdot (\delta x_0, \delta x_1).$$

Proof. As we showed in the discussion at the end of §2.3.2, we can find $\delta q_1' \in T_{q_1} Q$ such that $T\pi_{Q,S} \cdot \delta q_1' = \delta x_1$ and $(\delta q_0, \delta q_1') \in T_{(q_0,q_1)} J_d^{-1}(\mu)$. Let $\delta q_1 = \delta q_1' + \delta q_1''$. Thus $\delta q_1'' \in T_{q_1} Q$ is vertical, i.e., $T\pi_{Q,S} \cdot \delta q_1'' = 0$. Now,

$$(DL_d - \mathcal{A})(q_0, q_1) \cdot (\delta q_0, \delta q_1) = (DL_d - \mathcal{A})(q_0, q_1) \cdot (\delta q_0, \delta q_1') + (DL_d - \mathcal{A})(q_0, q_1) \cdot (0, \delta q_1'').$$

Using Equation 2.3.17, and the fact that $\mathcal{A}|J_d^{-1}(\mu)$ drops to a 1-form $\hat{\mathcal{A}}$ on $S \times S$, we get

$$(DL_d - \mathcal{A})(q_0, q_1) \cdot (\delta q_0, \delta q_1') = (D\hat{L}_d - \hat{\mathcal{A}})(x_0, x_1) \cdot (\delta x_0, \delta x_1).$$

Also, by a calculation similar to that used to derive Equation 2.3.19, we have that

$$(DL_d - \mathcal{A})(q_0, q_1) \cdot (0, \delta q_1'') = D_2 L_d(q_0, q_1) \cdot \delta q_1'' - \mathfrak{A}_\mu(q_1) \delta q_1'' = 0.$$

□

With this lemma, and Equation 2.3.26, we conclude that

$$\sum_{k=0}^{n-1}(D\hat{L}_d - \hat{\mathcal{A}})(x_k, x_{k+1}) \cdot (\delta x_k, \delta x_{k+1}) = D_1 L_d(q_0, q_1) \cdot \text{hor } \delta q_0 + D_2 L_d(q_{n-1}, q_n) \cdot \text{hor } \delta q_n. \tag{2.3.27}$$

If $\delta \mathbf{x}$ is a variation of $\mathbf{x}$ that vanishes at the endpoints, then hor $\delta q_0 = 0$, and hor $\delta q_1 = 0$. Therefore,

$$\sum_{k=0}^{n-1}(D\hat{L}_d - \hat{\mathcal{A}})(x_k, x_{k+1}) \cdot (\delta x_k, \delta x_{k+1}) = 0.$$

Equivalently,

$$\delta \sum_{k=0}^{n-1} \hat{L}_d(x_k, x_{k+1}) = \sum_{k=0}^{n-1} \hat{\mathcal{A}}(x_k, x_{k+1}) \cdot (\delta x_k, \delta x_{k+1}). \tag{2.3.28}$$

Equating terms involving δx_k on the left-hand side of Equation 2.3.28 to the corresponding terms on the right, we get the ***discrete Routh (DR) equations*** giving dynamics on $S \times S$:

$$D_2 \hat{L}_d(x_{k-1}, x_k) + D_1 \hat{L}_d(x_k, x_{k+1}) = \hat{\mathcal{A}}_2(x_{k-1}, x_k) + \hat{\mathcal{A}}_1(x_k, x_{k+1}). \tag{2.3.29}$$

Note that these equations depend on the value of momentum μ.

Thus, we have shown that if $\mathbf{q}$ is a discrete curve satisfying the discrete Euler–Lagrange equations, the curve $\mathbf{x}$, obtained by projecting $\mathbf{q}$ down to S, satisfies the DR equations (Equation 2.3.29).

Now we shall consider the converse, the discrete reduction procedure: Given a discrete curve $\mathbf{x}$ on S that satisfies the DR equations, is $\mathbf{x}$ the projection of a discrete curve $\mathbf{q}$ on Q that satisfies the DEL equations?

Let the pair (q_0, q_1) be a lift of (x_0, x_1) such that $J_d(q_0, q_1) = \mu$. Let $\mathbf{q} = \{q_0, \ldots, q_n\}$ be the solution of the DEL equations with initial condition (q_0, q_1). Note that $\mathbf{q}$ has momentum μ. Let $\mathbf{x}' = \{x'_0, \ldots, x'_n\}$ be the curve on S obtained by projecting $\mathbf{q}$. By our arguments above, $\mathbf{x}'$ solves the DR equations. However $\mathbf{x}'$ has the initial condition (x_0, x_1), which is the same as the initial condition of $\mathbf{x}$. Thus, by uniqueness of the solutions of the DR equations, $\mathbf{x}' = \mathbf{x}$. Thus $\mathbf{x}$ is the projection of a solution $\mathbf{q}$ of the DEL equations with momentum μ. Also, for a given initial condition q_0, there is a unique lift of $\mathbf{x}$ to a curve with momentum μ. Such a lift can be constructed using the method described in §2.3.2. Thus, lifting $\mathbf{x}$ to a curve with momentum μ yields a solution of the discrete Euler–Lagrange equations, which projects down to $\mathbf{x}$.

We summarize the results of this section in the following Theorem.

Theorem 2.3. *Let $\mathbf{x}$ is a discrete curve on S, and let $\mathbf{q}$ be a discrete curve on Q with momentum*

μ that is obtained by lifting $\mathbf{x}$. Then the following are equivalent.

1. $\mathbf{q}$ *solves the DEL equations.*

2. $\mathbf{q}$ *is a solution of the discrete Hamilton's variational principle,*

$$\delta \sum_{k=0}^{n-1} L_d(q_k, q_{k+1}) = 0,$$

for all variations $\delta\mathbf{q}$ of $\mathbf{q}$ that vanish at the endpoints.

3. $\mathbf{x}$ *solves the DR equations,*

$$D_2\hat{L}_d(x_{k-1}, x_k) + D_1\hat{L}_d(x_k, x_{k+1}) = \hat{\mathcal{A}}_2(x_{k-1}, x_k) + \hat{\mathcal{A}}_1(x_k, x_{k+1}).$$

4. $\mathbf{x}$ *is a solution of the reduced variational principle,*

$$\delta \sum_{k} \hat{L}_d(x_k, x_{k+1}) = \sum_{k=0}^{n-1} \hat{\mathcal{A}}(x_k, x_{k+1}) \cdot (\delta x_k, \delta x_{k+1}),$$

for all variations $\delta\mathbf{x}$ of $\mathbf{x}$ that vanish at the endpoints.

2.3.4 Preservation of the Reduced Discrete Symplectic Form

The DR equations define a discrete flow map, $\hat{F}_k : S \times S \to S \times S$. We already know that the flow of the DEL equations preserves the symplectic form Ω_{L_d} on $Q \times Q$. In this section we show that the reduced flow $\hat{F}_k$ preserves a *reduced* symplectic form $\Omega_{\mu,d}$ on $S \times S$, and that this reduced symplectic form is obtained by restricting Ω_{L_d} to $J_d^{-1}(\mu)$ and then dropping to $S \times S$. In other words,

$$\pi_{\mu,d}^* \Omega_{\mu,d} = i_{\mu,d}^* \Omega_{L_d}.$$

The continuous analogue of this equation is

$$\pi_\mu^* \Omega_\mu = i_\mu^* \Omega_Q.$$

Since the projections $\pi_{\mu,d}$ and π_μ involve a momentum shift, the reduced symplectic forms $\Omega_{\mu,d}$ and Ω_μ include magnetic terms.

Recall that $\hat{L}_d : S \times S \to \mathbb{R}$ is the reduced Lagrangian, and $D\hat{L}_d$ is a 1-form on $S \times S$. Define 1-forms $D\hat{L}_d^+$ and $D\hat{L}_d^-$ on $S \times S$ by

$$D\hat{L}_d^+(x_0, x_1) \cdot (\delta x_0, \delta x_1) = D\hat{L}_d(x_0, x_1) \cdot (0, \delta x_1) = D_2\hat{L}_d(x_0, x_1) \cdot \delta x_1,$$

$$D\hat{L}_d^-(x_0, x_1) \cdot (\delta x_0, \delta x_1) = D\hat{L}_d(x_0, x_1) \cdot (\delta x_0, 0) = D_1\hat{L}_d(x_0, x_1) \cdot \delta x_0.$$

Note that the partial derivatives $D_1\hat{L}_d$ and $D_2\hat{L}_d$ are both maps $S \times S \to T^*S$.

Define 2-forms $\mathcal{B}$ and $\hat{\mathcal{B}}$ on $Q \times Q$ and $S \times S$ as follows:

$$\mathcal{B} = \mathbf{d}\mathcal{A}, \quad \hat{\mathcal{B}} = \mathbf{d}\hat{\mathcal{A}}.$$

Since $\pi_{\mu,d}^*\hat{\mathcal{A}} = i_{\mu,d}^*\mathcal{A}$, we get $\pi_{\mu,d}^*\hat{\mathcal{B}} = i_{\mu,d}^*\mathcal{B}$. Thus $\hat{\mathcal{B}}$ can be obtained by restricting $\mathcal{B}$ to $J_d^{-1}(\mu)$ and then dropping to $J_d^{-1}(\mu)/G \approx S \times S$.

Since $\mathcal{A} = \pi_2^*\mathfrak{A}_\mu - \pi_1^*\mathfrak{A}_\mu$, it follows that $\mathcal{B} = \pi_2^*B_\mu - \pi_1^*B_\mu$, where $B_\mu = \mathbf{d}\mathfrak{A}_\mu$ is a 2-form on Q.

Now B_μ drops to a 2-form β_μ on S. Using this fact, we find that $\hat{\mathcal{B}} = \hat{\pi}_2^*\beta_\mu - \hat{\pi}_1^*\beta_\mu$. Here, $\hat{\pi}_1, \hat{\pi}_2 : S \times S \to S$ are projections onto the first and second components, respectively. If we define $\hat{\mathcal{B}}^+ := \hat{\pi}_2^*\beta_\mu$, and $\hat{\mathcal{B}}^- := -\hat{\pi}_1^*\beta_\mu$, then $\hat{\mathcal{B}} = \hat{\mathcal{B}}^- + \hat{\mathcal{B}}^+$.

We define a function $\mathcal{S} : S \times S \to \mathbb{R}$ by

$$\mathcal{S}(x_0, x_1) := \sum_{k=0}^{n-1} \hat{L}_d(x_k, x_{k+1}),$$

where $\mathbf{x} = \{x_0, \ldots, x_n\}$ is a solution of the DR equations with initial condition (x_0, x_1). Thus,

$$\mathcal{S}(x_0, x_1) = \sum_{k=0}^{n-1} \hat{L}_d(\hat{F}_k(x_0, x_1)).$$

Our goal in this section will be to show that symplecticity of the reduced flow follows from the fact that $\mathbf{d}^2\mathcal{S} = 0$.

Recall that if we lift $\mathbf{x}$ to a discrete curve $\mathbf{q}$ on Q with momentum μ, then $\mathbf{q}$ is a solution of the DEL equations. Let $(\delta x_0, \delta x_1) = \frac{d}{d\varepsilon}\Big|_{\varepsilon=0}(x_{0\varepsilon}, x_{1\varepsilon})$, and let $\mathbf{x}_\varepsilon = \{x_{0\varepsilon}, \ldots, x_{n\varepsilon}\}$ be a solution of the discrete Routh equations with initial condition $(x_{0\varepsilon}, x_{1\varepsilon})$. Let $\delta\mathbf{q}$ be any variation of $\mathbf{q}$ such that $T\pi_{Q,S} \cdot \delta q_i = \delta x_i$. Using Equation 2.3.27 in §2.3.3, we get

$$\begin{aligned}
\mathbf{d}\mathcal{S}(x_0, x_1)(\delta x_0, \delta x_1) &= \frac{d}{d\varepsilon}\Big|_{\varepsilon=0} \mathcal{S}(x_{0\varepsilon}, x_{1\varepsilon}) \\
&= \frac{d}{d\varepsilon}\Big|_{\varepsilon=0} \sum_{k=0}^{n-1} \hat{L}_d(x_{k\varepsilon}, x_{k+1\varepsilon}) \\
&= \sum_{k=0}^{n-1} D\hat{L}_d(x_k, x_{k+1}) \cdot (\delta x_k, \delta x_{k+1}) \\
&= D_1L_d(q_0, q_1) \cdot \operatorname{hor} \delta q_0 + D_2L_d(q_{n-1}, q_n) \cdot \operatorname{hor} \delta q_n
\end{aligned}$$

$$+\sum_{k=0}^{n-1}\hat{\mathcal{A}}(x_k,x_{k+1})\cdot(\delta x_k,\delta x_{k+1}).$$

Thus,

$$\begin{aligned}\mathbf{d}\mathcal{S}(x_0,x_1)(\delta x_0,\delta x_1)=&D_1L_d(q_0,q_1)\cdot\text{hor }\delta q_0+D_2L_d(q_{n-1},q_n)\cdot\text{hor }\delta q_n\\&+\sum_{k=0}^{n-1}(\hat{F}_k^*\hat{\mathcal{A}})(x_0,x_1)\cdot(\delta x_0,\delta x_1).\end{aligned}\tag{2.3.30}$$

We will eventually prove conservation of a reduced symplectic form by taking the exterior derivative of Equation 2.3.30. To do this, we need a number of preliminary calculations.

Lemma 2.4. $\mathbf{d}\left\{\sum_{k=0}^{n-1}(\hat{F}_k^*\hat{\mathcal{A}})\right\}=(\hat{F}_{n-1}^*\hat{\mathcal{B}}^+-\hat{\mathcal{B}}^+)-\hat{\mathcal{B}}$.

Proof. This is a straightforward verification using the facts that $\mathbf{d}\hat{\mathcal{A}}=\hat{\mathcal{B}}$, and that

$$\begin{aligned}(\hat{F}_k^*\hat{\mathcal{B}})(x_0,x_1)((\delta x_0,\delta x_1),(\delta x_0',\delta x_1'))&=\hat{\mathcal{B}}(x_k,x_{k+1})((\delta x_k,\delta x_{k+1}),(\delta x_k',\delta x_{k+1}'))\\&=\beta_\mu(x_{k+1})(\delta x_{k+1},\delta x_{k+1}')-\beta_\mu(x_k)(\delta x_k,\delta x_k').\end{aligned}$$

Here $\delta x_k,\delta x_k'$ are obtained by pushing forward $\delta x_0,\delta x_0'$, respectively, and $\delta x_{k+1},\delta x_{k+1}'$ are obtained by pushing forward $\delta x_1,\delta x_1'$, respectively. □

Lemma 2.5.

$$D_1L_d(q_0,q_1)\cdot\text{hor}\,\delta q_0=-D_2L_d(q_0,q_1)\cdot\text{hor}\,\delta q_1+(DL_d-\mathcal{A})(q_0,q_1)\cdot(\delta q_0,\delta q_1).$$

Proof.

$$\begin{aligned}D_1L_d(q_0,q_1)\cdot\text{hor }\delta q_0=&D_1L_d(q_0,q_1)\cdot\delta q_0-D_1L_d(q_0,q_1)\cdot\text{ver }\delta q_0\\=&DL_d(q_0,q_1)\cdot(\delta q_0,\delta q_1)-D_2L_d(q_0,q_1)\cdot\delta q_1-D_1L_d(q_0,q_1)\cdot\text{ver }\delta q_0\\=&DL_d(q_0,q_1)\cdot(\delta q_0,\delta q_1)-D_2L_d(q_0,q_1)\cdot\text{hor }\delta q_1\\&-D_2L_d(q_0,q_1)\cdot\text{ver }\delta q_1-D_1L_d(q_0,q_1)\cdot\text{ver }\delta q_0.\end{aligned}$$

As in Equation 2.3.19,

$$D_2L_d(q_0,q_1)\cdot\text{ver }\delta q_1=\mathfrak{A}_\mu(q_1)\cdot\delta q_1.$$

Similarly,

$$D_1 L_d(q_0, q_1) \cdot \text{ver } \delta q_0 = -\mathfrak{A}_\mu(q_0) \cdot \delta q_0.$$

Thus,

$$D_2 L_d(q_0, q_1) \cdot \text{ver } \delta q_1 + D_1 L_d(q_0, q_1) \cdot \text{ver } \delta q_0 = \mathcal{A}(q_0, q_1) \cdot (\delta q_0, \delta q_1).$$

The statement of the lemma now follows. □

Thus, Equation 2.3.30 can be rewritten as

$$\begin{aligned} \mathbf{d}\mathcal{S}(x_0, x_1)(\delta x_0, \delta x_1) =& (D_2 L_d(q_{n-1}, q_n) \cdot \text{hor } \delta q_n - D_2 L_d(q_0, q_1) \cdot \text{hor } \delta q_1) \\ &+ \sum_{k=0}^{n-1} (\hat{F}_k^* \hat{\mathcal{A}})(x_0, x_1) \cdot (\delta x_0, \delta x_1) + (DL_d - \mathcal{A})(q_0, q_1) \cdot (\delta q_0, \delta q_1) \\ =& (D_2 L_d(q_{n-1}, q_n) \cdot \text{hor } \delta q_n - D_2 L_d(q_0, q_1) \cdot \text{hor } \delta q_1) \\ &+ \sum_{k=0}^{n-1} (\hat{F}_k^* \hat{\mathcal{A}})(x_0, x_1) \cdot (\delta x_0, \delta x_1) + (D\hat{L}_d - \hat{\mathcal{A}})(x_0, x_1) \cdot (\delta x_0, \delta x_1). \end{aligned} \tag{2.3.31}$$

Lemma 2.6. $D_2 L_d(q_0, q_1) \cdot \text{hor}\, \delta q_1 = ((D\hat{L}_d)^+ - \hat{\mathcal{A}}^+)(x_0, x_1) \cdot (\delta x_0, \delta x_1)$.

Proof. Using Lemma 2.2, we get

$$\begin{aligned} D_2 L_d(q_0, q_1) \cdot \text{hor}\, \delta q_1 &= D_2 L_d(q_0, q_1) \cdot \delta q_1 - D_2 L_d(q_0, q_1) \cdot \text{ver}\, \delta q_1 \\ &= DL_d(q_0, q_1) \cdot (0, \delta q_1) - \mathfrak{A}_\mu(q_1) \cdot \delta q_1 \\ &= (DL_d - \mathcal{A})(q_0, q_1) \cdot (0, \delta q_1) \\ &= (D\hat{L}_d - \hat{\mathcal{A}})(x_0, x_1) \cdot (0, \delta x_1) \\ &= ((D\hat{L}_d)^+ - \hat{\mathcal{A}}^+)(x_0, x_1) \cdot (\delta x_0, \delta x_1). \end{aligned}$$

□

A consequence of this lemma is that

$$\begin{aligned} D_2 L_d(q_{n-1}, q_n) \cdot \text{hor } \delta q_n &= ((D\hat{L}_d)^+ - \hat{\mathcal{A}}^+)(x_{n-1}, x_n) \cdot (\delta x_{n-1}, \delta x_n) \\ &= (\hat{F}_{n-1}^*((D\hat{L}_d)^+ - \hat{\mathcal{A}}^+))(x_0, x_1) \cdot (\delta x_0, \delta x_1). \end{aligned}$$

Define the map $\hat{\mathbb{F}} : S \times S \to T^*S$ by

$$\hat{\mathbb{F}}(x_0, x_1) = D_2 \hat{L}_d(x_0, x_1) - \hat{\mathcal{A}}_2(x_0, x_1).$$

The map $\hat{\mathbb{F}}$ will play the role of a discrete Legendre transform. Let Θ_S be the canonical 1-form on T^*S.

Lemma 2.7. $(D\hat{L}_d)^+ - \hat{\mathcal{A}}^+ = \hat{\mathbb{F}}^*\Theta_S$.

Proof.

$$\begin{aligned}(\hat{\mathbb{F}}^*\Theta_S)(x_0,x_1)\cdot(\delta x_0,\delta x_1) &= \Theta_S(D_2\hat{L}_d(x_0,x_1) - \hat{\mathcal{A}}_2(x_0,x_1))\cdot T\hat{\mathbb{F}}\cdot(\delta x_0,\delta x_1)\\ &= (D_2\hat{L}_d(x_0,x_1) - \hat{\mathcal{A}}_2(x_0,x_1))\cdot T\pi_S\cdot T\hat{\mathbb{F}}\cdot(\delta x_0,\delta x_1),\end{aligned}$$

where $\pi_{T^*S,S} : T^*S \to S$ is the projection. Note that $\pi_{T^*S,S}\circ\hat{\mathbb{F}} = \hat{\pi}_2$, where $\hat{\pi}_2 : S\times S \to S$ is the projection onto the second component. Thus,

$$\begin{aligned}(\hat{\mathbb{F}}^*\Theta_S)(x_0,x_1)\cdot(\delta x_0,\delta x_1) &= (D_2\hat{L}_d(x_0,x_1) - \hat{\mathcal{A}}_2(x_0,x_1))\cdot T\hat{\pi}_2\cdot(\delta x_0,\delta x_1)\\ &= (D_2\hat{L}_d(x_0,x_1) - \hat{\mathcal{A}}_2(x_0,x_1))\cdot \delta x_1\\ &= ((D\hat{L}_d)^+ - \hat{\mathcal{A}}^+)(x_0,x_1)\cdot(\delta x_0,\delta x_1).\end{aligned}$$ □

Using Lemmas 2.6 and 2.7, Equation 2.3.31 can be rewritten as:

$$\mathbf{d}\mathcal{S} = (\hat{F}_{n-1}^*(\hat{\mathbb{F}}^*\Theta_S) - \hat{\mathbb{F}}^*\Theta_S) + \sum_{k=0}^{n-1}(\hat{F}_k^*\hat{\mathcal{A}}) + D\hat{L}_d - \hat{\mathcal{A}}.$$

Taking the exterior derivative on both sides of this equation and using Lemma 2.4 and the fact that $\mathbf{d}^2 = 0$ yields

$$0 = \hat{F}_{n-1}^*(\hat{\mathbb{F}}^*\Omega_S - \hat{\mathcal{B}}^+) - (\hat{\mathbb{F}}^*\Omega_S - \hat{\mathcal{B}}^+),$$

where $\Omega_S = -\mathbf{d}\Theta_S$ is the canonical 2-form on T^*S. Since $\pi_{T^*S,S}\circ\hat{\mathbb{F}} = \hat{\pi}_2$,

$$\hat{\mathcal{B}}^+ = \hat{\pi}_2^*\beta_\mu = \hat{\mathbb{F}}^*\pi_{T^*S,S}^*\beta_\mu.$$

Thus,

$$\hat{\mathbb{F}}^*\Omega_S - \hat{\mathcal{B}}^+ = \hat{\mathbb{F}}^*(\Omega_S - \pi_{T^*S,S}^*\beta_\mu).$$

We have thus proved the following Theorem.

Theorem 2.8. *The flow of the DR equations preserves the symplectic form*

$$\begin{aligned}\Omega_{\mu,d} &= \hat{\mathbb{F}}^*\Omega_S - \hat{\mathcal{B}}^+\\ &= (D_2\hat{L}_d - \hat{\mathcal{A}}_2)^*\Omega_S - \hat{\pi}_2^*\beta_\mu\end{aligned}$$

$$= \hat{\mathbb{F}}^*(\Omega_S - \pi^*_{T^*S,S}\beta_\mu).$$

We remark that the symplectic form $\Omega_{\mu,d}$ is just the pull-back by $\hat{\mathbb{F}}$ of the same symplectic form on T^*S that is obtained by the process of cotangent bundle reduction (see §2.2). The fact that $\Omega_{\mu,d}$ is closed follows from the closure of $(\Omega_S - \pi^*_{T^*S,S}\beta_\mu)$.

We will now complete our argument by showing that

$$\pi^*_{\mu,d}\Omega_{\mu,d} = i^*_{\mu,d}\Omega_{L_d}.$$

We showed in section §2.3.2 that the discrete Legendre transform $\mathbb{F}L_d : Q \times Q \to T^*Q$, $(q_0, q_1) \mapsto D_2L_d(q_0, q_1)$ maps $J_d^{-1}(\mu)$ to $J^{-1}(\mu)$, where J_d and J are the discrete and continuous momentum maps, respectively. For the rest of this section, let $\mathbb{F}' : J_d^{-1}(\mu) \to J^{-1}(\mu)$ be the restriction of $\mathbb{F}L_d$. Thus $\mathbb{F}' \circ i_\mu = i_{\mu,d} \circ \mathbb{F}L_d$, where $i_\mu : J^{-1}(\mu) \to T^*Q$ and $i_{\mu,d} : J_d^{-1}(\mu) \to Q \times Q$ are inclusions.

Recall that we had defined the map $\hat{\mathbb{F}} : S \times S \to T^*S$ as $D_2\hat{L}_d - \hat{\mathcal{A}}_2$.

Lemma 2.9. *The following diagram commutes.*

$$\begin{array}{ccc} J_d^{-1}(\mu) & \xrightarrow{\mathbb{F}'} & J^{-1}(\mu) \\ {\scriptstyle \pi_{\mu,d}}\downarrow & & \downarrow{\scriptstyle \pi_\mu} \\ S \times S & \xrightarrow{\hat{\mathbb{F}}} & T^*S \end{array}$$

Proof. Let $(q_0, q_1) \in J_d^{-1}(\mu)$. Thus $D_2L_d(q_0, q_1) \in J^{-1}(\mu)$, and

$$\pi_\mu(\mathbb{F}'(q_0, q_1)) = \pi_\mu(D_2L_d(q_0, q_1)).$$

Recall from §2.2 that $(D_2L_d(q_0, q_1) - \mathfrak{A}_\mu(q_1))$ annihilates all vertical tangent vectors and that $\pi_\mu(D_2L_d(q_0, q_1))$ is the element of $T^*_{x_1}S$ determined by $(D_2L_d(q_0, q_1) - \mathfrak{A}_\mu(q_1))$. For $\delta q_1 \in T_{q_1}Q$,

$$\langle D_2L_d(q_0, q_1) - \mathfrak{A}_\mu(q_1), \delta q_1\rangle = \langle D_2L_d(q_0, q_1) - \mathfrak{A}_\mu(q_1), \text{hor } \delta q_1\rangle.$$

Using the fact that $\mathfrak{A}_\mu(q_1)$ annihilates horizontal vectors, and Lemma 2.6, we obtain

$$\begin{aligned} \langle D_2L_d(q_0, q_1) - \mathfrak{A}_\mu(q_1), \delta q_1\rangle &= \langle D_2L_d(q_0, q_1), \text{hor } \delta q_1\rangle \\ &= D_2\hat{L}_d(x_0, x_1) \cdot \delta x_1 - \hat{\mathcal{A}}_2(x_0, x_1) \cdot \delta x_1\,. \end{aligned}$$

Thus,

$$\pi_\mu(D_2L_d(q_0, q_1)) = D_2\hat{L}_d(x_0, x_1) - \hat{\mathcal{A}}_2(x_0, x_1),$$

which means $\hat{\mathbb{F}} \circ \pi_{\mu,d} = \pi_\mu \circ \mathbb{F}'$. □

Using this lemma, we get

$$\begin{aligned} \pi_{\mu,d}^* \Omega_{\mu,d} &= \pi_{\mu,d}^* \hat{\mathbb{F}}^* (\Omega_S - \pi_{T^*S,S}^* \beta_\mu) \\ &= (\mathbb{F}')^* \pi_\mu^* (\Omega_S - \pi_{T^*S,S}^* \beta_\mu) \\ &= (\mathbb{F}')^* i_\mu^* \Omega_Q = i_{\mu,d}^* \mathbb{F} L_d^* \Omega_Q \\ &= i_{\mu,d}^* \Omega_{L_d}. \end{aligned}$$

Here, we have used the fact that $\pi_\mu^*(\Omega_S - \pi^* \beta_\mu) = i_\mu^* \Omega_Q$, which comes from the theory of cotangent bundle reduction. We have thus proved the following Theorem.

Theorem 2.10. *The flow of the DR equations preserves the symplectic form*

$$\Omega_{\mu,d} = \hat{\mathbb{F}}^* (\Omega_S - \pi_{T^*S,S}^* \beta_\mu).$$

$\Omega_{\mu,d}$ *can be obtained by dropping to* $S \times S$ *the restriction of* Ω_{L_d} *to* $J_d^{-1}(\mu)$*. In other words,*

$$\pi_{\mu,d}^* \Omega_{\mu,d} = i_{\mu,d}^* \Omega_{L_d}.$$

In proving Theorem 2.10, we started from the reduced variational equation (Equation 2.3.30). There is also an alternate route to proving symplecticity of the reduced flow which relies on the fact that discrete flow on $Q \times Q$ preserves the symplectic form Ω_{L_d}. We will give an outline of the steps involved, without giving all the details. The idea is to first show that the restriction to $J_d^{-1}(\mu)$ of the symplectic form Ω_{L_d} drops to a 2-form $\Omega_{\mu,d}$ on $S \times S$. The fact that the discrete flow on $Q \times Q$ preserves the symplectic form Ω_{L_d} is then used to show that the reduced flow preserves $\Omega_{\mu,d}$.

The outline of the steps involved is as follows.

1. Consider the 1-form Θ_{L_d} on $Q \times Q$ defined by $\Theta_{L_d}(q_0, q_1) \cdot (\delta q_0, \delta q_1) = D_2 L_d(q_0, q_1) \cdot \delta q_1$. Θ_{L_d} is G-invariant, and thus the Lie derivative $\mathcal{L}_{\xi_{Q \times Q}} \Theta_{L_d}$ is zero.

2. Since $\Omega_{L_d} = -\mathbf{d}\Theta_{L_d}$, Ω_{L_d} is G-invariant. If $i_{\mu,d} : J_d^{-1}(\mu) \to Q \times Q$ is the inclusion, $\Theta'_{L_d} = i_{\mu,d}^* \Theta_{L_d}$ and $\Omega'_{L_d} = i_{\mu,d}^* \Omega_{L_d}$ are the restrictions of Θ_{L_d} and Ω_{L_d}, respectively, to $J_d^{-1}(\mu)$. It is easy to check that Θ'_{L_d} and Ω'_{L_d} are invariant under the action of G on $J_d^{-1}(\mu)$.

3. If $\xi_{J_d^{-1}(\mu)}$ is an infinitesimal generator on $J_d^{-1}(\mu)$, then

$$\xi_{J_d^{-1}(\mu)} \lrcorner \, \Omega'_{L_d} = -\xi_{J_d^{-1}(\mu)} \lrcorner \, \mathbf{d}\Theta'_{L_d} = -\mathcal{L}_{\xi_{J_d^{-1}(\mu)}} \Theta'_{L_d} + \mathbf{d}\xi_{J_d^{-1}(\mu)} \lrcorner \, \Theta'_{L_d} = 0.$$

This follows from the G-invariance of Θ'_{L_d}, and the fact that $\Theta'_{L_d} \cdot \xi_{J_d^{-1}(\mu)} = \langle \mu, \xi \rangle$.

4. By steps 2 and 3, the form Ω'_{L_d} drops to a reduced form $\Omega_{\mu,d}$ on $J_d^{-1}(\mu)/G \approx S \times S$. Thus, if $\pi_{\mu,d} : J_d^{-1}(\mu) \to S \times S$ is the projection, then $\pi^*_{\mu,d}\Omega_{\mu,d} = \Omega'_{L_d}$. Note that the closure of $\Omega_{\mu,d}$ follows from the fact that Ω'_{L_d} is closed, which in turn follows from the closure of Ω_{L_d} and the relation $\Omega'_{L_d} = i^*_{\mu,d}\Omega_{L_d}$.

5. If $F_k : Q \times Q \to Q \times Q$ is the flow of the DEL equations, let F'_k be the restriction of this flow to $J_d^{-1}(\mu)$. We know that F'_k drops to the flow $\hat{F}_k$ of the DR equations on $S \times S$. Since F_k preserves Ω_{L_d}, F'_k preserves Ω'_{L_d}. Using this, it can be shown that $\hat{F}_k$ preserves $\Omega_{\mu,d}$. Note that it is sufficient to show that $\pi^*_{\mu,d}(\hat{F}^*_k\Omega_{\mu,d}) = \pi^*_{\mu,d}\Omega_{\mu,d}$.

6. It now remains to compute a formula for the reduced form $\Omega_{\mu,d}$. Using Lemma 2.9 (whose proof, in turn, relies on Lemma 2.6), it follows that

$$\begin{aligned}
\pi^*_{\mu,d}\Omega_{\mu,d} &= i^*_{\mu,d}\Omega_{L_d} = i^*_{\mu,d}\mathbb{F}L_d^*\Omega_Q = (\mathbb{F}')^* i^*_\mu \Omega_Q \\
&= (\mathbb{F}')^* \pi^*_\mu(\Omega_S - \pi^*_{T^*S,S}\beta_\mu) \\
&= \pi^*_{\mu,d}\hat{\mathbb{F}}^*(\Omega_S - \pi^*_{T^*S,S}\beta_\mu).
\end{aligned}$$

Thus $\pi^*_{\mu,d}\Omega_{\mu,d} = \pi^*_{\mu,d}\hat{\mathbb{F}}^*(\Omega_S - \pi^*_{T^*S,S}\beta_\mu)$, from which it follows that $\Omega_{\mu,d} = \hat{\mathbb{F}}^*(\Omega_S - \pi^*_{T^*S,S}\beta_\mu)$. Incidentally, this expression shows that $\Omega_{\mu,d}$ is nondegenerate provided the map $\hat{\mathbb{F}} = D_2\hat{L}_d - \hat{\mathcal{A}}_2$ is a local diffeomorphism.

2.3.5 Relating Discrete and Continuous Reduction

As we stated in §2.3.1, if the discrete Lagrangian L_d approximates the Jacobi solution of the Hamilton–Jacobi equation, then the DEL equations give us an integration scheme for the EL equations. In our commutative diagrams we will denote the relationship between the EL and DEL equations by a dashed arrow as follows:

$$(TQ, EL) \dashrightarrow (Q \times Q, DEL).$$

Thus, $\dashrightarrow$ can be read as "the corresponding discretization". By the continuous and discrete Noether theorems, we can restrict the flow of the EL and DEL equations to $J_L^{-1}(\mu)$ and $J_d^{-1}(\mu)$, respectively. We have seen that the flow on $J_L^{-1}(\mu)$ induces a reduced flow on $J_L^{-1}(\mu)/G \approx TS$, which is the flow of the Routh equations. Similarly, the discrete flow on $J_d^{-1}(\mu)$ induces a reduced discrete flow on $J_d^{-1}(\mu)/G \approx S \times S$, which is the flow of the discrete Routh equations. Since the DEL equations give us an integration algorithm for the EL equations, it follows that the DR equations give us an integration algorithm for the Routh equations.

Thus, to numerically integrate the Routh equations, we can follow either of the following approaches:

1. First solve the DEL equations to yield a discrete trajectory on Q, which can then be projected to a discrete trajectory on S.

2. Solve the DR equations to directly obtain a discrete trajectory on Q.

Either approach will yield the same result. We can express this situation by the following commutative diagram:

$$\begin{array}{ccc} (J_L^{-1}(\mu), EL) & \dashrightarrow & (J_d^{-1}(\mu), DEL) \\ {\scriptstyle \pi_{\mu,L}}\downarrow & & \downarrow{\scriptstyle \pi_{\mu,d}} \\ (TS, R) & \dashrightarrow & (S \times S, DR) \end{array} \tag{2.3.32}$$

The upper dashed arrow represents the fact that the DEL equations are an integration algorithm for the EL equations, and the lower dashed arrow represents the same relationship between the DR equations and the Routh equations. Note that for smooth group actions the order of accuracy will be equal for the reduced and unreduced algorithms. We will state this result precisely in the following corollary.

Corollary 2.11. *Given a discrete Lagrangian $L_d : Q \times Q \to \mathbb{R}$ of order r, and a smooth group action, the discrete Routh equations associated with the reduced discrete Lagrangian, $\hat{L}_d : S \times S \to \mathbb{R}$, obtained by dropping L_d to $S \times S$, is of order r as well.*

Proof. Recall that the order of the discrete Lagrangian is equal to the order of the push-forward discrete Lagrangian map, and as such, the discrete Euler–Lagrange equations yield a r-th order accurate approximation of the exact flow. When the group action is smooth, the projections $\pi_{\mu,L}$ and $\pi_{\mu,d}$ are smooth as well. Since the two projections agree when restricted to the position space, and the projections are smooth, the commutative diagram in Equation 2.3.32, together with the chain rule, implies that the discrete Routh equations yield a r-th order accurate approximation to the reduced flow. □

2.4 Relating the DEL Equations to Symplectic Runge–Kutta Algorithms

Symplectic Partitioned Runge–Kutta Methods. A well-studied class of numerical schemes for Hamiltonian and Lagrangian systems is the partitioned Runge–Kutta (PRK) algorithms (see

Hairer et al. [1993] and Hairer and Wanner [1996] for history and details). Stated for a regular Lagrangian system, a partitioned Runge–Kutta scheme is a map $F : T^*Q \to T^*Q$ defined by $F : (q_0, p_0) \mapsto (q_1, p_1)$, where

$$q_1 = q_0 + h \sum_{j=1}^{s} b_j \dot{Q}_j, \qquad p_1 = p_0 + h \sum_{j=1}^{s} \tilde{b}_j \dot{P}_j, \tag{2.4.1a}$$

$$Q_i = q_0 + h \sum_{j=1}^{s} a_{ij} \dot{Q}_j, \qquad P_i = p_0 + h \sum_{j=1}^{s} \tilde{a}_{ij} \dot{P}_j, \qquad i = 1, \dots, s, \tag{2.4.1b}$$

$$P_i = \frac{\partial L}{\partial \dot{q}}(Q_i, \dot{Q}_i), \qquad \dot{P}_i = \frac{\partial L}{\partial q}(Q_i, \dot{Q}_i), \qquad i = 1, \dots, s, \tag{2.4.1c}$$

where b_i, $\tilde{b}_i$, a_{ij} and $\tilde{a}_{ij}$ are real coefficients for $i, j = 1, \dots, s$ which define the method. Note that Equation 2.4.1c implicitly determined the Hamiltonian vector field $(\dot{Q}_i, \dot{P}_i)$ at the point $(Q_i, P_i) = \mathbb{F}L(Q_i, \dot{Q}_i)$.

The partitioned Runge–Kutta method, $F : T^*Q \to T^*Q$, approximates the flow map, $F_H^t : T^*Q \to T^*Q$, of the Hamiltonian system corresponding to the Lagrangian L, so that

$$F(q, p, h) = F_H^h(q, p) + \mathcal{O}(h^{r+1}),$$

where r, the order of the integration algorithm, is determined by the choice of the coefficients b_i, $\tilde{b}_i$, a_{ij} and $\tilde{a}_{ij}$.

As discussed in §2.2, the flow map F_H^t of the Hamiltonian system on T^*Q preserves the canonical symplectic form Ω on T^*Q. It can be shown that the partitioned Runge–Kutta method F preserves the canonical symplectic form if, and only if, the coefficients satisfy

$$b_i \tilde{a}_{ij} + \tilde{b}_j a_{ji} = b_i \tilde{b}_j, \qquad i, j = 1, \dots, s \tag{2.4.2a}$$

$$b_i = \tilde{b}_i, \qquad i = 1, \dots, s. \tag{2.4.2b}$$

Such schemes are known as symplectic partitioned Runge–Kutta (SPRK) methods.

Discrete Lagrangians for SPRK Methods. For any given time-step h, a symplectic partitioned Runge–Kutta method is a symplectic map $F : T^*Q \to T^*Q$. Therefore, as discussed in §2.3.1, there is a discrete Lagrangian L_d which generates it.

An explicit form for this discrete Lagrangian was found by Suris [1990], and is given by

$$L_d(q_0, q_1, h) = h \sum_{i=1}^{s} b_i L(Q_i, \dot{Q}_i),$$

where Q_i, $\dot{Q}_i$, P_i and $\dot{P}_i$ are such that Equations 2.4.1b and 2.4.1c are satisfied. It can then be shown, under assumptions (Equations 2.4.2a and 2.4.2b) on the coefficients, that the push-forward of the discrete Lagrangian map is exactly the symplectic partitioned Runge–Kutta method. The details of this calculation can be found in Suris [1990] or Marsden and West [2001].

For a partitioned Runge–Kutta method to be consistent, the coefficients must satisfy $\sum_{i=1}^{s} b_i = 1$. With this in mind, it can be readily seen that the L_d defined above is an approximation to the action over the interval $[0, h]$, as one would expect from §2.3.1.

Discrete Lagrangians from Polynomials and Quadrature. While the discrete Lagrangian given above generates any symplectic partitioned Runge–Kutta method, there is a subset of such methods for which the discrete Lagrangian has a particularly elegant form. These can be derived by approximating the action with polynomial trajectories and numerical quadrature.

As shown in §2.3.1, a discrete Lagrangian should be an approximation

$$L_d(q_0, q_1, h) \approx \operatorname*{ext}_{q \in \mathcal{C}(0,h)} S(q),$$

where $\mathcal{C}(0, h)$ is the space of trajectories $q : [0, h] \to Q$ with $q(0) = q_0$ and $q(h) = q_1$, and $S : \mathcal{C}(0, h) \to \mathbb{R}$ is the action $S(q) = \int_0^h L(q, \dot{q}) dt$.

To approximate this, we take a finite-dimensional approximation $\mathcal{C}_d(0, h) \subset \mathcal{C}(0, h)$ of the trajectory space,

$$\mathcal{C}_d(0, h) = \{q \in \mathcal{C}(0, h) \mid q \text{ is a polynomial of degree } s\},$$

and we approximate the action integral by numerical quadrature to give an approximate action $S_d : \mathcal{C}(0, h) \to \mathbb{R}$,

$$S_d(q) = h \sum_{i=1}^{s} b_i L(q(c_i h), \dot{q}(c_i h)),$$

where (b_i, c_i) is the maximal-order quadrature rule on the unit interval with quadrature points c_i. We now set the discrete Lagrangian to be

$$L_d(q_0, q_1, h) = \operatorname*{ext}_{q_d \in \mathcal{C}_d(0,h)} S_d(q_d),$$

which can be explicitly evaluated. This procedure corresponds to the Galerkin projection of the weak form of the ODE onto the space of piecewise polynomial trajectories, an interpretation which is further discussed in Marsden and West [2001].

Theorem 2.12. *Take a set of quadrature points c_i and let L_d be the corresponding discrete Lagrangian as described above. Then the integrator generated by this discrete Lagrangian is equivalent* *to the partitioned Runge–Kutta scheme defined by the coefficients*

$$\begin{aligned} b_i = \tilde{b}_i &= \int_0^1 l_{i,s}(\tau)\mathbf{d}\tau, \\ a_{ij} &= \int_0^{c_i} l_{j,s}(\tau)\mathbf{d}\tau, \\ \tilde{a}_{ij} &= \tilde{b}_j\left(1 - \frac{a_{ji}}{b_i}\right), \end{aligned} \tag{2.4.3}$$

where the $l_{i,s}(\tau)$ are the Lagrange polynomials associated with the c_i.

Proof. Evaluating the conditions which imply that q_d extremizes S_d and combining this with the definition of the push-forward of the discrete Euler–Lagrange equations give the desired result. See Marsden and West [2001] for details. □

2.5 Reduction of the Symplectic Runge–Kutta Algorithm

Consider the SPRK algorithm for mechanical systems described in §2.4. The equations defining this algorithm are

$$(q_1, p_1) = (q_0, p_0) + h\sum_j (b_j\dot{Q}_j, \tilde{b}_j\dot{P}_j), \tag{2.5.1a}$$

$$(Q_i, P_i) = (q_0, p_0) + h\sum_j (a_{ij}\dot{Q}_j, \tilde{a}_{ij}\dot{P}_j), \tag{2.5.1b}$$

$$(\dot{Q}_j, \dot{P}_j) = X_H(Q_j, P_j), \tag{2.5.1c}$$

for some coefficients $b_j, \tilde{b}_j, a_{ij}, \tilde{a}_{ij}$ satisfying Equation 2.4.2. These equations specify the push-forward discrete Lagrange map for some discrete Lagrangian, as discussed in §2.4. We will assume that there is an abelian group G that acts freely and properly on the configuration manifold Q, and that the Lagrangian and the Hamiltonian functions are invariant under the lifted actions of G on TQ and T^*Q, respectively. Locally, $Q \approx G \times S$, where $S = Q/G$ is the shape space. Let $\theta = (\theta^1, \dots, \theta^r)$ be local coordinates on G such that the group operation is addition, i.e., $\theta_1 \cdot \theta_2 = \theta_1 + \theta_2$. (Since the group is abelian, such coordinates can always be found.) Let $x = (x^1, \dots, x^s)$ be coordinates on S. In a local trivialization, (θ, x) are coordinates on Q. Let $(\theta, x, p_\theta, p_x)$ be canonical cotangent bundle coordinates on T^*Q, and $(\theta, x, \dot{\theta}, \dot{x})$ be canonical tangent bundle coordinates on TQ. It is easy to show that in these canonical coordinates on T^*Q, elements of the set $J^{-1}(\mu) \subset T^*Q$ are of the form (θ, x, μ, p_x). Also, since the Hamiltonian H on T^*Q is group invariant, $H(\theta, x, p_\theta, p_x)$ is independent of θ. Note that here we are implicitly assuming that the vector space structure used to define the SPRK method is that in which the group action is addition.

For the remainder of this section, we will adopt a local trivialization to express the SPRK method in which the group action is addition. Rewriting the symplectic partitioned Runge–Kutta algorithm in terms of this local trivialization gives

$$\theta_1 = \theta_0 + h\sum_j b_j \dot{\Theta}_j, \qquad (p_\theta)_1 = (p_\theta)_0 + h\sum_j \tilde{b}_j (\dot{P}_\theta)_j, \tag{2.5.2}$$

$$x_1 = x_0 + h\sum b_j \dot{X}_j, \qquad (p_x)_1 = (p_x)_0 + h\sum_j \tilde{b}_j (\dot{P}_x)_j, \tag{2.5.3}$$

$$\Theta_i = \theta_0 + h\sum_j a_{ij} \dot{\Theta}_j, \qquad (P_\theta)_i = (p_\theta)_0 + h\sum_j \tilde{a}_{ij} (\dot{P}_\theta)_j, \tag{2.5.4}$$

$$X_i = x_0 + h\sum a_{ij} \dot{X}_j, \qquad (P_x)_i = (p_x)_0 + h\sum_j \tilde{a}_{ij} (\dot{P}_x)_j, \tag{2.5.5}$$

and further,

$$\dot{\Theta}_j = \frac{\partial H}{\partial p_\theta}, \qquad (\dot{P}_\theta)_j = -\frac{\partial H}{\partial \theta}, \tag{2.5.6}$$

$$\dot{X}_j = \frac{\partial H}{\partial p_x}, \qquad (\dot{P}_x)_j = -\frac{\partial H}{\partial x}. \tag{2.5.7}$$

By group invariance, H does not depend on θ, and so $\partial H/\partial\theta = 0$. Thus $(\dot{P}_\theta)_j = 0$, and therefore, $(p_\theta)_1 = (P_\theta)_i = (p_\theta)_0$. Hence, if $(q_0, p_0) \in J^{-1}(\mu)$, then (q_1, p_1) and (Q_i, P_i) also lie on $J^{-1}(\mu)$. (We already know from the theory in the previous sections that the symplectic partitioned Runge–Kutta algorithm preserves momentum; what we have verified here is that the intermediate points (Q_i, P_i) do not move off the momentum surface.)

If $\mathfrak{A}$ is a connection on Q, it can be represented in local coordinates as

$$\mathfrak{A}(\theta, x)(\dot{\theta}, \dot{x}) = A(x)\dot{x} + \dot{\theta}.$$

Thus, the 1-form $\mathfrak{A}_\mu$ on Q is given by

$$\mathfrak{A}_\mu(\theta, x)(\dot{\theta}, \dot{x}) = \langle \mu, A(x)\dot{x} + \dot{\theta}\rangle = \begin{bmatrix} \mu & \mu A(x) \end{bmatrix} \begin{bmatrix} \dot{\theta} \\ \dot{x} \end{bmatrix}.$$

Thus, $\mathfrak{A}_\mu(\theta, x) = (\theta, x, \mu, \mu A(x))$.

As we have seen in §2.2, there is a projection $\pi_\mu : J^{-1}(\mu) \to T^*S$. If $\alpha_q \in J_q^{-1}(\mu)$, $(\alpha_q - \mathfrak{A}_\mu(q)) \in T_q^*Q$ annihilates all vertical tangent vectors at q, and $\pi_\mu(\alpha_q)$ is the element of T_x^*S determined by $(\alpha_q - \mathfrak{A}_\mu(q))$.

Suppose that in local coordinates, $\alpha_q = (\theta, x, \mu, p_x)$. Then, $(\alpha_q - \mathfrak{A}_\mu(q)) = (\theta, x, 0, p_x - \mu A(x))$.

Thus, $\pi_\mu(\theta, x, \mu, p_x) = (x, p_x - \mu A(x))$. Therefore, $T\pi_\mu : TJ^{-1}(\mu) \to T(T^*S)$ is given by

$$T\pi_\mu : (\dot{\theta}, \dot{x}, 0, \dot{p}_x) \mapsto (\dot{x}, \dot{p}_x - \mu \frac{\partial A}{\partial x}\dot{x}).$$

In components, $\mu A(x)$ can be represented as $\mu_a A_i^a(x)$ (sum over the repeated index a is implicit), and

$$\mu \frac{\partial A}{\partial x}\dot{x} = \mu_a \frac{\partial A_i^a}{\partial x^j}\dot{x}^j.$$

Let $(q, p) \in J^{-1}(\mu)$ and let $(\dot{q}, \dot{p}) = X_H(q, p)$. By Noether's theorem, we have that $(\dot{q}, \dot{p}) \in T_{(q,p)}(J^{-1}(\mu))$. In local coordinates,

$$(\dot{\theta}, \dot{x}, 0, \dot{p}_x) = X_H(\theta, x, \mu, p_x).$$

Now, by the theory of cotangent bundle reduction (see §2.2),

$$T\pi_\mu \cdot X_H(q, p) = X_{H_\mu}(\pi_\mu(q, p)),$$

i.e.,

$$(\dot{x}, \dot{p}_x - \mu \frac{\partial A}{\partial x}\dot{x}) = X_{H_\mu}(x, p_x - \mu A(x)).$$

If $(q_0, p_0) \in J^{-1}(\mu)$, we have seen how (Q_i, P_i) and (q_1, p_1) also lie in $J^{-1}(\mu)$. Let

$$\begin{aligned} \pi_\mu(q_0, p_0) &=: (x_0, s_0) = (x_0, (p_x)_0 - \mu A(x_0)), \\ \pi_\mu(Q_i, P_i) &=: (X_i, S_i) = (X_i, (P_x)_i - \mu A(X_i)), \\ \pi_\mu(q_1, p_1) &=: (x_1, s_1) = (x_1, (p_x)_1 - \mu A(x_1)). \end{aligned}$$

Then,

$$(\dot{X}_i, \dot{S}_i) := X_{H_\mu}(X_i, S_i) = (\dot{X}_i, (\dot{P}_x)_i - \mu \frac{\partial A}{\partial x}(X_i)\dot{X}_i). \tag{2.5.8}$$

Remark 2.1. *The Routh equations,*

$$\frac{\partial \hat{R}^\mu}{\partial x} - \frac{d}{dt}\frac{\partial \hat{R}^\mu}{\partial \dot{x}} = i_{\dot{x}}\beta_\mu(x),$$

define a vector field on TS which is related to the vector field X_{H_μ} by the reduced Legendre transform $\mathbb{F}\hat{R}^\mu$. The equations

$$s = \frac{\partial \hat{R}^\mu}{\partial \dot{x}}(x, \dot{x}), \tag{2.5.9}$$

and

$$\dot{s} = \frac{\partial \hat{R}^\mu}{\partial x}(x, \dot{x}) - i_{\dot{x}}\beta_\mu(x), \tag{2.5.10}$$

can be used to solve for $(\dot{x}, \dot{s})$ *in terms of* (x, s), *and thereby implicitly define the vector field* X_{H_μ}.

Recall that

$$(p_x)_1 = (p_x)_0 + h\sum_j \tilde{b}_j (\dot{P}_x)_j.$$

Adding and subtracting terms, this becomes

$$\begin{aligned}(p_x)_1 - \mu A(x_1) = (p_x)_0 - \mu A(x_0) + h\sum_j \tilde{b}_j\left[(\dot{P}_x)_j - \mu\frac{\partial A}{\partial x}(X_j)\dot{X}_j\right] \\ + \left[h\sum_j\left(\tilde{b}_j\mu\frac{\partial A}{\partial x}(X_j)\dot{X}_j\right) - (\mu A(x_1) - \mu A(x_0))\right].\end{aligned} \tag{2.5.11}$$

This can be rewritten as

$$s_1 = s_0 + h\sum_j \tilde{b}_j\dot{S}_j + \left[h\sum_j\left(\tilde{b}_j\mu\frac{\partial A}{\partial x}(X_j)\dot{X}_j\right) - (\mu A(x_1) - \mu A(x_0))\right]. \tag{2.5.12}$$

Similarly, it can be shown that

$$S_i = s_0 + h\sum_j \tilde{a}_{ij}\dot{S}_j + \left[h\sum_j\left(\tilde{a}_{ij}\mu\frac{\partial A}{\partial x}(X_j)\dot{X}_j\right) - (\mu A(X_i) - \mu A(x_0))\right]. \tag{2.5.13}$$

Putting the above equations together with the equations for x_1 and X_i, we get the following algorithm on T^*S:

$$x_1 = x_0 + h\sum b_j\dot{X}_j, \tag{2.5.14a}$$

$$s_1 = s_0 + h\sum_j \tilde{b}_j\dot{S}_j + \left[h\sum_j\left(\tilde{b}_j\mu\frac{\partial A}{\partial x}(X_j)\dot{X}_j\right) - (\mu A(x_1) - \mu A(x_0))\right], \tag{2.5.14b}$$

$$X_i = x_0 + h\sum a_{ij}\dot{X}_j, \tag{2.5.14c}$$

$$S_i = s_0 + h\sum_j \tilde{a}_{ij}\dot{S}_j + \left[h\sum_j\left(\tilde{a}_{ij}\mu\frac{\partial A}{\partial x}(X_j)\dot{X}_j\right) - (\mu A(X_i) - \mu A(x_0))\right], \tag{2.5.14d}$$

$$S_j = \frac{\partial \hat{R}^\mu}{\partial \dot{x}}(X_j, \dot{X}_j), \tag{2.5.14e}$$

$$\dot{S}_j = \frac{\partial \hat{R}^\mu}{\partial x}(X_j, \dot{X}_j) - i_{\dot{X}_j}\beta_\mu(X_j). \tag{2.5.14f}$$

We shall refer to this system of equations as the ***reduced symplectic partitioned Runge–Kutta (RSPRK)*** algorithm. Since we obtained this system by dropping the symplectic partitioned Runge–Kutta algorithm from $J^{-1}(\mu)$ to T^*S, it follows that this algorithm preserves the reduced symplectic form $\Omega_\mu = \Omega_S - \pi^*_{T^*S,S}\beta_\mu$ on T^*S.

Since the SPRK algorithm is an integration algorithm for the Hamiltonian vector field X_H on T^*Q, the RSPRK algorithm is an integration algorithm for the reduced Hamiltonian vector field X_{H_μ} on T^*S. The relationship between cotangent bundle reduction and the reduction of the SPRK algorithm can be represented by the following commutative diagram:

$$\begin{array}{ccc} (J^{-1}(\mu), X_H) & \dashrightarrow & (J^{-1}(\mu), SPRK) \\ \pi_\mu \big\downarrow & & \big\downarrow \pi_\mu \\ (T^*S, X_{H_\mu}) & \dashrightarrow & (T^*S, RSPRK) \end{array}$$

The dashed arrows here denote the corresponding discretization, as in Equation 2.3.32. We saw in §2.4 that the SPRK algorithm can be obtained by pushing forward the DEL equations by the discrete Legendre transform. By Lemma 2.9, this implies that the RSPRK algorithm can be obtained by pushing forward the DR equations by the reduced discrete Legendre transform $\hat{\mathbb{F}} = D_2\hat{L}_d - \hat{\mathcal{A}}_2$. These relationships are shown in the following commutative diagram:

$$\begin{array}{ccc} (J_d^{-1}(\mu), DEL) & \xrightarrow{\mathbb{F}L_d} & (J^{-1}(\mu), SPRK) \\ \pi_{\mu,d} \big\downarrow & & \big\downarrow \pi_\mu \\ (S \times S, DR) & \xrightarrow{\hat{\mathbb{F}}} & (T^*S, RSPRK) \end{array}$$

2.6 Putting Everything Together

Let us now recapitulate some of the main results of the previous sections.

We saw in §2.2 that the relationship between Routh reduction and cotangent bundle reduction can be represented by the following commutative diagram:

$$\begin{array}{ccc} (J_L^{-1}(\mu), EL) & \xrightarrow{\mathbb{F}L} & (J^{-1}(\mu), X_H) \\ \pi_{\mu,L} \big\downarrow & & \big\downarrow \pi_\mu \\ (TS, R) & \xrightarrow{\mathbb{F}\hat{R}^\mu} & (T^*S, X_{H_\mu}) \end{array}$$

We saw in §2.3.5 that if L_d approximates the Jacobi solution of the Hamilton–Jacobi equation, the relationship between discrete and continuous Routh reduction is described by the following diagram:

$$\begin{array}{ccc}
(J_L^{-1}(\mu), EL) & \dashrightarrow & (J_d^{-1}(\mu), DEL) \\
\downarrow{\scriptstyle \pi_{\mu,L}} & & \downarrow{\scriptstyle \pi_{\mu,d}} \\
(TS, R) & \dashrightarrow & (S \times S, DR)
\end{array}$$

The dashed arrows mean that the DEL equations are an integration algorithm for the EL equations, and that the DR equations are an integration algorithm for the Routh equations.

If L_d is defined as in §2.4, we saw that the algorithm on T^*Q obtained by pushing forward the DEL equation using the discrete Legendre transform $\mathbb{F}L_d$ is the symplectic partitioned Runge–Kutta algorithm (Equation 2.4.1), which is an integration algorithm for X_H. This is depicted as follows:

$$\begin{array}{ccc}
(J_L^{-1}(\mu), EL) & \dashrightarrow & (J_d^{-1}(\mu), DEL) \\
\downarrow{\scriptstyle \mathbb{F}L} & & \downarrow{\scriptstyle \mathbb{F}L_d} \\
(J^{-1}(\mu), X_H) & \dashrightarrow & (J^{-1}(\mu), SPRK)
\end{array}$$

The SPRK algorithm on $J^{-1}(\mu) \subset T^*Q$ induces the RSPRK algorithm on $J^{-1}(\mu)/G \approx T^*S$. As we saw in §2.5, this reduction process is related to cotangent bundle reduction and to discrete Routh reduction as shown in the following diagram:

$$\begin{array}{ccccc}
(J^{-1}(\mu), X_H) & \dashrightarrow & (J^{-1}(\mu), SPRK) & \xleftarrow{\mathbb{F}L_d} & (J_d^{-1}(\mu), DEL) \\
\downarrow{\scriptstyle \pi_{\mu}} & & \downarrow{\scriptstyle \pi_{\mu}} & & \downarrow{\scriptstyle \pi_{\mu,d}} \\
(T^*S, X_{H_\mu}) & \dashrightarrow & (T^*S, RSPRK) & \xleftarrow{\hat{\mathbb{F}}} & (S \times S, DR)
\end{array}$$

Putting all the above commutative diagrams together into one diagram, we obtain Figure 2.1.

2.7 Links with the Classical Routh Equations

The Routhian function $\hat{R}^\mu$ that we have been using is not the same as the classical Routhian defined by Routh [1877]. The classical Routhian, which we shall denote $\hat{R}_c^\mu$, is a function on TS that is related to our Routhian by the equation

$$\hat{R}_c^\mu(x, \dot{x}) = \hat{R}^\mu(x, \dot{x}) + \langle \mu, A(x)\dot{x} \rangle.$$

Recall from §2.2 that the map $A(x) : T_xS \to \mathfrak{g}$ is the restriction of the connection $\mathfrak{A}$ to T_xS. (T_xS is identified with the subspace $T_xS \times \{0\}$ of $T_gG \times T_xS$, which in turn is identified with T_qQ.) Note

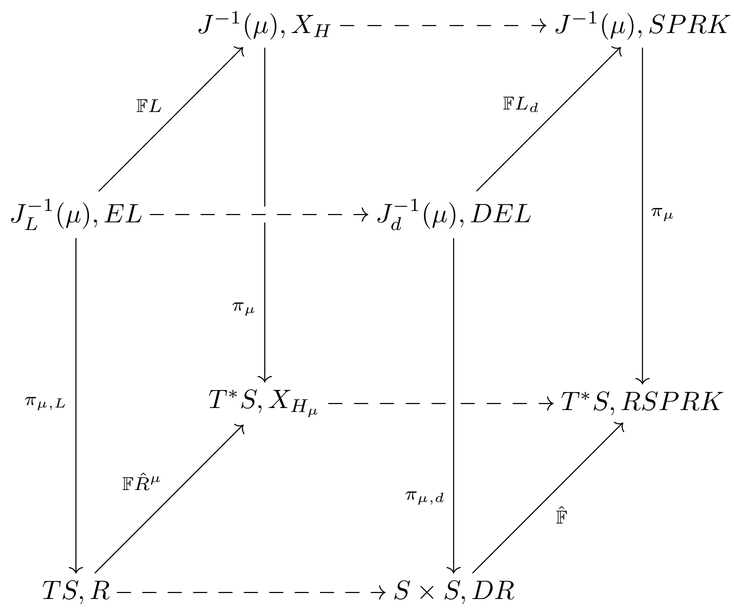


Figure 2.1: Complete commutative cube. Dashed arrows represent discretization from the continuous systems on the left face to the discrete systems on the right face. Vertical arrows represent reduction from the full systems on the top face to the reduced systems on the bottom face. Front and back faces represent Lagrangian and Hamiltonian viewpoints, respectively.

that the map $A(x)$ depends on our choice of local trivialization. Thus $\hat{R}^\mu_c$, too, depends on the trivialization.

The classical Routh equations are

$$\frac{\partial \hat{R}^\mu_c}{\partial x} - \frac{d}{dt}\frac{\partial \hat{R}^\mu_c}{\partial \dot{x}} = 0. \tag{2.7.1}$$

It can be verified (see, for example, Marsden and Ratiu [1999]) that these equations are equivalent to the modern Routh equations (Equation 2.2.3), which we restate here:

$$\frac{\partial \hat{R}^\mu}{\partial x} - \frac{d}{dt}\frac{\partial \hat{R}^\mu}{\partial \dot{x}} = i_{\dot{x}}\beta_\mu(x). \tag{2.7.2}$$

Thus the classical and the modern Routh equation define the same vector field X on TS.

To obtain dynamics on T^*S, we could use the fiber derivative of either the modern Routhian $\mathbb{F}\hat{R}^\mu$ or that of the classical Routhian $\mathbb{F}\hat{R}^\mu_c$. In coordinates on TS and T^*S, these fiber derivatives are

$$\mathbb{F}\hat{R}^\mu : (x, \dot{x}) \in TS \mapsto (x, \frac{\partial \hat{R}^\mu}{\partial \dot{x}}(x, \dot{x})) \in T^*S, \tag{2.7.3}$$

$$\mathbb{F}\hat{R}^{\mu}_{c} : (x, \dot{x}) \in TS \mapsto (x, \frac{\partial \hat{R}^{\mu}_{c}}{\partial \dot{x}}(x, \dot{x})) = (x, \frac{\partial \hat{R}^{\mu}}{\partial \dot{x}}(x, \dot{x}) + \mu A(x)) \in T^*S. \tag{2.7.4}$$

Note that the map $\mathbb{F}\hat{R}^{\mu}_{c}$ depends upon the trivialization.

We have seen in §2.2 that by pushing forward the dynamics on TS by $\mathbb{F}\hat{R}^{\mu}$, we obtain the vector field X_{H_μ} on T^*S. Recall that the restriction of the Hamiltonian vector field X_H to $J^{-1}(\mu)$ is π_μ-related to X_{H_μ}, where $\pi_\mu : J^{-1}(\mu) \to T^*S$ is the projection. Also recall that X_{H_μ} is Hamiltonian with respect to the non-canonical symplectic structure $\Omega_\mu = \Omega_S - \pi^*_{T^*S,S}\beta_\mu$ on T^*S.

If, on the other hand, we use $\mathbb{F}\hat{R}^{\mu}_{c}$ to push forward the dynamics from TS to T^*S, we obtain a vector field (which we shall call $X_{H'}$) that is Hamiltonian with respect to the *canonical* symplectic structure Ω_S on T^*S.

Consider the following symplectic partitioned Runge–Kutta scheme for integrating $X_{H'}$:

$$x_1 = x_0 + h\sum_{j=1}^{s} b_j \dot{X}_j, \qquad y_1 = y_0 + h\sum_{j=1}^{s} \tilde{b}_j \dot{Y}_j, \tag{2.7.5a}$$

$$X_i = x_0 + h\sum_{j=1}^{s} a_{ij} \dot{X}_j, \qquad Y_i = y_0 + h\sum_{j=1}^{s} \tilde{a}_{ij} \dot{Y}_j, \qquad i = 1, \ldots, s, \tag{2.7.5b}$$

$$Y_i = \frac{\partial \hat{R}^{\mu}_{c}}{\partial \dot{x}}(X_i, \dot{X}_i), \qquad \dot{Y}_i = \frac{\partial \hat{R}^{\mu}_{c}}{\partial x}(X_i, \dot{X}_i), \qquad i = 1, \ldots, s, \tag{2.7.5c}$$

for some coefficients $b_j, \tilde{b}_j, a_{ij}, \tilde{a}_{ij}$ satisfying Equation 2.4.2. It follows from that condition that this scheme preserves the canonical symplectic structure Ω_S. A particularly simple scheme of this form, that is second-order, was developed independently by Sanyal et al. [2003].

A natural question to ask at this point is how the above integration scheme for the reduced dynamics is related to the RSPRK scheme (Equation 2.5.14). To answer this question, consider the map $\sigma := \mathbb{F}\hat{R}^{\mu}_{c} \circ (\mathbb{F}\hat{R}^{\mu})^{-1} : T^*S \to T^*S$. In coordinates, $\sigma : (x, s) \mapsto (x, y) = (x, s + \mu A(x))$. Note that the σ transforms X_{H_μ} to $X_{H'}$, i.e., $X_{H'} = \sigma_* X_{H_\mu}$. It can be verified that this map σ also transforms the RSPRK scheme (Equation 2.5.14) to the above SPRK scheme for $X_{H'}$. Thus, these two schemes for integrating the reduced dynamics are equivalent, and are related to each other by a momentum shift.

Though the derivation for the SPRK scheme for $X_{H'}$ (Equation 2.7.5) is shorter than the reduction process through which we obtained the RSPRK scheme (Equation 2.5.14), there are several reasons to prefer the RSPRK scheme. Firstly, the classical Routhian $\hat{R}^{\mu}_{c}$ and therefore the fiber derivative $\mathbb{F}\hat{R}^{\mu}_{c}$ and the vector field $X_{H'}$ are dependent on the trivialization. Consequently, the SPRK scheme for $X_{H'}$ is non-intrinsic. On the other hand, as we saw in §2.5, the RSPRK scheme (Equation 2.5.14) is derived by dropping the SPRK scheme (Equation 2.5.1) for X_H onto the quotient $T^*S = J^{-1}(\mu)/G_\mu$ in a manner that is independent of the trivialization. (Though the equations defining the RSPRK scheme have terms involving the map $A(x)$, which is trivialization dependent, the trivialization dependence "cancels out", causing the overall scheme to be trivialization independent.)

Secondly, since the vector field $X_{H'}$ and the SPRK scheme (Equation 2.7.5) are not derived by a reduction process, it is not possible to fit them in a natural way into a commutative diagram like that depicted in Figure 2.1.

Furthermore, the classical theory of Routh reduction does not generalize to the case of non-abelian symmetry groups, whereas the intrinsic, modern version does (see, for example, Marsden and Scheurle [1993a,b], Jalnapurkar and Marsden [2000], and Marsden et al. [2000b]). Thus, to develop numerical algorithms for the reduced dynamics of systems with non-abelian symmetry, one would need to build on the intrinsic approach developed in this paper.

2.8 Forced and Constrained Systems

2.8.1 Constrained Coordinate Formalism

It is often desirable for computational reasons to realize the configuration space as a constraint manifold Q in a containing space V.

Assume that the constraint manifold Q can be expressed as the preimage of a regular value of a G-invariant constraint function, $g : V \to \mathbb{R}^m$. Then, $g^{-1}(0) = Q \subset V$ is a constraint manifold of codimension m.

On the constraint manifold Q, the discrete Hamilton's variational principle states that

$$\delta \sum_{k=0}^{n-1} L_d(q_k, q_{k+1}) = 0$$

for all variations $\delta \mathbf{q}$ of $\mathbf{q}$ that vanish at the endpoints. By the Lagrange multiplier theorem, in the containing space V, this is equivalent to the ***discrete Hamilton's variational principle with constraints***,

$$\delta \left[\sum_{k=0}^{n-1} L_d(v_k, v_{k+1}) + \sum_{k=0}^{n} \lambda_k^T g(v_k) \right] = 0,$$

for all variations $\delta \mathbf{v}$ of $\mathbf{v}$ that vanish at the endpoints.

As the variations are arbitrary and vanish at the endpoints, this is equivalent to the ***discrete Euler–Lagrange equations with constraints***,

$$\begin{aligned} D_2 L_d(v_{k-1}, v_k) + D_1 L_d(v_k, v_{k+1}) + \lambda_k^T Dg(v_k) &= 0, \\ g(v_k) &= 0. \end{aligned}$$

In the case of higher-order discrete Lagrangians, one must be careful about the choice constrained discrete Lagrangians. In particular, the internal sample points used in defining the constrained discrete Lagrangian must lie on the constraint manifold Q. In practice, this corresponds to the inclusion of Lagrange multiplier terms for each of the internal sample points in the variational definition of the higher-order constrained discrete Lagrangian.

Consider the preshape space, $U = V/G$. As the constraint function $g : V \to \mathbb{R}^m$ is G-invariant, this induces the function $\hat{g} : U \to \mathbb{R}^m$.

In addition, we have a G-invariant discrete Lagrangian, $L_d^V : V \times V \to \mathbb{R}$, and the discrete Lagrangian on $Q \times Q$ is simply the restriction, i.e., $L_d^Q = L_d^V\big|_{Q\times Q}$. The discrete momentum maps are related by the following lemma.

Lemma 2.13. *The discrete momentum map, $J_d^Q : Q \times Q \to \mathfrak{g}^*$, is obtained from $J_d^V : V \times V \to \mathfrak{g}^*$ by restriction, i.e., $J_d^Q = J_d^V\big|_{Q\times Q}$.*

Proof. Since $q_0 \in Q \subset V$, $\xi_Q(q_0) \in T_{q_0}Q \hookrightarrow T_{q_0}V$. Q is G-invariant, thus, the group orbits lie on Q, and in particular, $\xi_Q(q_0) = \xi_V(q_0)$. The result then follows from the calculation:

$$\begin{aligned} J_d^Q(q_0, q_1) \cdot \xi &= D_1 L_d^Q(q_0, q_1) \cdot \xi_Q(q_0) \\ &= D_1 L_d^Q(q_0, q_1) \cdot \xi_V(q_0) \\ &= D_1 L_d^V(q_0, q_1) \cdot \xi_V(q_0) \\ &= J_d^V(q_0, q_1) \cdot \xi. \end{aligned}$$ □

Since the discrete momentum map on the constraint manifold is obtained by restriction, and in our subsequent discussion, all the forms are evaluated on the constraint manifold, we shall abuse notation and omit the superscripts denoting the spaces. We are thereby able to formulate the main theorem of this section.

Theorem 2.14. *Let $\mathbf{x}$ be a discrete curve on S, and let $\mathbf{y}$ be a discrete curve on U. Then, the following are equivalent.*

1. $\mathbf{x}$ *solves the discrete Routh equations,*

$$D_2\hat{L}_d(x_{k-1}, x_k) + D_1\hat{L}_d(x_k, x_{k+1}) = \hat{\mathcal{A}}_2(x_{k-1}, x_k) + \hat{\mathcal{A}}_1(x_k, x_{k+1}).$$

2. $\mathbf{x}$ *is a solution of the reduced variational principle,*

$$\delta \sum_{k=0}^{n-1} \hat{L}_d(x_k, x_{k+1}) = \sum_{k=0}^{n-1} \hat{\mathcal{A}}(x_k, x_{k+1}) \cdot (\delta x_k, \delta x_{k+1}),$$

for all variations $\delta\mathbf{x}$ *of* $\mathbf{x}$ *that vanish at the endpoints.*

3. $\mathbf{y}$ *solves the discrete (reduced) Routh equations with constraints,*

$$\begin{aligned} D_2\hat{L}_d\left(y_{k-1},y_k\right)+D_1\hat{L}_d\left(y_k,y_{k+1}\right)+\lambda_k^T D\hat{g}\left(y_k\right)&=\hat{\mathcal{A}}_2\left(y_{k-1},y_k\right)+\hat{\mathcal{A}}_1\left(y_k,y_{k+1}\right),\\ \hat{g}\left(y_k\right)&=0.\end{aligned}$$

4. $\mathbf{y}$ *is a solution of the reduced discrete variational principle,*

$$\delta\left[\sum_{k=0}^{n-1}\hat{L}_d\left(y_k,y_{k+1}\right)+\sum_{k=0}^{n}\lambda_k^T\hat{g}\left(y_k\right)\right]=\sum_{k=0}^{n-1}\hat{\mathcal{A}}\left(y_k,y_{k+1}\right)\cdot\left(\delta y_k,\delta y_{k+1}\right),$$

for all variations $\delta\mathbf{y}$ *of* $\mathbf{y}$ *that vanish at the endpoints, and* $\hat{g}\left(y_k\right)=0$.

Proof. If $\mathbf{q}$ is a lift of $\mathbf{x}$ onto the μ-momentum surface, then the first two statements are equivalent to the discrete Hamilton's variational principle, which states that

$$\delta\sum_{k=0}^{n-1}L_d\left(q_k,q_{k+1}\right)=0,$$

for all variations $\delta\mathbf{q}$ of $\mathbf{q}$ that vanish at the endpoints. By the Lagrange multiplier theorem, this is equivalent to the discrete Hamilton's variational principle with constraints,

$$\delta\left[\sum_{k=0}^{n-1}L_d\left(v_k,v_{k+1}\right)+\sum_{k=0}^{n}\lambda_k^T g\left(v_k\right)\right]=0,$$

for all variations $\delta\mathbf{v}$ of $\mathbf{v}$ that vanish at the endpoints.

As the variations are arbitrary and vanish at the endpoints, this is equivalent to the discrete Euler–Lagrange equations with constraints,

$$\begin{aligned} D_2L_d\left(v_{k-1},v_k\right)+D_1L_d\left(v_k,v_{k+1}\right)+\lambda_k^T Dg\left(v_k\right)&=0,\\ g\left(v_k\right)&=0.\end{aligned}$$

Let $\mathbf{v}$ be a solution of the discrete Euler–Lagrange equations with constraints. Then,

$$\begin{aligned}&\delta\left[\sum_{k=0}^{n-1}L_d\left(v_k,v_{k+1}\right)+\sum_{k=0}^{n}\lambda_k^T g\left(v_k\right)\right]\\ &\quad=\left.\frac{d}{d\epsilon}\right|_{\epsilon=0}\left[\sum_{k=0}^{n-1}L_d\left(v_{k_\epsilon},v_{{k+1}_\epsilon}\right)+\sum_{k=0}^{n}\lambda_{k_\epsilon}^T g\left(v_{k_\epsilon}\right)\right]\end{aligned}$$

$$
\begin{aligned}
&= D_1 L_d\left(v_0, v_1\right) \cdot \delta v_0 + \sum_{k=1}^{n-1}\left(D_2 L_d\left(v_{k-1}, v_k\right) + D_1 L_d\left(v_k, v_{k+1}\right)\right) \cdot \delta v_k \\
&\quad + D_2 L_d\left(v_{n-1}, v_n\right) \cdot \delta v_n + \sum_{k=0}^{n} \underbrace{g\left(v_k\right)}_{0} \cdot \delta \lambda_k + \lambda_0^T D g\left(v_0\right) \cdot \delta v_0 \\
&\quad + \sum_{k=1}^{n-1}\left(\lambda_k^T D g\left(v_k\right)\right) \cdot \delta v_k + \lambda_n^T D g\left(v_n\right) \cdot \delta v_n \\
&= \left(D_1 L_d\left(v_0, v_1\right) + \lambda_0^T D g\left(v_0\right)\right) \cdot \delta v_0 + \left(D_2 L_d\left(v_{n-1}, v_n\right) + \lambda_n^T D g\left(v_n\right)\right) \cdot \delta v_n \\
&\quad + \sum_{k=1}^{n-1} \underbrace{\left[D_2 L_d\left(v_{k-1}, v_k\right) + D_1 L_d\left(v_k, v_{k+1}\right) + \lambda_k^T D g\left(v_k\right)\right]}_{0} \\
&= \left(D_1 L_d\left(v_0, v_1\right) + \lambda_0^T D g\left(v_0\right)\right) \cdot \delta v_0 + \left(D_2 L_d\left(v_{n-1}, v_n\right) + \lambda_n^T D g\left(v_n\right)\right) \cdot \delta v_n .
\end{aligned}
$$

Therefore, we have that $\mathbf{v}$ solves the discrete Euler–Lagrange equations with constraints if, and only if,

$$
\begin{aligned}
&\left.\frac{d}{d\epsilon}\right|_{\epsilon=0}\left[\sum_{k=0}^{n-1} L_d\left(v_{k_\epsilon}, v_{k+1_\epsilon}\right) + \sum_{k=0}^{n} \lambda_{k_\epsilon}^T g\left(v_{k_\epsilon}\right)\right] \\
&\quad = \left(D_1 L_d\left(v_0, v_1\right) + \lambda_0^T D g\left(v_0\right)\right) \cdot \delta v_0 + \left(D_2 L_d\left(v_{n-1}, v_n\right) + \lambda_n^T D g\left(v_n\right)\right) \cdot \delta v_n ,
\end{aligned}
$$

for all variations, including those that do not vanish at the endpoints.

Let $\mathbf{y}$ be the projection of $\mathbf{v}$, the solution of the DEL equations with constraints, onto the preshape space V/G, and $\delta \mathbf{y} = \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \mathbf{y}_\epsilon$ be a variation of $\mathbf{y}$. By construction,

$$
\hat{g}\left(y_{k_\epsilon}\right) = g\left(v_{k_\epsilon}\right).
$$

The terms $\lambda_0^T D g\left(v_0\right)$ and $\lambda_n^T D g\left(v_n\right)$ correspond to forces of constraint, and are therefore normal to the constraint manifold. Since the constraint manifold Q is G-invariant, the group orbits lie on the constraint manifold. As a consequence, the forces of constraint annihilate vertical variations, implying that

$$
\begin{aligned}
\lambda_0^T D g\left(v_0\right) \cdot \operatorname{ver} \delta v_0 &= 0, \\
\lambda_n^T D g\left(v_n\right) \cdot \operatorname{ver} \delta v_n &= 0.
\end{aligned}
$$

From which we conclude,

$$
\left.\frac{d}{d\epsilon}\right|_{\epsilon=0}\left[\sum_{k=0}^{n-1} L_d\left(v_{k_\epsilon}, v_{k+1_\epsilon}\right) + \sum_{k=0}^{n} \lambda_{k_\epsilon}^T g\left(v_{k_\epsilon}\right)\right]
$$

$$
\begin{aligned}
&= \left(D_1 L_d\left(v_0, v_1\right) + \lambda_0^T D g\left(v_0\right)\right) \cdot \delta v_0 + \left(D_2 L_d\left(v_{n-1}, v_n\right) + \lambda_n^T D g\left(v_n\right)\right) \cdot \delta v_n \\
&= \left(D_1 L_d\left(v_0, v_1\right) + \lambda_0^T D g\left(v_0\right)\right) \cdot \operatorname{hor} \delta v_0 + \left(D_2 L_d\left(v_{n-1}, v_n\right) + \lambda_n^T D g\left(v_n\right)\right) \cdot \operatorname{hor} \delta v_n \\
&\quad - \mathfrak{A}_\mu\left(v_0\right) \cdot \delta v_0 + \mathfrak{A}_\mu\left(v_n\right) \cdot \delta v_n \\
&= \left(D_1 L_d\left(v_0, v_1\right) + \lambda_0^T D g\left(v_0\right)\right) \cdot \operatorname{hor} \delta v_0 + \left(D_2 L_d\left(v_{n-1}, v_n\right) + \lambda_n^T D g\left(v_n\right)\right) \cdot \operatorname{hor} \delta v_n \\
&\quad + \sum_{k=0}^{n-1} \mathcal{A}\left(v_k, v_{k+1}\right) \cdot \left(\delta v_k, \delta v_{k+1}\right),
\end{aligned}
$$

where we used Equation 2.3.19 for the second to last equality. Then,

$$
\begin{aligned}
&\left(D_1 L_d\left(v_0, v_1\right) + \lambda_0^T D g\left(v_0\right)\right) \cdot \operatorname{hor} \delta v_0 + \left(D_2 L_d\left(v_{n-1}, v_n\right) + \lambda_n^T D g\left(v_n\right)\right) \cdot \operatorname{hor} \delta v_n \\
&\quad = \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \left[\sum_{k=0}^{n-1} L_d\left(v_{k_\epsilon}, v_{k+1_\epsilon}\right) + \sum_{k=0}^{n} \lambda_{k_\epsilon}^T g\left(v_{k_\epsilon}\right)\right] - \sum_{k=0}^{n-1} \mathcal{A}\left(v_k, v_{k+1}\right) \cdot \left(\delta v_k, \delta v_{k+1}\right).
\end{aligned}
$$

From Lemma 2.2, and the fact that $\hat{g}\left(y_{k_\epsilon}\right) = g\left(v_{k_\epsilon}\right)$, this can be rewritten in terms of the reduced quantities,

$$
\begin{aligned}
&\left(D_1 L_d\left(v_0, v_1\right) + \lambda_0^T D g\left(v_0\right)\right) \cdot \operatorname{hor} \delta v_0 + \left(D_2 L_d\left(v_{n-1}, v_n\right) + \lambda_n^T D g\left(v_n\right)\right) \cdot \operatorname{hor} \delta v_n \\
&\quad = \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \left[\sum_{k=0}^{n-1} \hat{L}_d\left(y_{k_\epsilon}, y_{k+1_\epsilon}\right) + \sum_{k=0}^{n} \lambda_{k_\epsilon}^T \hat{g}\left(y_{k_\epsilon}\right)\right] - \sum_{k=0}^{n-1} \hat{\mathcal{A}}\left(y_k, y_{k+1}\right) \cdot \left(\delta y_k, \delta y_{k+1}\right).
\end{aligned}
$$

If the variations $\delta \mathbf{y}$ vanishes at the endpoints, i.e., $\delta y_0 = \delta y_n = 0$, then hor $\delta v_0 =$ hor $\delta v_n = 0$, and therefore

$$
\delta \left[\sum_{k=0}^{n-1} \hat{L}_d\left(y_k, y_{k+1}\right) + \sum_{k=0}^{n} \lambda_k^T \hat{g}\left(y_k\right)\right] = \sum_{k=0}^{n-1} \hat{\mathcal{A}}\left(y_k, y_{k+1}\right) \cdot \left(\delta y_k, \delta y_{k+1}\right),
$$

for all variations $\delta \mathbf{y}$ of $\mathbf{y}$ that vanish at the endpoints, and $\hat{g}\left(y_k\right) = 0$.

Since the variations are arbitrary and vanish at the endpoints, this is equivalent to the ***Discrete Routh equations with constraints***,

$$
\begin{aligned}
D_2 \hat{L}_d\left(y_{k-1}, y_k\right) + D_1 \hat{L}_d\left(y_k, y_{k+1}\right) + \lambda_k^T D \hat{g}\left(y_k\right) &= \hat{\mathcal{A}}_2\left(y_{k-1}, y_k\right) + \hat{\mathcal{A}}_1\left(y_k, y_{k+1}\right), \\
\hat{g}\left(y_k\right) &= 0.
\end{aligned}
$$

Conversely, if $\mathbf{y}$ satisfies the reduced variational principle, and $\mathbf{v}$ is its lift onto the μ-momentum surface, then a construction analogous to the derivation of the discrete Routh equations shows that $\mathbf{v}$ satisfies the discrete Hamilton's variational principle with constraints. □

2.8.2 Routh Reduction with Forcing

Mechanical systems with external forcing are governed by the ***Lagrange–d'Alembert variational principle***,

$$\delta \int L\left(q\left(t\right),\dot{q}\left(t\right)\right) dt + \int F\left(q\left(t\right),\dot{q}\left(t\right)\right) \cdot \delta q dt = 0.$$

We define the ***discrete Lagrange–d'Alembert principle*** (Kane et al. [2000]) to be

$$\delta \sum_{k=0}^{n-1} L_d\left(q_k, q_{k+1}\right) + \sum_{k=0}^{n-1} F_d\left(q_k, q_{k+1}\right) \cdot \left(\delta q_k, \delta q_{k+1}\right) = 0,$$

for all variations $\delta \mathbf{q}$ of $\mathbf{q}$ that vanish at the endpoints. F_d is a 1-form on $Q \times Q$, and approximates the impulse integral between the points q_k and q_{k+1}, just as the discrete Lagrangian L_d approximates the action integral. We define the 1-forms F_d^+ and F_d^- on $Q \times Q$ and the maps $F_d^1, F_d^2 : Q \times Q \to T^*Q$ by the relations

$$\begin{aligned} F_d^+\left(q_0, q_1\right) \cdot \left(\delta q_0, \delta q_1\right) &= F_d^2\left(q_0, q_1\right) \cdot \delta q_1 = F_d\left(q_0, q_1\right) \cdot \left(0, \delta q_1\right), \\ F_d^-\left(q_0, q_1\right) \cdot \left(\delta q_0, \delta q_1\right) &= F_d^1\left(q_0, q_1\right) \cdot \delta q_0 = F_d\left(q_0, q_1\right) \cdot \left(\delta q_0, 0\right). \end{aligned}$$

The discrete Lagrange–d'Alembert principle may then be rewritten as

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

for all variations $\delta \mathbf{q}$ of $\mathbf{q}$ that vanish at the endpoints. This is equivalent to the ***forced discrete Euler–Lagrange equations***,

$$D_2 L_d\left(q_{k-1}, q_k\right) + D_1 L_d\left(q_k, q_{k+1}\right) + F_d^1\left(q_k, q_{k+1}\right) + F_d^2\left(q_{k-1}, q_k\right) = 0.$$

As we are concerned with mechanical systems with symmetry, we shall restrict our discussion to discrete forces that are invariant under the diagonal action of G on $Q \times Q$. In particular, for all $\xi \in \mathfrak{g}$, and all variations $\left(\delta q_0, \delta q_1\right)$ of $\left(q_0, q_1\right)$,

$$F_d\left(\exp\left(t\xi\right) q_0, \exp\left(t\xi\right) q_1\right) \cdot \left(\delta q_0, \delta q_1\right) = F_d\left(q_0, q_1\right) \cdot \left(\delta q_0, \delta q_1\right).$$

Since the Routh reduction technique requires that the momentum map be conserved, we shall further restrict our discussion to G-invariant forcing that satisfies the discrete Noether theorem. This constrains our choice of forcing, as the following lemma illustrates.

Lemma 2.15. *Let* $\mathbf{q}$ *be a discrete curve on* Q *that solves the forced discrete Euler–Lagrange equa-*

tions. Then, the discrete Noether theorem is satisfied if, and only if,

$$\left(F_d^2\left(q_{k-1}, q_k\right) + F_d^1\left(q_k, q_{k+1}\right)\right) \cdot \operatorname{ver} \delta q_k = 0.$$

Proof. Given $\xi \in \mathfrak{g}$, consider the ξ-component of J_d, given by

$$J_d^\xi\left(q_0, q_1\right) = \left\langle J_d\left(q_0, q_1\right), \xi\right\rangle.$$

We compute the evolution of J_d^ξ along the flow of the forced discrete Euler–Lagrange equations:

$$\begin{aligned} & J_d^\xi\left(q_1, q_2\right) - J_d^\xi\left(q_0, q_1\right) \\ & \quad = J_d\left(q_1, q_2\right) \cdot \xi - J_d\left(q_0, q_1\right) \cdot \xi \\ & \quad = -D_1 L_d\left(q_1, q_2\right) \cdot \xi_Q\left(q_1\right) - D_2 L_d\left(q_0, q_1\right) \cdot \xi_Q\left(q_1\right) \\ & \quad = -D_1 L_d\left(q_1, q_2\right) \cdot \xi_Q\left(q_1\right) - D_2 L_d\left(q_0, q_1\right) \cdot \xi_Q\left(q_1\right) \\ & \qquad + \underbrace{\left[D_2 L_d\left(q_0, q_1\right) + D_1 L_d\left(q_1, q_2\right) + F_d^2\left(q_0, q_1\right) + F_d^1\left(q_1, q_2\right)\right]}_{0} \cdot \xi_Q\left(q_1\right) \\ & \quad = \left[F_d^2\left(q_0, q_1\right) + F_d^1\left(q_1, q_2\right)\right] \cdot \xi_Q\left(q_1\right). \end{aligned}$$

Since $J_d : Q \times Q \rightarrow \mathfrak{g}^*$, the discrete Noether theorem is satisfied if, and only if, $J_d^\xi\left(q_1, q_2\right) - J_d^\xi\left(q_0, q_1\right) = 0$, for all $\xi \in \mathfrak{g}$. As the vertical space ver_{q_1} is given by

$$\operatorname{ver}_{q_1} = \left\{\xi_Q\left(q_1\right) \mid \xi \in \mathfrak{g}\right\},$$

this is equivalent to $F_d^2\left(q_0, q_1\right) + F_d^1\left(q_1, q_2\right)$ vanishing on all vertical vectors. □

For the rest of our discussion, we shall specialize to the case whereby $F_d^2\left(q_0, q_1\right)$ and $F_d^1\left(q_1, q_2\right)$ individually vanish on vertical vectors, which is a sufficient condition for momentum conservation.

The discrete forcing term F_d is an invariant 1-form under the diagonal action of G on $Q \times Q$, and vanishes on vertical vectors. By restricting F_d to $J_d^{-1}(\mu)$, it drops to $\hat{F}_d : S \times S \rightarrow T^*S \times T^*S$.

In this context, we may formulate a discrete Routh reduction theory for the discrete Lagrange–d'Alembert principle.

Theorem 2.16. *Let* $\mathbf{x}$ *be a discrete curve on* S*, and let* $\mathbf{q}$ *be a discrete curve on* Q *with momentum* μ *that is obtained by lifting* $\mathbf{x}$*. Then, the following are equivalent.*

1. $\mathbf{q}$ *solves the forced discrete Euler–Lagrange equations,*

$$D_2 L_d\left(q_{k-1}, q_k\right) + D_1 L_d\left(q_k, q_{k+1}\right) + F_d^2\left(q_{k-1}, q_k\right) + F_d^1\left(q_k, q_{k+1}\right) = 0.$$

2. $\mathbf{q}$ *is a solution of the discrete Lagrange–d'Alembert variational principle,*

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

for all variations $\delta\mathbf{q}$ *of* $\mathbf{q}$ *that vanish at the endpoints.*

3. $\mathbf{x}$ *solves the Discrete Routh equations with forcing,*

$$\begin{aligned} D_2\hat{L}_d\left(x_{k-1}, x_k\right) + D_1\hat{L}_d\left(x_k, x_{k+1}\right) + \hat{F}_d^2\left(x_{k-1}, x_k\right) + \hat{F}_d^1\left(x_k, x_{k+1}\right) \\ = \hat{\mathcal{A}}_2\left(x_{k-1}, x_k\right) + \hat{\mathcal{A}}_1\left(x_k, x_{k+1}\right). \end{aligned}$$

4. $\mathbf{x}$ *is a solution of the reduced variational principle,*

$$\begin{aligned} \delta \sum_{k=0}^{n-1} \hat{L}_d\left(x_k, x_{k+1}\right) + \sum_{k=0}^{n-1} \left[\hat{F}_d^1\left(x_k, x_{k+1}\right) \cdot \delta x_k + \hat{F}_d^2\left(x_k, x_{k+1}\right) \cdot \delta x_{k+1}\right] \\ = \sum_{k=0}^{n-1} \hat{\mathcal{A}}\left(x_k, x_{k+1}\right) \cdot \left(\delta x_k, \delta x_{k+1}\right), \end{aligned}$$

for all variations $\delta\mathbf{x}$ *of* $\mathbf{x}$ *that vanish at the endpoints.*

Proof. We begin with the discrete Lagrange–d'Alembert variational principle,

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

for all variations $\delta\mathbf{q}$ of $\mathbf{q}$ that vanish at the endpoints.

Since the variations are arbitrary and vanish at the endpoints, this is equivalent to the forced discrete Euler–Lagrange equations,

$$D_2L_d\left(q_{k-1}, q_k\right) + D_1L_d\left(q_k, q_{k+1}\right) + F_d^2\left(q_{k-1}, q_k\right) + F_d^1\left(q_k, q_{k+1}\right) = 0.$$

Let $\mathbf{q}$ be a solution of the forced discrete Euler–Lagrange equations, then,

$$\begin{aligned} &\delta \sum_{k=0}^{n-1} L_d\left(q_k, q_{k+1}\right) + \sum_{k=0}^{n-1} \left[F_d^1\left(q_k, q_{k+1}\right) \cdot \delta q_k + F_d^2\left(q_k, q_{k+1}\right) \cdot \delta q_{k+1}\right] \\ &\quad = \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \sum_{k=0}^{n-1} L_d\left(q_{k_\epsilon}, q_{k+1_\epsilon}\right) + \sum_{k=0}^{n-1} \left[F_d^1\left(q_k, q_{k+1}\right) \cdot \delta q_k + F_d^2\left(q_k, q_{k+1}\right) \cdot \delta q_{k+1}\right] \\ &\quad = D_1L_d\left(q_0, q_1\right) \cdot \delta q_0 + \sum_{k=1}^{n-1} \left(D_2L_d\left(q_{k-1}, q_k\right) + D_1L_d\left(q_k, q_{k+1}\right)\right) \cdot \delta q_k \end{aligned}$$

$$
\begin{aligned}
&+ D_2 L_d\left(q_{n-1}, q_n\right) \cdot \delta q_n + F_d^1\left(q_0, q_1\right) \cdot \delta q_0 \\
&+ \sum_{k=1}^{n-1} \big(F_d^1\left(q_k, q_{k+1}\right) + F_d^2\left(q_{k-1}, q_k\right)\big) \cdot \delta q_k + F_d^2\left(q_{n-1}, q_n\right) \cdot \delta q_n \\
= &\big(D_1 L_d\left(q_0, q_1\right) + F_d^1\left(q_0, q_1\right)\big) \cdot \delta q_0 + \big(D_2 L_d\left(q_{n-1}, q_n\right) + F_d^2\left(q_{n-1}, q_n\right)\big) \cdot \delta q_n \\
&+ \sum_{k=1}^{n-1} \underbrace{\left[D_2 L_d\left(q_{k-1}, q_k\right) + D_1 L_d\left(q_k, q_{k+1}\right) + F_d^2\left(q_{k-1}, q_k\right) + F_d^1\left(q_k, q_{k+1}\right)\right]}_{0} \cdot \delta q_k \\
= &\big(D_1 L_d\left(q_0, q_1\right) + F_d^1\left(q_0, q_1\right)\big) \cdot \delta q_0 + \big(D_2 L_d\left(q_{n-1}, q_n\right) + F_d^2\left(q_{n-1}, q_n\right)\big) \cdot \delta q_n .
\end{aligned}
$$

Conversely, for an arbitrary discrete curve $\mathbf{q}$ and an arbitrary variation $\delta\mathbf{q}$, the final equality only holds if $\mathbf{q}$ satisfies

$$
D_2 L_d\left(q_{k-1}, q_k\right) + D_1 L_d\left(q_k, q_{k+1}\right) + F_d^2\left(q_{k-1}, q_k\right) + F_d^1\left(q_k, q_{k+1}\right) = 0,
$$

which is the forced DEL equation.

Therefore, we have that $\mathbf{q}$ solves the forced discrete Euler–Lagrange equations if, and only if,

$$
\begin{aligned}
&\left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \sum_{k=0}^{n-1} L_d\left(q_{k_\epsilon}, q_{k+1_\epsilon}\right) + \sum_{k=0}^{n-1} \left[F_d^1\left(q_k, q_{k+1}\right) \cdot \delta q_k + F_d^2\left(q_k, q_{k+1}\right) \cdot \delta q_{k+1}\right] \\
&\quad = \big(D_1 L_d\left(q_0, q_1\right) + F_d^1\left(q_0, q_1\right)\big) \cdot \delta q_0 + \big(D_2 L_d\left(q_{n-1}, q_n\right) + F_d^2\left(q_{n-1}, q_n\right)\big) \cdot \delta q_n ,
\end{aligned}
$$

for all variations, including those that do not vanish at the endpoints.

Let $\mathbf{x}$ be the projection of $\mathbf{q}$, the solution of the forced DEL equations, onto the shape space S, and $\delta\mathbf{x} = \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \mathbf{x}_\epsilon$ be a variation of $\mathbf{x}$. Since (q_k, q_{k+1}) is on the μ-momentum surface, and $(\delta q_k, \delta q_{k+1})$ is tangent to the momentum surface, we have by the construction of $\hat{F}_d$ the following relations

$$
\begin{aligned}
&\hat{F}_d^1\left(x_k, x_{k+1}\right) \cdot \delta x_k + \hat{F}_d^2\left(x_k, x_{k+1}\right) \cdot \delta x_{k+1} \\
&\quad = \hat{F}_d\left(x_k, x_{k+1}\right) \cdot \left(\delta x_k, 0\right) + \hat{F}_d\left(x_k, x_{k+1}\right) \cdot \left(0, \delta x_{k+1}\right) \\
&\quad = \hat{F}_d\left(x_k, x_{k+1}\right) \cdot \left(\delta x_k, \delta x_{k+1}\right) \\
&\quad = F_d\left(q_k, q_{k+1}\right) \cdot \left(\delta q_k, \delta q_{k+1}\right) \\
&\quad = F_d\left(q_k, q_{k+1}\right) \cdot \left(\delta q_k, 0\right) + F_d\left(q_k, q_{k+1}\right) \cdot \left(0, \delta q_{k+1}\right) \\
&\quad = F_d^1\left(q_k, q_{k+1}\right) \cdot \delta q_k + F_d^2\left(q_k, q_{k+1}\right) \cdot \delta q_{k+1} .
\end{aligned}
$$

This allows us to rewrite the sum over discrete forces in the discrete Lagrange–d'Alembert principle in terms of a sum over the reduced discrete forces,

$$\frac{d}{d\epsilon}\bigg|_{\epsilon=0} \sum_{k=0}^{n-1} L_d\left(q_{k_\epsilon}, q_{k+1_\epsilon}\right) + \sum_{k=0}^{n-1}\left[\hat{F}_d^1\left(x_k, x_{k+1}\right)\cdot \delta x_k + \hat{F}_d^2\left(x_k, x_{k+1}\right)\cdot \delta x_{k+1}\right]$$
$$= \left(D_1 L_d\left(q_0, q_1\right) + F_d^1\left(q_0, q_1\right)\right)\cdot \delta q_0 + \left(D_2 L_d\left(q_{n-1}, q_n\right) + F_d^2\left(q_{n-1}, q_n\right)\right)\cdot \delta q_n.$$

Splitting the variations into horizontal and vertical components, and using the assumption that the discrete forces vanish on vertical vectors, we have

$$\begin{aligned}
&\left(D_1 L_d\left(q_0, q_1\right) + F_d^1\left(q_0, q_1\right)\right)\cdot \delta q_0 + \left(D_2 L_d\left(q_{n-1}, q_n\right) + F_d^2\left(q_{n-1}, q_n\right)\right)\cdot \delta q_n \\
&\quad = \left(D_1 L_d\left(q_0, q_1\right) + F_d^1\left(q_0, q_1\right)\right)\cdot \left(\text{ver }\delta q_0 + \text{hor }\delta q_0\right) \\
&\qquad + \left(D_2 L_d\left(q_{n-1}, q_n\right) + F_d^2\left(q_{n-1}, q_n\right)\right)\cdot \left(\text{ver }\delta q_n + \text{hor }\delta q_n\right) \\
&\quad = \left(D_1 L_d\left(q_0, q_1\right) + F_d^1\left(q_0, q_1\right)\right)\cdot \text{hor }\delta q_0 + \left(D_2 L_d\left(q_{n-1}, q_n\right) + F_d^2\left(q_{n-1}, q_n\right)\right)\cdot \text{hor }\delta q_n \\
&\qquad - \mathfrak{A}_\mu\left(q_0\right)\cdot \delta q_0 + \mathfrak{A}_\mu\left(q_n\right)\cdot \delta q_n \\
&\quad = \left(D_1 L_d\left(q_0, q_1\right) + F_d^1\left(q_0, q_1\right)\right)\cdot \text{hor }\delta q_0 + \left(D_2 L_d\left(q_{n-1}, q_n\right) + F_d^2\left(q_{n-1}, q_n\right)\right)\cdot \text{hor }\delta q_n \\
&\qquad + \sum_{k=0}^{n-1} \mathcal{A}\left(q_k, q_{k+1}\right)\cdot \left(\delta q_k, \delta q_{k+1}\right),
\end{aligned}$$

where, as before, we used Equation 2.3.19 for the second to last equality. Then,

$$\begin{aligned}
&\left(D_1 L_d\left(q_0, q_1\right) + F_d^1\left(q_0, q_1\right)\right)\cdot \text{hor }\delta q_0 + \left(D_2 L_d\left(q_{n-1}, q_n\right) + F_d^2\left(q_{n-1}, q_n\right)\right)\cdot \text{hor }\delta q_n \\
&\quad = \frac{d}{d\epsilon}\bigg|_{\epsilon=0} \sum_{k=0}^{n-1} L_d\left(q_{k_\epsilon}, q_{k+1_\epsilon}\right) + \sum_{k=0}^{n-1}\left[\hat{F}_d^1\left(x_k, x_{k+1}\right)\cdot \delta x_k + \hat{F}_d^2\left(x_k, x_{k+1}\right)\cdot \delta x_{k+1}\right] \\
&\qquad - \sum_{k=0}^{n-1} \mathcal{A}\left(q_k, q_{k+1}\right)\cdot \left(\delta q_k, \delta q_{k+1}\right).
\end{aligned}$$

If the variations $\delta\mathbf{x}$ vanishes at the endpoints, i.e., $\delta x_0 = \delta x_n = 0$, then hor $\delta q_0 =$ hor $\delta q_n = 0$, and therefore,

$$\delta \sum_{k=0}^{n-1} \hat{L}_d\left(x_{k_\epsilon}, x_{k+1_\epsilon}\right) + \sum_{k=0}^{n-1}\left[\hat{F}_d^1\left(x_k, x_{k+1}\right)\cdot \delta x_k + \hat{F}_d^2\left(x_k, x_{k+1}\right)\cdot \delta x_{k+1}\right]$$
$$= \sum_{k=0}^{n-1} \hat{\mathcal{A}}\left(x_k, x_{k+1}\right)\cdot \left(\delta x_k, \delta x_{k+1}\right),$$

for all variations $\delta\mathbf{x}$ of $\mathbf{x}$ that vanish at the endpoints.

Since the variations are arbitrary and vanish at the endpoints, this is equivalent to the ***Discrete***

Routh equations with forcing,

$$
\begin{aligned}
D_2\hat{L}_d\left(x_{k-1},x_k\right)+D_1\hat{L}_d\left(x_k,x_{k+1}\right)+\hat{F}_d^2\left(x_{k-1},x_k\right)+\hat{F}_d^1\left(x_k,x_{k+1}\right)\\
=\hat{\mathcal{A}}_2\left(x_{k-1},x_k\right)+\hat{\mathcal{A}}_1\left(x_k,x_{k+1}\right).
\end{aligned}
$$

Conversely, if $\mathbf{x}$ satisfies the reduced variational principle, and $\mathbf{q}$ is its lift onto the μ-momentum surface, then a construction analogous to the derivation of the discrete Routh equations show that $\mathbf{q}$ satisfies the discrete Lagrange–d'Alembert principle. □

2.8.3 Routh Reduction with Constraints and Forcing

By applying the techniques of the previous sections, we may synthesize the formalisms involving constraints and forcing. We shall state, without proof, the relevant equations in the following theorem.

Theorem 2.17. *Let* $\mathbf{x}$ *be a discrete curve on* S*, and let* $\mathbf{q}$ *be a discrete curve on* Q *with momentum* μ *that is obtained by lifting* $\mathbf{x}$*. Let* $\mathbf{y}$ *be a discrete curve on* U *obtained from* $\mathbf{x}$ *by the inclusion* $S=\hat{g}^{-1}(0)\hookrightarrow U$*, and let* $\mathbf{v}$ *be a discrete curve on* V *with momentum* μ *that is obtained by lifting* $\mathbf{y}$*. Then, the following are equivalent.*

1. $\mathbf{v}$ *solves the forced discrete Euler–Lagrange equations with constraints,*

$$
\begin{aligned}
D_2L_d\left(v_{k-1},v_k\right)+D_1L_d\left(v_k,v_{k+1}\right)+F_d^2\left(v_{k-1},v_k\right)+F_d^1\left(v_k,v_{k+1}\right)+\lambda_k^TDg\left(v_k\right)=0,\\
g\left(v_k\right)=0.
\end{aligned}
$$

2. $\mathbf{v}$ *is a solution of the discrete Lagrange–d'Alembert variational principle with constraints,*

$$
\begin{aligned}
\delta\left[\sum_{k=0}^{n-1}L_d\left(v_k,v_{k+1}\right)+\sum_{k=0}^{n}\lambda_k^Tg\left(v_k\right)\right]\\
+\sum_{k=0}^{n-1}\left[F_d^1\left(v_k,v_{k+1}\right)\cdot\delta v_k+F_d^2\left(v_k,v_{k+1}\right)\cdot\delta v_{k+1}\right]=0,
\end{aligned}
$$

for all variations $\delta\mathbf{v}$ *of* $\mathbf{v}$ *that vanish at the endpoints, and* $g\left(v_k\right)=0$.

3. $\mathbf{y}$ *solves the Discrete Routh equations with forcing and constraints,*

$$
\begin{aligned}
D_2\hat{L}_d\left(y_{k-1},y_k\right)+D_1\hat{L}_d\left(y_k,y_{k+1}\right)+\hat{F}_d^2\left(y_{k-1},y_k\right)+\hat{F}_d^1\left(y_k,y_{k+1}\right)+\lambda_k^TD\hat{g}\left(y_k\right)\\
=\hat{\mathcal{A}}_2\left(y_{k-1},y_k\right)+\hat{\mathcal{A}}_1\left(y_k,y_{k+1}\right),\\
\hat{g}\left(y_k\right)=0.
\end{aligned}
$$

4. $\mathbf{y}$ *is a solution of the reduced variational principle,*

$$\delta\left[\sum_{k=0}^{n-1}\hat{L}_d\left(y_k,y_{k+1}\right)+\sum_{k=0}^{n}\lambda_k^T\hat{g}\left(y_k\right)\right]$$
$$+\sum_{k=0}^{n-1}\left[\hat{F}_d^1\left(y_k,y_{k+1}\right)\cdot\delta y_k+\hat{F}_d^2\left(y_k,y_{k+1}\right)\cdot\delta y_{k+1}\right]=\sum_{k=0}^{n-1}\hat{\mathcal{A}}\left(y_k,y_{k+1}\right)\cdot\left(\delta y_k,\delta y_{k+1}\right),$$

for all variations $\delta\mathbf{y}$ *of* $\mathbf{y}$ *that vanish at the endpoints, and* $\hat{g}\left(y_k\right)=0$.

2.9 Example: J_2 Satellite Dynamics

2.9.1 Configuration Space and Lagrangian

An illustrative and important example of a system with an abelian symmetry group is that of a single satellite in orbit about an oblate Earth. The general aspects and background for this problem are discussed in Prussing and Conway [1993], and some interesting aspects of the geometry underlying it are discussed in Chang and Marsden [2003].

The configuration manifold Q is $\mathbb{R}^3$, and the Lagrangian for the system has the form, kinetic minus potential energy,

$$L(q,\dot{(q)})=\frac{1}{2}M_s\|\dot{q}\|^2-M_sV(q),$$

where M_s is the mass of the satellite and $V:\mathbb{R}^3\to\mathbb{R}$ is the gravitational potential due to the Earth, truncated at the first term in the expansion in the ellipticity,

$$V(q)=\frac{GM_e}{\|q\|}+\frac{GM_eR_e^2J_2}{\|q\|^3}\left(\frac{3}{2}\frac{(q^3)^2}{\|q\|^2}-\frac{1}{2}\right).$$

Here, G is the gravitational constant, M_e is the mass of the Earth, R_e is the radius of the Earth, J_2 is a small non-dimensional parameter describing the degree of ellipticity, and q^3 is the third component of q.

We will now assume that we are working in non-dimensional coordinates, so that

$$L(q,\dot{q})=\frac{1}{2}\|\dot{q}\|^2-\left[\frac{1}{\|q\|}+\frac{J_2}{\|q\|^3}\left(\frac{3}{2}\frac{(q^3)^2}{\|q\|^2}-\frac{1}{2}\right)\right]. \tag{2.9.1}$$

This corresponds to choosing space and time coordinates in which the radius of the Earth is 1 and the period of orbit at zero altitude is 2π when $J_2=0$ (spherical Earth).

2.9.2 Symmetry Action

The symmetry of interest to us is that of rotation about the vertical (q^3) axis, so the symmetry group is the unit circle S^1. Using cylindrical coordinates, $q = (r, \theta, z)$, for the configuration, the symmetry action is $\phi : (r, \theta, z) \mapsto (r, \theta + \phi, z)$. Since $\|q\|$, $\|\dot{q}\|$, and $q^3 = z$ are all invariant under this transformation, so too is the Lagrangian.

This action is clearly not free on all of $Q = \mathbb{R}^3$, as the z-axis is invariant for all group elements. This is not a serious obstacle, however, as the lifted action is free on $T(Q \setminus (0,0,0))$ and this is enough to permit the application of the intrinsic Routh reduction theory outlined in §2.2. Alternatively, one can simply take $Q = \mathbb{R}^3 \setminus \{(0,0,z) \mid z \in \mathbb{R}\}$ and then the theory literally applies.

The shape space, $S = Q/G$, is the half-plane $S = \mathbb{R}^+ \times \mathbb{R}$ and we will take coordinates (r, z) on S. In doing so, we are implicitly defining a global diffeomorphism $S \times G \to Q$ given by $((r, z), \theta) \mapsto (r, \theta, z)$.

The Lie algebra $\mathfrak{g}$ for $G = S^1$ is the real line $\mathfrak{g} = \mathbb{R}$, and we will identify the dual with the real line itself, $\mathfrak{g}^* \cong \mathbb{R}$. For a Lie algebra element $\xi \in \mathfrak{g}$, the corresponding infinitesimal generator is given by

$$\xi_Q : (r, \theta, z) \mapsto ((r, \theta, z), (0, \xi, 0)).$$

Recall that the Lagrange momentum map, $J_L : TQ \to \mathfrak{g}^*$, is defined by

$$J_L(v_q) \cdot \xi = \langle \mathbb{F}L(v_q), \xi_Q(q) \rangle,$$

so we have

$$J_L((r, \theta, z), (\dot{r}, \dot{\theta}, \dot{z})) \cdot \xi = \Big\langle (\dot{r}, r^2\dot{\theta}, \dot{z}), (0, \xi, 0) \Big\rangle = r^2\dot{\theta}\xi,$$

and

$$J_L((r, \theta, z), (\dot{r}, \dot{\theta}, \dot{z})) = r^2\dot{\theta}.$$

This momentum map is simply the vertical component of the standard angular momentum.

Consider the Euclidean metric on $\mathbb{R}^3$, which corresponds to the kinetic energy norm in the Lagrangian. From this metric we define the mechanical connection, $\mathfrak{A} : TQ \to \mathfrak{g}$, which is given by $\mathfrak{A}((r, \theta, z), (\dot{r}, \dot{\theta}, \dot{z})) = \dot{\theta}$. The 1-form $\mathfrak{A}_\mu$ on Q is thus given by $\mathfrak{A}_\mu = \mu \mathbf{d}\theta$. Taking the exterior derivative of this expression gives $\mathbf{d}\mathfrak{A}_\mu = \mu \mathbf{d}^2\theta = 0$, and so the reduced 2-form is $\beta_\mu = 0$.

2.9.3 Equations of Motion

Computing the Euler–Lagrange equations for the Lagrangian (Equation 2.9.1) gives the equations of motion,

$$\ddot{q} = -\nabla_q \left[\frac{1}{\|q\|} + \frac{J_2}{\|q\|^3} \left(\frac{3}{2} \frac{(q^3)^2}{\|q\|^2} - \frac{1}{2} \right) \right].$$

To calculate the reduced equations, we begin by calculating the Routhian,

$$\begin{aligned} R^\mu(r,\theta,z,\dot{r},\dot{\theta},\dot{z}) &= L(r,\theta,z,\dot{r},\dot{\theta},\dot{z}) - \mathfrak{A}_\mu(r,\theta,z) \cdot (\dot{r},\dot{\theta},\dot{z}) \\ &= \frac{1}{2}\|(\dot{r},\dot{\theta},\dot{z})\|^2 - \left[\frac{1}{r} + \frac{J_2}{r^3} \left(\frac{3}{2} \frac{z^2}{r^2} - \frac{1}{2} \right) \right] - \mu\dot{\theta}. \end{aligned}$$

We now choose a fixed value μ of the momentum and restrict ourselves to the space $J_L^{-1}(\mu)$, on which $\dot{\theta} = \mu$. The reduced Routhian, $\hat{R}^\mu : TS \to \mathbb{R}$, is the restricted Routhian dropped to the tangent bundle of the shape space. In coordinates, this is

$$\hat{R}^\mu(r,z,\dot{r},\dot{z}) = \frac{1}{2}\|(\dot{r},\dot{z})\|^2 - \left[\frac{1}{r} + \frac{J_2}{r^3} \left(\frac{3}{2} \frac{z^2}{r^2} - \frac{1}{2} \right) \right] - \frac{1}{2}\mu^2.$$

Recalling that $\beta_\mu = 0$, the Routh equations (Equation 2.2.3) can now be evaluated to give

$$(\ddot{r},\ddot{z}) = -\nabla_{(r,z)} \left[\frac{1}{r} + \frac{J_2}{r^3} \left(\frac{3}{2} \frac{z^2}{r^2} - \frac{1}{2} \right) \right],$$

which describes the motion on the shape space.

To recover the unreduced Euler–Lagrange equations from the Routh equations, one uses the procedure of reconstruction. This is covered in detail in Marsden et al. [1990], Marsden [1992] and Marsden et al. [2000b].

2.9.4 Discrete Lagrangian System

We now discretize this system with the discrete Lagrangian used in Theorem 2.12. Recall that the push-forward discrete Lagrange map associated with this discrete Lagrangian is a symplectic partitioned Runge–Kutta method with coefficients given by Equation 2.4.3.

Given a point $(q_0,q_1) \in Q \times Q$ we will take (q_0,p_0) and (q_1,p_1) to be the associated discrete Legendre transforms. As the discrete momentum map is the pull-back of the canonical momentum map, we have that

$$J_{L_d}(q_0,q_1) = (p_\theta)_0 = (p_\theta)_1.$$

Take a fixed momentum map value μ and restrict L_d to the set $J_{L_d}^{-1}(\mu)$. Dropping this to $S \times S$ now gives the reduced discrete Lagrangian, $\hat{L}_d : S \times S \to \mathbb{R}$.

As discussed in §2.5, the fact that we have taken coordinates in which the group action is addition in θ means that the push-forward discrete Lagrange map associated with the reduced discrete Lagrangian is the reduced method given by Equation 2.5.14. In fact, as the mechanical connection has $A(r, z) = 0$ and $\beta_\mu = 0$, the push-forward discrete Lagrange map is exactly a partitioned Runge–Kutta method with Hamiltonian equal to the reduced Routhian. As we saw in §2.7, these are generically related by a momentum shift, rather than being equal.

Given a trajectory of the reduced discrete system, we can reconstruct a trajectory of the unreduced discrete system by solving for the θ component of Equation 2.5.1. Correspondingly, a trajectory of the unreduced discrete system can be projected onto the shape space to give a trajectory of the reduced discrete system.

2.9.5 Example Trajectories

Solutions of the Spherical Earth System. Consider initially the system with $J_2 = 0$. This corresponds to the case of a spherical Earth, and so the equations reduce to the standard Kepler problem. As this is an integrable system, the trajectories consist of periodic orbits.

A slightly inclined circular trajectory is shown in Figure 2.2, in both the unreduced and reduced pictures. Note that the graph of the reduced trajectory is a quadratic, as $\|q\| = \sqrt{r^2 + z^2}$ is a constant.

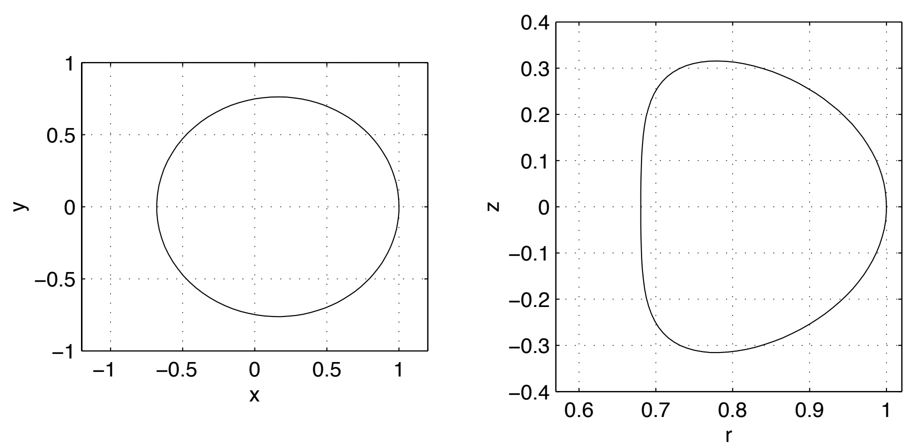


Figure 2.2: Unreduced (left) and reduced (right) views of an inclined elliptic trajectory for the continuous time system with $J_2 = 0$ (spherical Earth).

We will now investigate the effect of two different perturbations to the system, one due to taking non-zero J_2 and the other due to the numerical discretization.

The J_2 Effect. Taking $J_2 = 0.05$ (which is close the actual value for the Earth), the system becomes near-integrable and experiences breakup of the KAM tori. This can be seen in Figure 2.3, where the same initial condition is used as in Figure 2.2.

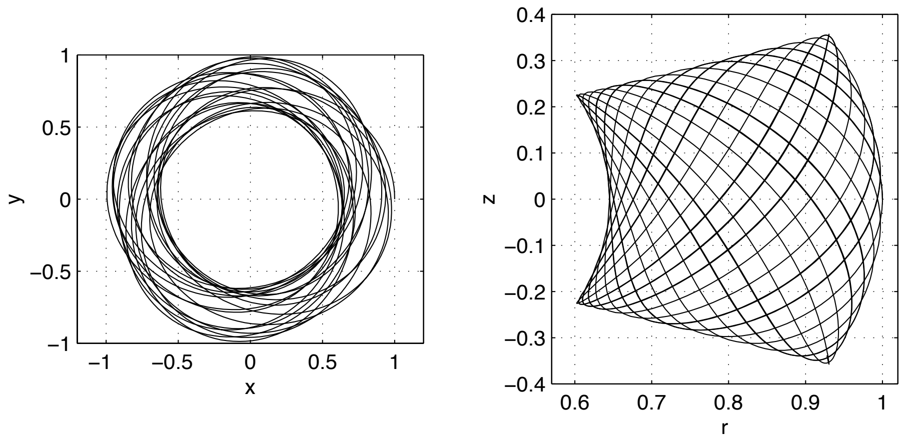


Figure 2.3: Unreduced (left) and reduced (right) views of an inclined elliptic trajectory for the continuous time system with $J_2 = 0.05$. Observe that the non-spherical terms introduce precession of the near-elliptic orbit in the symmetry direction.

Due to the fact that the reduced trajectory is no longer a simple curve, there is a geometric-phase-like effect which causes precession of the orbit. This precession can be seen in the thickening of the unreduced trajectory.

Solutions of the Discrete System for a Spherical Earth. We now consider the discrete system with $J_2 = 0$, for the second-order Gauss–Legendre discrete Lagrangian with timestep of $h = 0.3$. The trajectory with the same initial condition as above is given in Figure 2.4.

As can be seen from the reduced trajectory, the discretization has caused a similar breakup of the periodic orbit as was produced by the non-zero J_2. The effect of this is to, once again, induce precession of the orbit in the unreduced trajectory, in a way which is difficult to distinguish from the perturbation above due to non-zero J_2 when only the unreduced picture is considered. If the reduced pictures are consulted, however, then it is immediately clear that the system is much closer to the continuous time system with $J_2 = 0$ than to the system with non-zero J_2.

Solutions of the Discrete System with J_2 Effect. Finally, we consider the discrete system with non-zero $J_2 = 0.05$. The resulting trajectory is shown in Figure 2.5, and, clearly, it is not easy to determine from the unreduced picture whether the precession is due to the J_2 perturbation, the discretization, or some combination of the two.

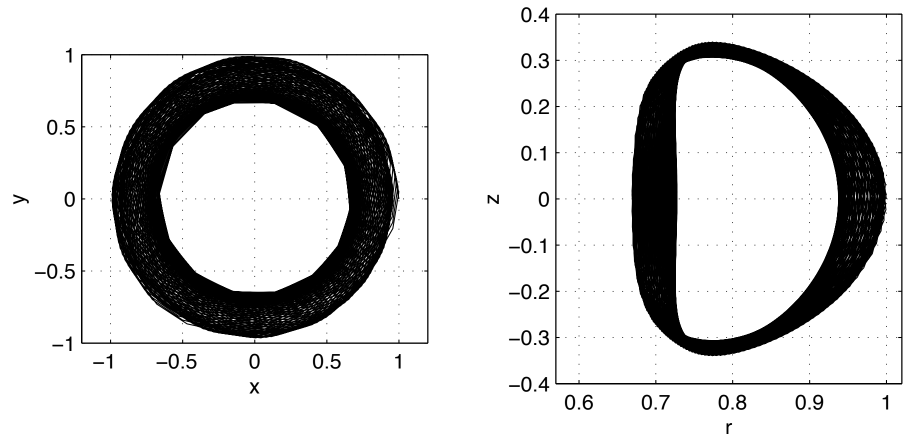


Figure 2.4: Unreduced (left) and reduced (right) views of an inclined trajectory of the discrete system with step-size $h = 0.3$ and $J_2 = 0$. The initial condition is the same as that used in Figure 2.2. The numerically introduced precession means that the unreduced picture looks similar to that of Figure 2.3 with non-zero J_2, whereas, by considering the reduced picture we can see the correct resemblance to the $J_2 = 0$ case of Figure 2.2.

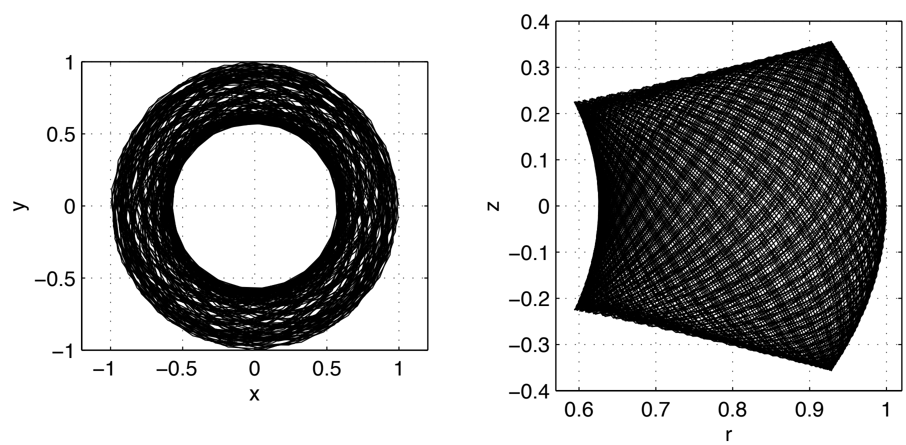


Figure 2.5: Unreduced (left) and reduced (right) views of an inclined trajectory of the discrete system with step-size $h = 0.3$ and $J_2 = 0.05$. The initial condition is the same as that used in Figure 2.3. The unreduced picture is similar to that of both Figures 2.3 and 2.4. By considering the reduced picture, we obtain the correct resemblance to Figure 2.3.

Taking the reduced trajectories, however, immediately shows that this discrete time system is structurally much closer to the non-zero J_2 system than to the original $J_2 = 0$ system. This confusion arises because both the J_2 term and the discretization introduce perturbations which act in the symmetry direction.

While this system is sufficiently simple that one can run simulations with such small timesteps that the discretization artifacts become negligible, this is not possible in general. This example demonstrates how knowledge of the geometry of the system can be important in understanding the discretization process, and how this can give insight into the behavior of numerical simulations. In particular, understanding how the discretization interacts with the symmetry action is extremely important.

2.9.6 Coordinate Systems

In this example, we have chosen cylindrical coordinates, thus making the group action addition in θ. One can always do this, as an abelian Lie group is isomorphic to a product of copies of $\mathbb{R}$ and S^1, but it may sometimes be preferable to work in coordinates in which the group action is not addition. For example, cartesian coordinates in the present example.

It may be easier, both in terms of computational expense, and in the simplicity of expressions, if we adopt a coordinate system in which the group action is not addition. We can still apply the Discrete Routh equations to obtain an integration scheme on $S \times S$. The push-forward of this under $\hat{\mathbb{F}}$ yields an integration scheme on T^*S. The trajectories on the shape space that we obtain in this manner could be different from those we would get with the RSPRK method. However, in both cases we would have conservation of symplectic structure, momentum, and the order of accuracy would be the same. One could choose whichever approach is cheaper and easier.

2.10 Example: Double Spherical Pendulum

2.10.1 Configuration Space and Lagrangian

We consider the example of the double spherical pendulum which has a non-trivial magnetic term and constraints. The configuration manifold Q is $S^2 \times S^2$, and the embedding linear space V is $\mathbb{R}^3 \times \mathbb{R}^3$.

The position vectors of each pendulum with respect to their pivot point are denoted by $\mathbf{q}_1$ and $\mathbf{q}_2$, as illustrated in Figure 2.6. These vectors are constrained to have lengths l_1 and l_2, respectively, and the pendula masses are denoted by m_1 and m_2.

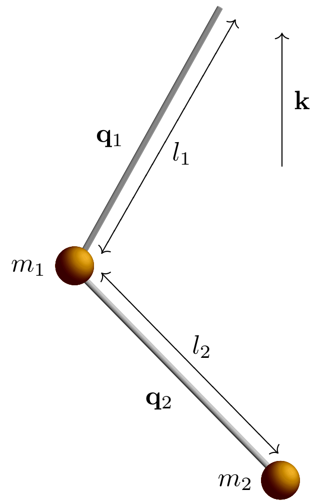


Figure 2.6: Double spherical pendulum.

The Lagrangian for the system has the form, kinetic minus potential energy,

$$L(\mathbf{q}_1, \mathbf{q}_2, \dot{\mathbf{q}}_1, \dot{\mathbf{q}}_2) = \frac{1}{2} m_1 \|\dot{\mathbf{q}}_1\|^2 + \frac{1}{2} m_2 \|\dot{\mathbf{q}}_1 + \dot{\mathbf{q}}_2\|^2 - m_1 g \mathbf{q}_1 \cdot \mathbf{k} - m_2 g (\mathbf{q}_1 + \mathbf{q}_2) \cdot \mathbf{k},$$

where g is the gravitational constant, and $\mathbf{k}$ is the unit vector in the z direction. The constraint function, $c : V \to \mathbb{R}^2$, is given by

$$c(\mathbf{q}_1, \mathbf{q}_2) = (\|\mathbf{q}_1\| - l_1, \|\mathbf{q}_2\| - l_2).$$

Using cylindrical coordinates, $\mathbf{q}_i = (r_i, \theta_i, z_i)$, for the configuration, we can express the Lagrangian as

$$\begin{aligned} L(q, \dot{q}) = & \frac{1}{2} m_1 \left(\dot{r}_1^2 + r_1^2 \dot{\theta}_1^2 + \dot{z}_1^2 \right) + \frac{1}{2} m_2 \Big\{ \dot{r}_1^2 + r_1^2 \dot{\theta}_1^2 + \dot{r}_2^2 + r_2^2 \dot{\theta}_2^2 \\ & + 2 \left(\dot{r}_1 \dot{r}_2 + r_1 r_2 \dot{\theta}_1 \dot{\theta}_2 \right) \cos\varphi + 2 \left(r_1 \dot{r}_2 \dot{\theta}_1 - r_2 \dot{r}_1 \dot{\theta}_2 \right) \sin\varphi + (\dot{z}_1 + \dot{z}_2)^2 \Big\} \\ & - m_1 g z_1 - m_2 g (z_1 + z_2), \end{aligned}$$

where $\varphi = \theta_2 - \theta_1$. Furthermore, we can automatically satisfy the constraints by performing the following substitutions,

$$z_i = \sqrt{l_i^2 - r_i^2}, \qquad \dot{z}_i = -\frac{r_i \dot{r}_i}{\sqrt{l_i^2 - r_i^2}}.$$

2.10.2 Symmetry Action

The symmetry of interest to us is the simultaneous rotation of the two pendula about vertical (z) axis, so the symmetry group is the unit circle S^1. Using cylindrical coordinates, $\mathbf{q}_i = (r_i, \theta_i, z_i)$, for the configuration, the symmetry action is $\phi : (r_i, \theta_i, z_i) \mapsto (r_i, \theta_i + \phi, z_i)$. Since $\|\mathbf{q}_i\|$, $\|\dot{\mathbf{q}}_i\|$, $\|\dot{\mathbf{q}}_1 + \dot{\mathbf{q}}_2\|$, and $\mathbf{q}_i \cdot \mathbf{k}$ are all invariant under this transformation, so too is the Lagrangian.

This action is clearly not free on all of $V = \mathbb{R}^3 \times \mathbb{R}^3$, as the z-axis is invariant for all group elements. However, this does not pose a problem computationally, as long as the trajectories do not pass through the downward hanging configuration, corresponding to $r_1 = r_2 = 0$. To treat the downward handing configuration properly, we would need to develop a discrete Lagrangian analogue of the continuous theory of singular reduction described in Ortega and Ratiu [2001].

The Lie algebra $\mathfrak{g}$ for $G = S^1$ is the real line $\mathfrak{g} = \mathbb{R}$, and we will identify the dual with the real line itself $\mathfrak{g}^* \cong \mathbb{R}$. For a Lie algebra element $\xi \in \mathfrak{g}$, the corresponding infinitesimal generator is given by

$$\xi_Q : (r_1, \theta_1, z_1, r_2, \theta_2, z_2) \mapsto ((r_1, \theta_1, z_1, r_2, \theta_2, z_2), (0, \xi, 0, 0, \xi, 0)).$$

Recall that the Lagrange momentum map $J_L : TQ \to \mathfrak{g}^*$ is defined by

$$J_L(v_q) \cdot \xi = \langle \mathbb{F}L(v_q), \xi_Q(q) \rangle,$$

so we have

$$\begin{aligned}
&J_L((r_1, \theta_1, z_1, r_2, \theta_2, z_2), (\dot{r}_1, \dot{\theta}_1, \dot{z}_1, \dot{r}_2, \dot{\theta}_2, \dot{z}_2)) \cdot \xi \\
&\quad = \Big\langle \Big(m_1 \dot{r}_1 + m_2 \left[\dot{r}_1 + \dot{r}_2 \cos\varphi - r_2 \dot{\theta}_2 \sin\varphi \right], \\
&\qquad m_1 r_1^2 \dot{\theta}_1 + m_2 \left[r_1^2 \dot{\theta}_1 + r_1 r_2 \dot{\theta}_2 \cos\varphi + r_1 \dot{r}_2 \sin\varphi \right], \\
&\qquad m_1 \dot{z}_1 + m_2 \left[\dot{z}_1 + \dot{z}_2 \right], m_2 \left[\dot{r}_2 + \dot{r}_1 \cos\varphi + r_1 \dot{\theta}_1 \sin\varphi \right], \\
&\qquad m_2 \left[r_2^2 \dot{\theta}_2 + r_1 r_2 \dot{\theta}_1 \cos\varphi - r_2 \dot{r}_1 \sin\varphi \right], m_2 \left[\dot{z}_1 + \dot{z}_2 \right] \Big), (0, \xi, 0, 0, \xi, 0) \Big\rangle \\
&\quad = \Big((m_1 + m_2) r_1^2 \dot{\theta}_1 + m_2 r_2^2 \dot{\theta}_2 + m_2 r_1 r_2 \left(\dot{\theta}_1 + \dot{\theta}_2 \right) \cos\varphi + (r_1 \dot{r}_2 - r_2 \dot{r}_1) \sin\varphi \Big) \xi,
\end{aligned}$$

and

$$\begin{aligned}
&J_L((r_1, \theta_1, z_1, r_2, \theta_2, z_2), (\dot{r}_1, \dot{\theta}_1, \dot{z}_1, \dot{r}_2, \dot{\theta}_2, \dot{z}_2)) \\
&\quad = (m_1 + m_2) r_1^2 \dot{\theta}_1 + m_2 r_2^2 \dot{\theta}_2 + m_2 r_1 r_2 \left(\dot{\theta}_1 + \dot{\theta}_2 \right) \cos\varphi + (r_1 \dot{r}_2 - r_2 \dot{r}_1) \sin\varphi.
\end{aligned}$$

This momentum map is simply the vertical component of the standard angular momentum.

The locked inertia tensor is given by Marsden [1992],

$$\begin{aligned}\mathbb{I}(\mathbf{q}_1\mathbf{q}_2) &= m_1\|\mathbf{q}_1^\perp\|^2 + m_2\|(\mathbf{q}_1+\mathbf{q}_2)^\perp\|^2\\ &= m_1r_1^2 + m_2(r_1^2+r_2^2+2r_1r_2\cos\varphi).\end{aligned}$$

Furthermore, the mechanical connection is given by

$$\begin{aligned}\alpha(\mathbf{q}_1,\mathbf{q}_2,\dot{\mathbf{q}}_1,\dot{\mathbf{q}}_2) &= \mathbb{I}(\mathbf{q}_1,\mathbf{q}_2)^{-1}J_L(\mathbf{q}_1,\mathbf{q}_2,\dot{\mathbf{q}}_1,\dot{\mathbf{q}}_2)\\ &= \frac{(m_1+m_2)\,r_1^2\dot\theta_1 + m_2r_2^2\dot\theta_2 + m_2r_1r_2\left(\dot\theta_1+\dot\theta_2\right)\cos\varphi + (r_1\dot r_2 - r_2\dot r_1)\sin\varphi}{m_1r_1^2 + m_2(r_1^2+r_2^2+2r_1r_2\cos\varphi)}.\end{aligned}$$

As a 1-form, it is given by

$$\begin{aligned}\alpha(\mathbf{q}_1,\mathbf{q}_2) = &\frac{1}{m_1r_1^2 + m_2(r_1^2+r_2^2+2r_1r_2\cos\varphi)}\\ &\times\left[(m_1+m_2)\,r_1^2\mathbf{d}\theta_1 + m_2r_2^2\mathbf{d}\theta_2 + m_2r_1r_2\left(\mathbf{d}\theta_1+\mathbf{d}\theta_2\right)\cos\varphi\right.\\ &\quad\left.+\,(r_1\mathbf{d}r_2 - r_2\mathbf{d}r_1)\sin\varphi\right].\end{aligned}$$

The μ-component of the mechanical connection is given by

$$\begin{aligned}\alpha_\mu(\mathbf{q}_1,\mathbf{q}_2) = &\frac{\mu}{m_1r_1^2 + m_2(r_1^2+r_2^2+2r_1r_2\cos\varphi)}\\ &\times\left\{\left[(m_1+m_2)\,r_1^2 + m_2r_1r_2\cos\varphi\right]\mathbf{d}\theta_1 + \left[m_2r_2^2 + m_2r_1r_2\cos\varphi\right]\mathbf{d}\theta_2\right\}.\end{aligned}$$

Taking the exterior derivative of this 1-form yields a non-trivial magnetic term on the reduced space,

$$\begin{aligned}\mathbf{d}\alpha_\mu = &\frac{\mu}{\left[m_1r_1^2 + m_2\left(r_1^2+r_2^2+2r_1r_2\cos\varphi\right)\right]^2}\\ &\times\{m_2r_2\left[2\left(m_1+m_2\right)r_1r_2 + \left(m_1r_1^2 + m_2(r_1^2+r_2^2)\right)\cos\varphi\right]\mathbf{d}r_1\wedge\mathbf{d}\theta_1\\ &\quad - m_2r_1\left[2\left(m_1+m_2\right)r_1r_2 + \left(m_1r_1^2 + m_2(r_1^2+r_2^2)\right)\cos\varphi\right]\mathbf{d}r_2\wedge\mathbf{d}\theta_1\\ &\quad + m_2r_1r_2\sin\varphi[m_1r_1^2 + m_2(r_1^2-r_2^2)]\mathbf{d}\theta_2\wedge\mathbf{d}\theta_1\\ &\quad - m_2r_2\left[2\left(m_1+m_2\right)r_1r_2 + \left(m_1r_1^2 + m_2(r_1^2+r_2^2)\right)\cos\varphi\right]\mathbf{d}r_1\wedge\mathbf{d}\theta_2\\ &\quad + m_2r_1\left[2\left(m_1+m_2\right)r_1r_2 + \left(m_1r_1^2 + m_2(r_1^2+r_2^2)\right)\cos\varphi\right]\mathbf{d}r_2\wedge\mathbf{d}\theta_2\\ &\quad + m_2r_1r_2\sin\varphi[m_1r_1^2 + m_2(r_1^2-r_2^2)]\mathbf{d}\theta_1\wedge\mathbf{d}\theta_2\}.\end{aligned}$$

This 2-form drops to the quotient space to yield

$$
\begin{aligned}
\beta_\mu = & \frac{\mu}{\left[m_1 r_1^2 + m_2\left(r_1^2 + r_2^2 + 2r_1 r_2 \cos\varphi\right)\right]^2} \\
& \times \left\{ m_2 r_2 \left[2\left(m_1+m_2\right) r_1 r_2 + \left(m_1 r_1^2 + m_2(r_1^2+r_2^2)\right)\cos\varphi\right] \mathbf{d}\varphi \wedge \mathbf{d}r_1 \right. \\
& \qquad \left. - m_2 r_1 \left[2\left(m_1+m_2\right) r_1 r_2 + \left(m_1 r_1^2 + m_2(r_1^2+r_2^2)\right)\cos\varphi\right] \mathbf{d}\varphi \wedge \mathbf{d}r_2 \right\} \\
= & \frac{\mu m_2 \left[2\left(m_1+m_2\right) r_1 r_2 + \left(m_1 r_1^2 + m_2(r_1^2+r_2^2)\right)\cos\varphi\right]}{\left[m_1 r_1^2 + m_2\left(r_1^2 + r_2^2 + 2r_1 r_2 \cos\varphi\right)\right]^2} \mathbf{d}\varphi \wedge (r_2 \mathbf{d}r_1 - r_1 \mathbf{d}r_2).
\end{aligned}
$$

The local representation of the connection can be computed from the expression

$$
\begin{aligned}
& \alpha(\theta_1, r_1, r_2, \varphi)(\dot\theta_1, \dot r_1, \dot r_2, \dot\varphi) \\
& = A(r_1, r_2, \varphi) \begin{bmatrix} \dot r_1 \\ \dot r_2 \\ \dot\varphi \end{bmatrix} + \dot\theta_1 \\
& = \frac{m_2}{m_1 r_1^2 + m_2(r_1^2 + r_2^2 + 2r_1 r_2 \cos\varphi)} \begin{bmatrix} -r_2 \sin\varphi & r_1 \sin\varphi & r_2^2 + r_1 r_2 \cos\varphi \end{bmatrix} \begin{bmatrix} \dot r_1 \\ \dot r_2 \\ \dot\varphi \end{bmatrix} + \dot\theta_1.
\end{aligned}
$$

From this, we observe that

$$
A(r_1, r_2, \varphi) = \frac{m_2}{m_1 r_1^2 + m_2(r_1^2 + r_2^2 + 2r_1 r_2 \cos\varphi)} \begin{bmatrix} -r_2 \sin\varphi & r_1 \sin\varphi & r_2^2 + r_1 r_2 \cos\varphi \end{bmatrix}.
$$

The amended potential V_μ is given by

$$
\begin{aligned}
V_\mu(q) &= V(q) + \frac{1}{2}\langle \mu, \mathbb{I}(q)^{-1}\mu \rangle \\
&= \left[m_1 g \mathbf{q}_1 + m_2 g(\mathbf{q}_1 + \mathbf{q}_2)\right] \cdot \mathbf{k} + \frac{1}{2} \cdot \frac{\mu^2}{m_1 \|\mathbf{q}_1^\perp\|^2 + m_2 \|(\mathbf{q}_1 + \mathbf{q}_2)^\perp\|^2} \\
&= -m_1 g \sqrt{l_1^2 - r_1^2} - m_2 g \left(\sqrt{l_1^2 - r_1^2} + \sqrt{l_2^2 - r_2^2}\right) + \frac{1}{2} \cdot \frac{\mu^2}{m_1 r_1^2 + m_2(r_1^2 + r_2^2 + 2r_1 r_2 \cos\varphi)}.
\end{aligned}
$$

The Routhian has the following expression on the momentum level set,

$$
R^\mu = \frac{1}{2}\|\operatorname{hor}(q, v)\|^2 - V_\mu.
$$

Recall that $\operatorname{hor}(v_q) = v_q - \xi_Q(v_q)$, where $\xi = \alpha(v_q)$, and $\xi_Q(v_q) = (0, \xi, 0, 0, \xi, 0)$. Then, we obtain

$$
\operatorname{hor}(v_q) = v_q - (0, \alpha(v_q), 0, 0, \alpha(v_q), 0)
$$

$$= (\dot{r}_1, \dot{\theta}_1 - \alpha(v_q), \dot{z}_1, \dot{r}_2, \dot{\theta}_2 - \alpha(v_q), \dot{z}_2).$$

From this, we conclude that

$$\begin{aligned}
&\frac{1}{2}\|\operatorname{hor}(q,v)\|^2 \\
&= \frac{1}{2}\begin{bmatrix} \dot{r}_1 \\ \dot{\theta}_1 - \alpha \\ \dot{z}_1 \\ \dot{r}_2 \\ \dot{\theta}_2 - \alpha \\ \dot{z}_2 \end{bmatrix}^T \begin{bmatrix} m_1 + m_2 & 0 & 0 & m_2\cos\varphi & -m_2 r_2 \sin\varphi & 0 \\ 0 & (m_1+m_2) r_1^2 & 0 & m_2 r_1 \sin\varphi & m_2 r_1 r_2 \cos\varphi & 0 \\ 0 & 0 & m_1 + m_2 & 0 & 0 & 0 \\ m_2 \cos\varphi & m_2 r_1 \sin\varphi & 0 & m_2 & 0 & 0 \\ -m_2 r_2 \sin\varphi & m_2 r_1 r_2 \cos\varphi & 0 & 0 & m_2 r_2^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & m_2 \end{bmatrix} \begin{bmatrix} \dot{r}_1 \\ \dot{\theta}_1 - \alpha \\ \dot{z}_1 \\ \dot{r}_2 \\ \dot{\theta}_2 - \alpha \\ \dot{z}_2 \end{bmatrix} \\
&= \frac{1}{2}\left\{(m_1+m_2) r_1^2 + 2 m_2 r_1 r_2 \cos\varphi + m_2 r_2^2\right\}\alpha^2 \\
&\quad - \left\{ m_1 r_1^2 \dot{\theta}_1 + m_2 \left[r_1 r_2 (\dot{\theta}_1 + \dot{\theta}_2)\cos\varphi + (r_1 \dot{r}_2 - r_2 \dot{r}_1)\sin\varphi + (r_1^2 \dot{\theta}_1 + r_2^2 \dot{\theta}_2)\right]\right\}\alpha \\
&\quad + \frac{1}{2} m_1 (\dot{r}_1^2 + r_1^2 \dot{\theta}_1^2 + \dot{z}_1^2) \\
&\quad + \frac{1}{2} m_2 \Big\{ \dot{r}_1^2 + r_1^2 \dot{\theta}_1^2 + \dot{r}_2^2 + r_2^2 \dot{\theta}_2^2 + 2(\dot{r}_1 \dot{r}_2 + r_1 r_2 \dot{\theta}_1 \dot{\theta}_2)\cos\varphi \\
&\qquad\qquad + 2(r_1 \dot{r}_2 \dot{\theta}_1 - r_2 \dot{r}_1 \dot{\theta}_2)\sin\varphi + (\dot{z}_1 + \dot{z}_2)^2 \Big\},
\end{aligned}$$

where $\alpha = \frac{\mu}{\mathbb{I}}$.

These combine to yield an expression for the Routhian R^μ, which drops to TS to give $\hat{R}^\mu$, and allow us to apply the Reduced Symplectic Partitioned Runge–Kutta algorithm.

2.10.3 Example Trajectories

We have computed the reduced trajectory of the double spherical pendulum using the fourth-order RSPRK algorithm on the Routh equations, and the fourth-order SPRK algorithm on the classical Routh equations.

As discussed in §2.7, these two methods should yield equivalent reduced dynamics, related to each other by a momentum shift, and in particular, their trajectories in position space should agree. We first consider the evolution of r_1, r_2, and φ, using the RSPRK algorithm on the Routh equations, as well as the projection of the relative position of m_2 with respect to m_1 onto the xy plane as seen in Figure 2.7.

Figure 2.8 illustrates that the energy behavior of the trajectory is very good, as is typical of variational integrators, and does not exhibit a spurious drift. In comparison, when a non-symplectic fourth-order Runge–Kutta is applied to the unreduced dynamics, with time-steps that were a quarter

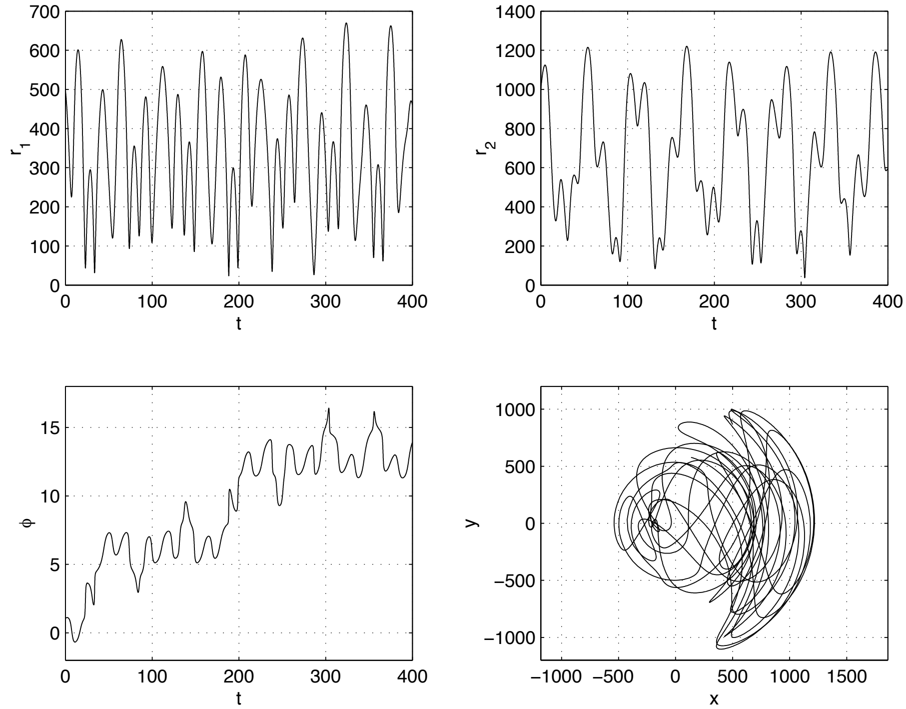


Figure 2.7: Time evolution of r_1, r_2, φ, and the trajectory of m_2, relative to m_1, using RSPRK.

of that used in the symplectic method, and we notice a systematic drift in the energy behavior.

Finally, we consider the relative error between the position trajectories and energy obtained from the RSPRK algorithm applied to the Routh equations as compared to the trajectories from the SPRK algorithm applied to the classical Routh equations. As Figure 2.9 clearly illustrates, these agree very well, as expected theoretically.

2.10.4 Computational Considerations

The choice of whether to compute in the unreduced space, and then project onto the shape space to obtain the reduced dynamics, or to compute the reduced dynamics directly using either the Discrete Routh equations, or the RSPRK algorithm, depends on the nature of the problem to be simulated.

Given a configuration space of dimension n, and a symmetry group of dimension m, we are faced with the option of implementing a conceptually simpler algorithm in $2n$ dimensions, as compared to a more geometrically involved algorithm in $2(n-m)$ dimensions. Whether the additional effort associated with implementing the reduced algorithm is justified depend on a number of factors, including the relative dimension of the configuration space and the symmetry group, the computational complexity of the iterative schemes used to solve the resulting implicit system of equations, and any additional structure that may arise in either the reduced or unreduced system.

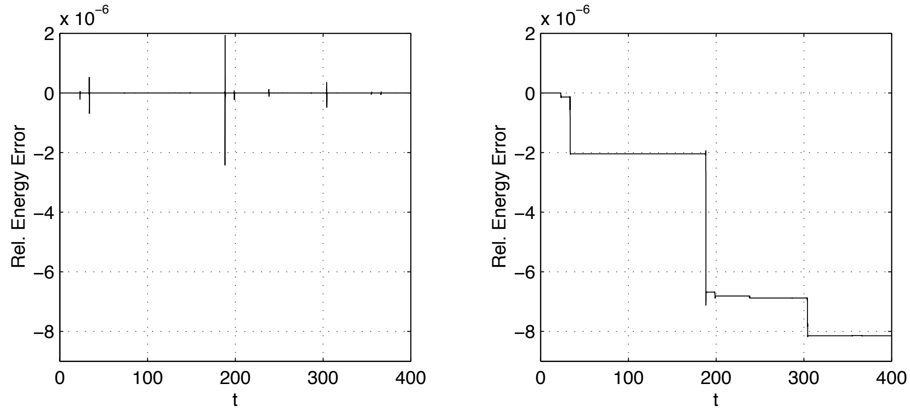


Figure 2.8: Relative energy drift $(E - E_0)/E_0$ using RSPRK (left) compared to the relative energy drift in a non-symplectic RK (right).

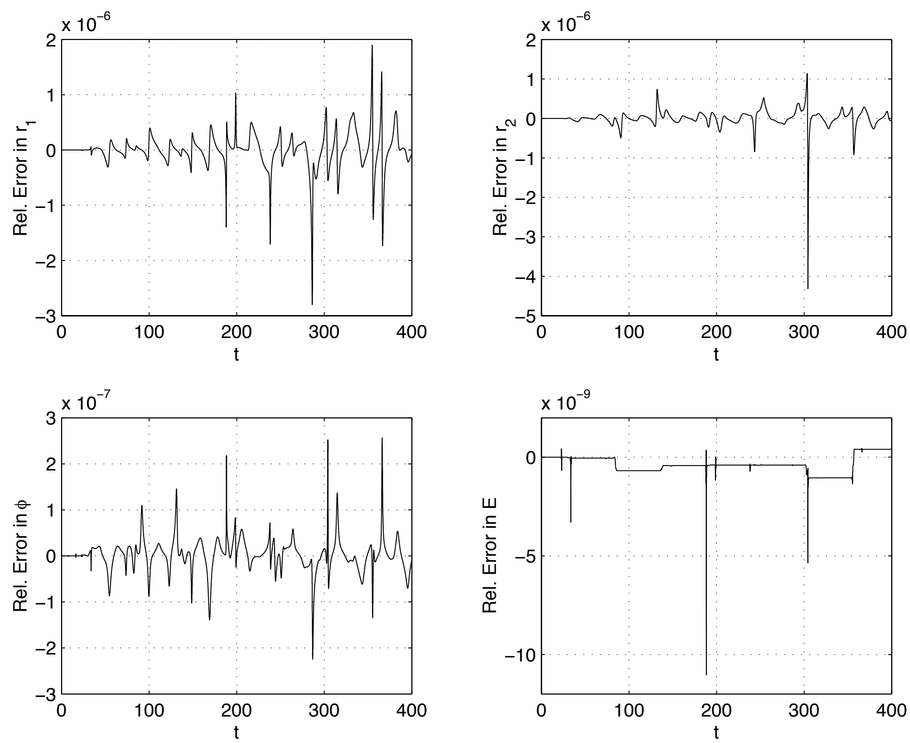


Figure 2.9: Relative error in r_1, r_2, φ, and E between RSPRK and SPRK.

For instance, if longtime or repeated simulations are desired of systems with high-dimensional symmetry groups, it can be advantageous to compute in the reduced space directly. An example of this situation, which is of current engineering interest, is simulating the dynamical behavior of connected networks of systems with their own internal symmetries.

If the systems to be connected are all identical, the geometric quantities that need to be computed, such as the mechanical connection, have a particularly simple repeated form, and the additional upfront effort in implementing the reduced algorithm can result in substantial computational savings.

Non-intrinsic numerical schemes such as the Symplectic Partitioned Runge–Kutta algorithm applied to the classical Routh equations can have undesirable numerical properties due to the need for coordinate-dependent local trivializations and the presence of coordinate singularities in these local trivializations, such as those encountered while using Euler angles for rigid-body dynamics. In the presence of non-trivial magnetic terms in the symplectic form, this can necessitate frequent changes of coordinate charts, as documented in Wisdom et al. [1984] and Patrick [1991]. In such instances, the coordinate changes can account for an overwhelming portion of the total computational effort. In contrast, intrinsic methods do not depend on a particular choice of coordinate system, and as such allow for the use of global charts through the use of containing vector spaces with constraints enforced using Lagrange multipliers.

Coordinate singularities can affect the quality of the simulation in subtle ways that may depend on the choice of numerical scheme. In the energy behavior of the simulation of the double spherical pendulum, we notice spikes in the energy corresponding to times when r_1 or r_2 are close to 0. While these errors accumulate in the non-symplectic method, the energy error in the symplectic method remains well-behaved. However, sharp spikes can be avoided altogether by evolving the equations as a constrained system with $V = \mathbb{R}^3 \times \mathbb{R}^3$, and constraint function $g(\mathbf{v}_1, \mathbf{v}_2) = (\|\mathbf{v}_1\| - l_1, \|\mathbf{v}_2\| - l_2)$ that is imposed using Lagrange multipliers, as opposed to choosing local coordinates that automatically satisfy the constraints. Here, the increased cost of working in the six-dimensional linear space V with constraints is offset by not having to transform between charts of $S^2_{l_1} \times S^2_{l_2}$, which can be significant if the trajectories are particularly chaotic.

While in simple examples, the effect of choosing local coordinates that allow the use of non-intrinsic schemes can be properly corrected for, this is not true in general for more complicated examples. Here, intrinsic schemes such as those we have developed in this paper for dealing with reduced dynamics and constrained systems are preferable, since they do not depend on a particular choice of local trivialization, and as such do not require frequent coordinate transformations.

2.11 Conclusions and Future Work

In summary, we have derived the Discrete Routh equations on $S \times S$, which are symplectic with respect to a non-canonical symplectic form, and retains the good energy behavior typically associated with variational integrators. Furthermore, when the group action can be expressed as addition, we obtain the Reduced Symplectic Partitioned Runge–Kutta algorithm on T^*S, that can be considered as a discrete analogue of cotangent bundle reduction. In addition, the theory has been extended to include constraints and forcing. By providing an understanding of how the reduced and unreduced formulations are related at a discrete level, we enable the user to freely choose whichever formulation is most appropriate, and provides the most insight into the problem at hand.

Certainly one of the obvious things to do in the future is to extend this reduction procedure to the case of nonabelian symmetry groups following the nonabelian version of Routh reduction given in Jalnapurkar and Marsden [2000] and Marsden et al. [2000b]. There are also several problems, including the averaged J_2 problem, in which one can also carry out discrete reduction by stages and in particular relate it to the semidirect product work of Bobenko and Suris [1999]. This is motivated by the fact that the semidirect product reduction theory of Holm et al. [1998] is a special case of reduction by stages (at least without the momentum map constraint), as was shown in Cendra et al. [1998]. In further developing discrete reduction theory, the discrete theory of connections on principal bundles developed in Leok et al. [2003] and Chapter 4 is particularly relevant, as it provides an intrinsic method of representing the reduced space $(Q \times Q)/G$ as $(S \times S) \oplus \tilde{G}$.

Another component that is needed in this work is a good discrete version of the calculus of differential forms. Note that in our work we found, being directed by mechanics, that the right discrete version of the magnetic 2-form is the difference of two connection 1-forms. It is expected that we could recover such a magnetic 2-form by considering the discrete exterior derivative of a discrete connection form in a finite discretization of space-time, and taking the continuum limit in the spatial discretization. Developing a discrete analogue of Stokes' Theorem would also provide insight into the issue of discrete geometric phases. Some work on a discrete theory of exterior calculus can be found in Desbrun et al. [2003a] and Chapter 3.

Of course, extensions of this work to the context of PDEs, especially fluid mechanics, would be very interesting.

Chapter 3

Discrete Exterior Calculus

In collaboration with Mathieu Desbrun, Anil N. Hirani, and Jerrold E. Marsden.

Abstract

We present a theory and applications of discrete exterior calculus on simplicial complexes of arbitrary finite dimension. This can be thought of as calculus on a discrete space. Our theory includes not only discrete differential forms but also discrete vector fields and the operators acting on these objects. This allows us to address the various interactions between forms and vector fields (such as Lie derivatives) which are important in applications. Previous attempts at discrete exterior calculus have addressed only differential forms. We also introduce the notion of a circumcentric dual of a simplicial complex. The importance of dual complexes in this field has been well understood, but previous researchers have used barycentric subdivision or barycentric duals. We show that the use of circumcentric duals is crucial in arriving at a theory of discrete exterior calculus that admits both vector fields and forms.

3.1 Introduction

This work presents a theory of ***discrete exterior calculus*** (DEC) motivated by potential applications in computational methods for field theories such as elasticity, fluids, and electromagnetism. In addition, it provides much needed mathematical machinery to enable a systematic development of numerical schemes that mirror the approach of geometric mechanics.

This theory has a long history that we shall outline below in §3.2, but we aim at a comprehensive, systematic, as well as useful, treatment. Many previous works, as we shall review, are incomplete both in terms of the objects that they treat as well as the types of meshes that they allow.

Our vision of this theory is that it should proceed *ab initio* as a discrete theory that parallels the continuous one. General views of the subject area of DEC are common in the literature (see, for instance, Mattiussi [2000]), but they usually stress the process of discretizing a continuous theory and the overall approach is tied to this goal. However, if one takes the point of view that the discrete theory can, and indeed should, stand in its own right, then the range of application areas naturally is enriched and increases.

Convergence and consistency considerations alone are inadequate to discriminate between the various choices of discretization available to the numerical analyst, and only by requiring, when appropriate, that the discretization exhibits discrete analogues of continuous properties of interest can we begin to address the question of what makes a discrete theory a canonical discretization of a continuous one.

Applications to Variational Problems. One of the major application areas we envision is to variational problems, be they in mechanics or optimal control. One of the key ingredients in this direction that we imagine will play a key role in the future is that of AVI's (asynchronous variational integrators) designed for the numerical integration of mechanical systems, as in Lew et al. [2003]. These are integration algorithms that respect some of the key features of the continuous theory, such as their multi-symplectic nature and exact conservation laws. They do so by discretizing the underlying variational principles of mechanics rather than discretizing the equations. It is well-known (see the reference just mentioned for some of the literature) that variational problems come equipped with a rich exterior calculus structure and so on the discrete level, such structures will be enhanced by the availability of a discrete exterior calculus. One of the objectives of this chapter is to fill this gap.

Structured Constraints. There are many constraints in numerical algorithms that naturally involve differential forms, such as the divergence constraint for incompressibility of fluids, as well as the fact that differential forms are naturally the fields in electromagnetism, and some of Maxwell's equations are expressed in terms of the divergence and curl operations on these fields. Preserving, as in the mimetic differencing literature, such features directly on the discrete level is another one of the goals, overlapping with our goals for variational problems.

Lattice Theories. Periodic crystalline lattices are of important practical interest in material science, and the anisotropic nature of the material properties arises from the geometry and connectivity of the intermolecular bonds in the lattice. It is natural to model these lattices as inherently discrete objects, and an understanding of discrete curvature that arises from DEC is particularly relevant, since part of the potential energy arises from stretched bonds that can be associated with discrete curvature in the underlying relaxed configuration of the lattice. In particular, this could yield a more detailed geometric understanding of what happens at grain boundaries. Lattice defects can also be associated with discrete curvature when appropriately interpreted. The introduction of a discrete notion of curvature will lay the foundations for a better understanding of the role of geometry in the material properties of solids.

Some of the Key Theoretical Accomplishments. Our development of discrete exterior calculus includes discrete differential forms, the Hodge star operator, the wedge product, the exterior derivative, as well as contraction and the Lie derivative. For example, this approach leads to the proper definition of discrete divergence and curl operators and has already resulted in applications like a discrete Hodge type decomposition of 3D vector fields on irregular grids—see Tong et al. [2003].

Context. We present the theory and some applications of DEC in the context of simplicial complexes of arbitrary finite dimension.

Methodology. We believe that the correct way to proceed with this program is to develop, as we have already stressed, *ab initio*, a calculus on discrete manifolds which parallels the calculus on smooth manifolds of arbitrary finite dimension. Chapters 6 and 7 of Abraham et al. [1988] are a good source for the concepts and definitions in the smooth case. However we have tried to make this chapter as self-contained as possible. Indeed, one advantage of developing a calculus on discrete manifolds, as we do here, is pedagogical. By using concrete examples of discrete two- and three-dimensional spaces one can explain most of calculus on manifolds at least formally as we will do using the examples in this chapter. The machinery of Riemannian manifolds and general manifold theory from the smooth case is, strictly speaking, not required in the discrete world. The technical terms that are used in this introduction will be defined in subsequent sections, but they should be already familiar to someone who knows the usual exterior calculus on smooth manifolds.

The Objects in DEC. To develop a discrete theory, one must define discrete differential forms along with vector fields and operators involving these. Once discrete forms and vector fields are defined, a calculus can be developed by defining the discrete exterior derivative ($\mathbf{d}$), codifferential ($\boldsymbol{\delta}$) and Hodge star ($*$) for operating on forms, discrete wedge product ($\wedge$) for combining forms, discrete flat ($\flat$) and sharp ($\sharp$) operators for going between vector fields and 1-forms and discrete contraction operator ($\mathbf{i}_X$) for combining forms and vector fields. Once these are done, one can then define other useful operators. For example, a discrete Lie derivative ($\pounds_X$) can be *defined* by requiring that the Cartan magic (or homotopy) formula hold. A discrete divergence in any dimension can be defined. A discrete Laplace–deRham operator (Δ) can be defined using the usual definition of $\mathbf{d}\boldsymbol{\delta} + \boldsymbol{\delta}\mathbf{d}$. When applied to functions, this is the same as the discrete Laplace–Beltrami operator (∇^2), which is the defined as $\text{div} \circ \text{curl}$. We define all these operators in this chapter.

The discrete manifolds we work with are simplicial complexes. We will recall the standard formal definitions in §3.3 but familiar examples of simplicial complexes are meshes of triangles embedded in $\mathbb{R}^3$ and meshes made up of tetrahedra occupying a portion of $\mathbb{R}^3$. We will assume that the angles and lengths on such discrete manifolds are computed in the embedding space $\mathbb{R}^N$ using the standard metric of that space. In other words, in this chapter we do not address the issue of how to discretize a given smooth Riemannian manifold, and how to embed it in $\mathbb{R}^N$, since there may be many ways to do this. For example, SO(3) can be embedded in $\mathbb{R}^9$ with a constraint, or as the unit quaternions in $\mathbb{R}^4$. Another potentially important consideration in discretizing the manifold is that the topology of the simplicial complex should be the same as the manifold to be discretized. This can be verified using the methods of computational homology (see, for example, Kaczynski et al. [2004]), or discrete Morse theory (see, for example, Forman [2002]; Wood [2003]). For the purposes of discrete exterior calculus, only local metric information is required, and we will comment towards the end of §3.3 how to address the issue of embedding in a local fashion, as well as the criterion for a good global embedding.

Our development in this chapter is for the most part formal in that we choose appropriate geometric definitions of the various objects and quantities involved. For the most part, we do not prove that these definitions converge to the smooth counterparts. The definitions are chosen so as to make some important theorems like the generalized Stokes' theorem true by definition. Moreover, in the cases where previous results are available, we have checked that the operators we obtain match the ones obtained by other means, such as variational derivations.

3.2 History and Previous Work

The use of simplicial chains and cochains as the basic building blocks for a discrete exterior calculus has appeared in several papers. See, for instance, Sen et al. [2000], Adams [1996], Bossavit [2002c], and references therein. These authors view forms as linearly interpolated versions of smooth differential forms, a viewpoint originating from Whitney [1957], who introduced the Whitney and deRham maps that establish an isomorphism between simplicial cochains and Lipschitz differential forms.

We will, however, view discrete forms as real-valued linear functions on the space of chains. These are inherently discrete objects that can be paired with chains of oriented simplices, or their geometric duals, by the bilinear pairing of evaluation. In the next chapter, where we consider applications involving the curvature of a discrete space, we will relax the condition that discrete forms are real-valued, and consider group-valued forms.

Intuitively, this natural pairing of evaluation can be thought of as integration of the discrete form over the chain. This difference from the work of Sen et al. [2000] and Adams [1996] is apparent in the definitions of operations like the wedge product as well.

There is also much interest in a discrete exterior calculus in the computational electromagnetism community, as represented by Bossavit [2001, 2002a,b,c], Gross and Kotiuga [2001], Hiptmair [1999, 2001a,b, 2002], Mattiussi [1997, 2000], Nicolaides and Wang [1998], Teixeira [2001], and Tonti [2002].

Many of the authors cited above, for example, Bossavit [2002c], Sen et al. [2000], and Hiptmair [2002], also introduce the notions of dual complexes in order to construct the Hodge star operator. With the exception of Hiptmair, they use barycentric duals. This works if one develops a theory of discrete forms and does not introduce discrete vector fields. We show later that to introduce discrete vector fields into the theory the notion of circumcentric duals seems to be important.

Other authors, such as Moritz [2000]; Moritz and Schwalm [2001]; Schwalm et al. [1999], have incorporated vector fields into the cochain based approach to exterior calculus by identifying vector fields with cochains, and having them supported on the same mesh. This is ultimately an unsatisfactory approach, since dual meshes are essential as a means of encoding physically relevant phenomena such as fluxes across boundaries.

The use of primal and dual meshes arises most often as staggered meshes in finite volume and finite difference methods. In fluid computations, for example, the density is often a cell-centered quantity, which can either be represented as a primal object by being associated with the 3-cell, or as a dual object associated with the 0-cell at the center of the 3-cell. Similarly, the flux across boundaries can be associated with the 2-cells that make up the boundary, or the 1-cell which is normal to the boundary.

Another approach to a discrete exterior calculus is presented in Dezin [1995]. He defines a one-dimensional discretization of the real line in much the same way we would. However, to generalize to higher dimensions he introduces a tensor product of this space. This results in logically rectangular meshes. Our calculus, however, is defined over simplicial meshes. A further difference is that like other authors in this field, Dezin [1995] does not introduce vector fields into his theory.

A related effort for three-dimensional domains with logically rectangular meshes is that of Mansfield and Hydon [2001], who established a variational complex for difference equations by constructing a discrete homotopy operator. We construct an analogous homotopy operator for simplicial meshes in proving the discrete Poincaré lemma.

3.3 Primal Simplicial Complex and Dual Cell Complex

In constructing the discretization of a continuous problem in the context of our formulation of discrete exterior calculus, we first discretize the manifold of interest as a simplicial complex. While this is typically in the form of a simplicial complex that is embedded into Euclidean space, it is only necessary to have an abstract simplicial complex, along with a local metric defined on adjacent vertices. This abstract setting will be addressed further toward the end of this section.

We will now recall some basic definitions of simplices and simplicial complexes, which are standard from simplicial algebraic topology. A more extensive treatment can be found in Munkres [1984].

Definition 3.1. *A k-**simplex** is the convex span of $k+1$ geometrically independent points,*

$$\sigma^k = [v_0, v_1, \ldots, v_k] = \left\{ \sum_{i=0}^{k} \alpha^i v_i \;\middle|\; \alpha^i \geq 0, \sum_{i=0}^{n} \alpha^i = 1 \right\}.$$

*The points $v_0, \ldots, v_k$ are called the **vertices** of the simplex, and the number k is called the **dimension** of the simplex. Any simplex spanned by a (proper) subset of $\{v_0, \ldots, v_k\}$ is called a **(proper) face** of σ^k. If σ^l is a proper face of σ^k, we denote this by $\sigma^l \prec \sigma^k$.*

Example 3.1. *Consider 3 non-collinear points v_0, v_1 and v_2 in $\mathbb{R}^3$. Then, these three points individually are examples of 0-simplices, to which an orientation is assigned through the choice of a sign. Examples of 1-simplices are the oriented line segments $[v_0, v_1]$, $[v_1, v_2]$ and $[v_0, v_2]$. By writing the vertices in that order we have given orientations to these 1-simplices, i.e., $[v_0, v_1]$ is oriented from v_0 to v_1. The triangle $[v_0, v_1, v_2]$ is a 2-simplex oriented in counterclockwise direction. Note that the orientation of $[v_0, v_2]$ does not agree with that of the triangle.*

Definition 3.2. *A **simplicial complex** K in $\mathbb{R}^N$ is a collection of simplices in $\mathbb{R}^N$, such that,*

1. *Every face of a simplex of K is in K.*

2. *The intersection of any two simplices of K is a face of each of them.*

Definition 3.3. *A **simplicial triangulation** of a polytope $|K|$ is a simplicial complex K such that the union of the simplices of K recovers the polytope $|K|$.*

Definition 3.4. *If L is a subcollection of K that contains all faces of its elements, then L is a simplicial complex in its own right, and it is called a **subcomplex** of K. One subcomplex of K is the collection of all simplices of K of dimension at most k, which is called the k**-skeleton** of K, and is denoted $K^{(k)}$.*

Circumcentric Subdivision. We will also use the notion of a circumcentric dual or Voronoi mesh of the given primal mesh. We will point to the importance of this choice later on in §3.7 and 3.9. We call the Voronoi dual a circumcentric dual since the dual of a simplex is its circumcenter (equidistant from all vertices of the simplex).

Definition 3.5. *The **circumcenter** of a k-simplex σ^k is given by the center of the k-circumsphere, where the k-circumsphere is the unique k-sphere that has all $k+1$ vertices of σ^k on its surface. Equivalently, the circumcenter is the unique point in the k-dimensional affine space that contains the k-simplex that is equidistant from all the $k+1$ nodes of the simplex. We will denote the circumcenter of a simplex σ^k by $c(\sigma^k)$.*

The circumcenter of a simplex σ^k can be obtained by taking the intersection of the normals to the $(k-1)$-dimensional faces of the simplex, where the normals are emanating from the circumcenter of the face. This allows us to recursively compute the circumcenter.

If we are given the nodes which describe the primal mesh, we can construct a simplicial triangulation by using the Delaunay triangulation, since this ensures that the circumcenter of a simplex is always a point within the simplex. Otherwise we assume that a nice mesh has been given to us, i.e., it is such that the circumcenters lie within the simplices. While this is not be essential for our theory it makes some proofs simpler. For some computations the Delaunay triangulation is desirable in that it reduces the maximum aspect ratio of the mesh, which is a factor in determining the rate at which the corresponding numerical scheme converges. But in practice there are many problems for which Delaunay triangulations are a bad idea. See, for example, Schewchuck [2002]. We will address such computational issues in a separate work.

Definition 3.6. *The **circumcentric subdivision** of a simplicial complex is given by the collection of all simplices of the form*

$$[c(\sigma_0), \ldots, c(\sigma_k)],$$

where $\sigma_0 \prec \sigma_1 \prec \ldots \prec \sigma_k$, or equivalently, that σ_i is a proper face of σ_j for all $i < j$.

Circumcentric Dual. We construct a circumcentric dual to a k-simplex using the circumcentric duality operator, which is introduced below.

Definition 3.7. *The **circumcentric duality operator** is given by*

$$\star\left(\sigma^k\right) = \sum_{\sigma^k \prec \sigma^{k+1} \prec \ldots \prec \sigma^n} \epsilon_{\sigma^k,\ldots,\sigma^n} \left[c(\sigma^k), c(\sigma^{k+1}), \ldots, c(\sigma^n)\right],$$

where the $\epsilon_{\sigma^k,\ldots,\sigma^n}$ coefficient ensures that the orientation of $\left[c(\sigma^k), c(\sigma^{k+1}), \ldots, c(\sigma^n)\right]$ is consistent with the orientation of the primal simplex, and the ambient volume-form.

Orienting σ^k is equivalent to choosing a ordered basis, which we shall denote by $dx^1 \wedge \ldots \wedge dx^k$. Similarly, $\left[c(\sigma^k), c(\sigma^{k+1}), \ldots, c(\sigma^n)\right]$ has an orientation denoted by $dx^{k+1} \wedge \ldots \wedge dx^n$. If the orientation corresponding to $dx^1 \wedge \ldots \wedge dx^n$ is consistent with the volume-form on the manifold, then $\epsilon_{\sigma^k,\ldots,\sigma^n} = 1$, otherwise it takes the value -1.

We immediately see from the construction of the circumcentric duality operator that the dual elements can be realized as a submesh of the first circumcentric subdivision, since it consists of elements of the form $[c(\sigma_0), \ldots, c(\sigma_k)]$, which are, by definition, part of the first circumcentric subdivision.

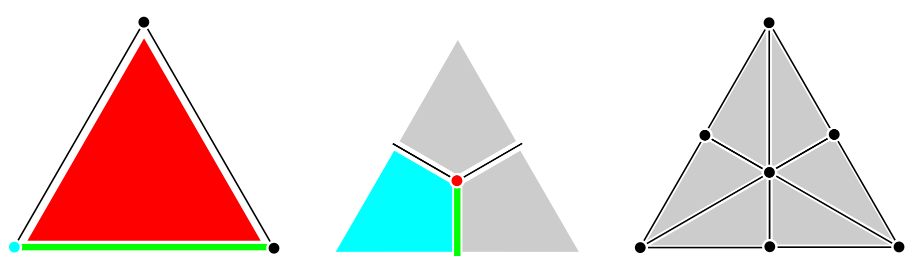
Example 3.2. *The circumcentric duality operator maps a 0-simplex into the convex hull generated by the circumcenters of n-simplices that contain the 0-simplex,*

$$\star(\sigma^0) = \left\{ \sum \alpha_{\sigma^n} c\left(\sigma^n\right) \,\middle|\, \alpha_{\sigma^n} \geq 0, \sum \alpha_{\sigma^n} = 1, \sigma^0 \prec \sigma^n \right\},$$

and the circumcentric duality operator maps a $n-$simplex into the circumcenter of the $n-$simplex,

$$\star(\sigma^n) = c(\sigma^n).$$

This is more clearly illustrated in Figure 3.1, where the primal and dual elements are color coded to represent the dual relationship between the elements in the primal and dual mesh.



(a) Primal (b) Dual (c) First subdivision

Figure 3.1: Primal, and dual meshes, as chains in the first circumcentric subdivision.

The choice of a circumcentric dual is significant, since it allows us to recover geometrically important objects such as normals to $(n-1)$-dimensional faces, which are obtained by taking their circumcentric dual, whereas, if we were to use a barycentric dual, the dual to a $(n-1)$-dimensional face would not be normal to it.

Orientation of the Dual Cell. Notice that given an oriented simplex σ^k, which is represented by $[v_0,\ldots,v_k]$, the orientation is equivalently represented by $(v_1-v_0)\wedge(v_2-v_1)\wedge\ldots\wedge(v_k-v_{k-1})$, which we denote by,

$$[v_0,\ldots,v_k]\sim(v_1-v_0)\wedge(v_2-v_1)\wedge\ldots\wedge(v_k-v_{k-1}),$$

which is an equivalence at the level of orientation. It would be nice to express our criterion for determining the orientation of the dual cell in terms of the $(k+1)$-vertex representation.

To determine the orientation of the $(n-k)$-simplex given by $[c(\sigma^k),c(\sigma^{k+1}),\ldots,c(\sigma^n)]$, or equivalently, $dx^{k+1}\wedge\ldots\wedge dx^n$, we consider the n-simplex given by $[c(\sigma^0),\ldots,c(\sigma^n)]$, where $\sigma^0\prec\ldots\prec\sigma^k$. This is related to the expression $dx^1\wedge\ldots\wedge dx^n$, up to a sign determined by the relative orientation of $[c(\sigma^0),\ldots,c(\sigma^k)]$ and σ^k. Thus, we have that

$$dx^1\wedge\ldots\wedge dx^n\sim\operatorname{sgn}([c(\sigma^0),\ldots,c(\sigma^k)],\sigma^k)[c(\sigma^0),\ldots,c(\sigma^n)]\,.$$

Then, we need to check that $dx^1\wedge\ldots\wedge dx^n$ is consistent with the volume-form on the manifold, which is represented by the orientation of σ^n. Thus, we have that the correct orientation for the $[c(\sigma^k),c(\sigma^{k+1}),\ldots,c(\sigma^n)]$ term is given by,

$$\operatorname{sgn}([c(\sigma^0),\ldots,c(\sigma^k)],\sigma^k)\cdot\operatorname{sgn}([c(\sigma^0),\ldots,c(\sigma^n)],\sigma^n).$$

These two representations of the choice of orientation for the dual cells are equivalent, but the combinatorial definition above might be preferable for the purposes of implementation.

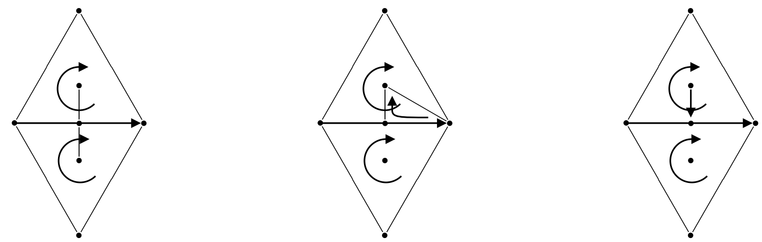
Example 3.3. *We would like to compute the orientation of the dual of a* 1*-simplex, in two dimensions, given the orientation of the two neighboring* 2*-simplices.*

Given a simplicial complex, as shown in Figure 3.2(a), we consider a 2*-simplex of the form* $[c(\sigma^0),c(\sigma^1),c(\sigma^2)]$*, which is illustrated in Figure 3.2(b).*

Notice that the orientation is consistent with the given orientation of the 2*-simplex, but it is not consistent with the orientation of the primal* 1*-simplex, so the orientation should be reversed, to give the dual cell illustrated in Figure 3.2(c).*

We summarize the results for the induced orientation of dual cells for the other 2*-simplices of the form* $[c(\sigma^0),c(\sigma^1),c(\sigma^2)]$*, in Table 3.1.*

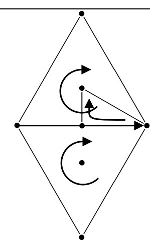
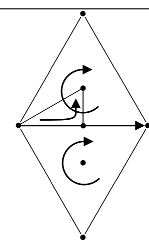
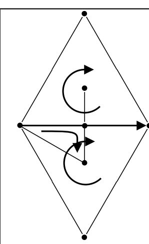
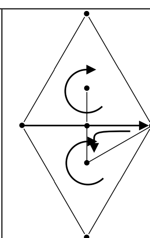
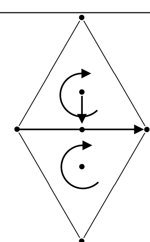
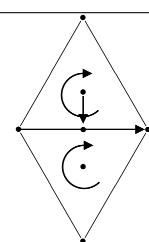
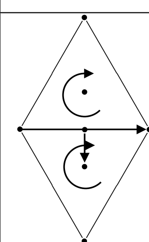
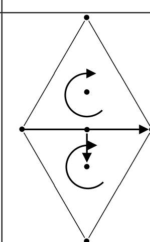
Orientation of the Dual of a Dual Cell. While the circumcentric duality operator is a map from the primal simplicial complex to the dual cell complex, we can formally extend the circumcentric duality operator to a map from the dual cell complex to the primal simplicial complex. However,



(a) Simplicial complex (b) 2-simplex (c) $\star\sigma^1$

Figure 3.2: Orienting the dual of a cell.

Table 3.1: Determining the induced orientation of a dual cell.

$[c(\sigma^0), c(\sigma^1), c(\sigma^2)]$				
$\text{sgn}([c(\sigma^0), c(\sigma^1)], \sigma^1)$	$-$	$+$	$+$	$-$
$\text{sgn}([c(\sigma^0), c(\sigma^1), c(\sigma^2)], \sigma^2)$	$+$	$-$	$+$	$-$
$\text{sgn}([c(\sigma^0), c(\sigma^1)], \sigma^1)$ $\cdot\,\text{sgn}([c(\sigma^0), c(\sigma^1), c(\sigma^2)], \sigma^2)$ $\cdot[c(\sigma^1), c(\sigma^2)]$				

we need to be slightly careful about the orientation of primal simplex we recover from applying the circumcentric duality operator twice.

We have that, $\star\star(\sigma^k) = \pm\sigma^k$, where the sign is chosen to ensure the appropriate choice of orientation. If, as before, σ^k has an orientation represented by $dx^1 \wedge \ldots \wedge dx^k$, and $\star\sigma^k$ has an orientation represented by $dx^{k+1} \wedge \ldots \wedge dx^n$, then the orientation of $\star\star(\sigma^k)$ is chosen so that $dx^{k+1} \wedge \ldots \wedge dx^n \wedge dx^1 \wedge \ldots \wedge dx^k$ is consistent with the ambient volume-form. Since, by construction, $\star(\sigma^k)$, $dx^1 \wedge \ldots \wedge dx^n$ has an orientation consistent with the ambient volume-form, we need only compare $dx^{k+1} \wedge \ldots \wedge dx^n \wedge dx^1 \wedge \ldots \wedge dx^k$ with $dx^1 \wedge \ldots \wedge dx^n$. Notice that it takes $n-k$ transpositions to get the dx^1 term in front of the $dx^{k+1} \wedge \ldots \wedge dx^n$ terms, and we need to do this k times for each term of $dx^1 \wedge \ldots \wedge dx^k$, so it follows that the sign is simply given by $(-1)^{k(n-k)}$, or equivalently,

$$\star\star(\sigma^k) = (-1)^{k(n-k)}\sigma^k. \tag{3.3.1}$$

A similar relationship holds if we use a dual cell instead of the primal simplex σ^k.

Support Volume of a Primal Simplex and Its Dual Cell. We can think of a cochain as being constructed out of a basis consisting of cosimplices or cocells with value 1 on a single simplex or cell, and 0 otherwise. The way to visualize this cosimplex is that it is associated with a differential form that has support on what we will refer to as the ***support volume*** associated with a given simplex or cell.

Definition 3.8. *The **support volume** of a simplex σ^k is a n-volume given by the convex hull of the geometric union of the simplex and its circumcentric dual. This is given by*

$$V_{\sigma^k} = \mathrm{convexhull}(\sigma^k, \star\sigma^k) \cap |K|.$$

The intersection with $|K|$ is necessary to ensure that the support volume does not extend beyond the polytope $|K|$ which would otherwise occur if $|K|$ is nonconvex.

We extend the notion of a support volume to a dual cell $\star\sigma^k$ by similarly defining

$$V_{\star\sigma^k} = \mathrm{convexhull}(\star\sigma^k, \star\star\sigma^k) \cap |K| = V_{\sigma^k}.$$

To clarify this definition, we will consider some examples of simplices, their dual cells, and their corresponding support volumes. For two-dimensional simplicial complexes, this is illustrated in Table 3.2.

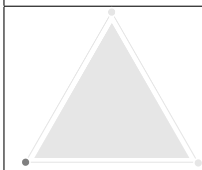
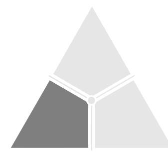
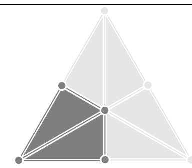
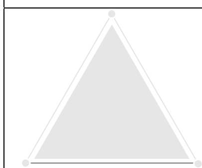
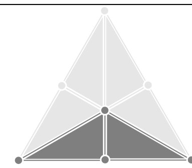
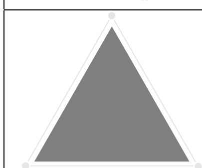
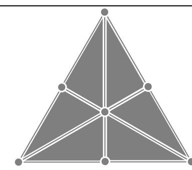
The support volume has the nice property that at each dimension, it partitions the polytope $|K|$ into distinct non-intersecting regions associated with each individual k-simplex. For any two distinct k-simplices, the intersection of their corresponding support volumes have measure zero, and the union of the support volumes of all k-simplices recovers the original polytope $|K|$.

Notice, from our construction, that the support volume of a simplex and its dual cell are the same, which suggests that there is an identification between cochains on k-simplices and cochains on $(n-k)$-cells. This is indeed the case, and is a concept associated with the Hodge star for differential forms.

Examples of simplices, their dual cells, and the corresponding support volumes in three dimensions are given in Table 3.3.

In our subsequent discussion, we will assume that we are given a simplicial complex K of di-

Table 3.2: Primal simplices, dual cells, and support volumes in two dimensions.

Primal Simplex	Dual Cell	Support Volume
 σ^0, 0-simplex	 $\star\sigma^0$, 2-cell	 $V_{\sigma^0} = V_{\star\sigma^0}$
 σ^1, 1-simplex	$\star\sigma^1$, 1-cell	 $V_{\sigma^1} = V_{\star\sigma^1}$
 σ^2, 2-simplex	$\star\sigma^2$, 0-cell	 $V_{\sigma^2} = V_{\star\sigma^2}$

mension n in $\mathbb{R}^N$. Thus, the highest-dimensional simplex in the complex is of dimension n and each 0-simplex (vertex) is in $\mathbb{R}^N$. One can obtain this, for example, by starting from 0-simplices, i.e., vertices, and then constructing a Delaunay triangulation, using the vertices as sites. Often, our examples will be for two-dimensional discrete surfaces in $\mathbb{R}^3$ made up of triangles (here $n = 2$ and $N = 3$) or three-dimensional manifolds made of tetrahedra, possibly embedded in a higher-dimensional space.

Cell Complexes. The circumcentric dual of a primal simplicial complex is an example of a cell complex. The definition of a cell complex follows.

Definition 3.9. *A* ***cell complex*** $\star K$ *in* $\mathbb{R}^N$ *is a collection of cells in* $\mathbb{R}^N$ *such that,*

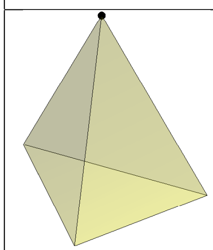
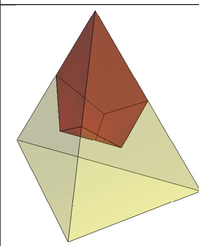
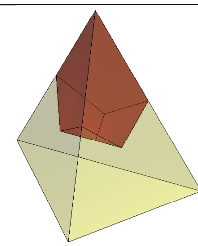
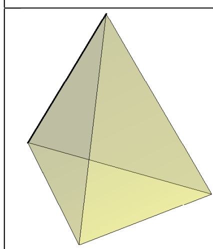
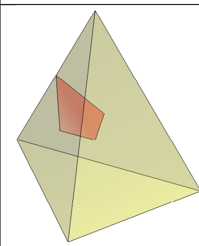
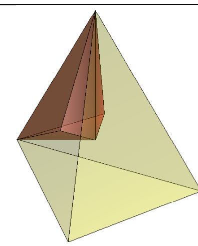
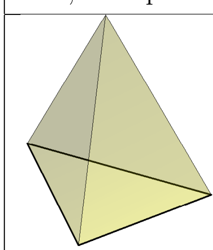
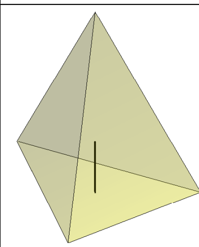
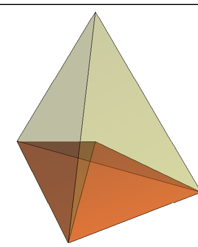
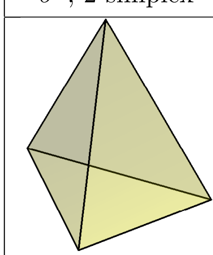
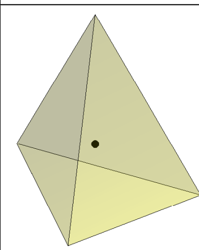
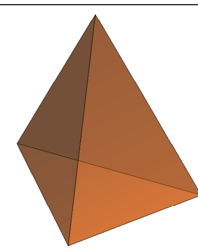
1. *There is a partial ordering of cells in* $\star K$*,* $\hat{\sigma}^k \prec \hat{\sigma}^l$*, which is read as* $\hat{\sigma}^k$ *is a face of* $\hat{\sigma}^l$*.*

2. *The intersection of any two cells in* $\star K$*, is either a face of each of them, or it is empty.*

3. *The boundary of a cell is expressible as a sum of its proper faces.*

We will see in the next section that the notion of boundary in the circumcentric dual has to be modified slightly from the geometric notion of a boundary in order for the circumcentric dual to be made into a cell complex.

Table 3.3: Primal simplices, dual cells, and support volumes in three dimensions.

Primal Simplex	Dual Cell	Support Volume
 σ^0, 0-simplex	 $\star\sigma^0$, 3-cell	 $V_{\sigma^0} = V_{\star\sigma^0}$
 σ^1, 1-simplex	 $\star\sigma^1$, 2-cell	 $V_{\sigma^1} = V_{\star\sigma^1}$
 σ^2, 2-simplex	 $\star\sigma^2$, 1-cell	 $V_{\sigma^2} = V_{\star\sigma^2}$
 σ^3, 3-simplex	 $\star\sigma^3$, 0-cell	 $V_{\sigma^3} = V_{\star\sigma^3}$

3.4 Local and Global Embeddings

While it is computationally more convenient to have a global embedding of the simplicial complex into a higher-dimensional ambient space to account for non-flat manifolds it suffices to have an abstract simplicial complex along with a local metric on vertices. The metric is local in the sense that distances between two vertices are only defined if they are part of a common n-simplex in the abstract simplicial complex. Then, the local metric is a map $d : \{(v_0, v_1) \mid v_0, v_1 \in K^{(0)}, [v_0, v_1] \prec \sigma^n \in K\} \to \mathbb{R}$.

The axioms for a ***local metric*** are as follows,

Positive. $d(v_0, v_1) \geq 0$, and $d(v_0, v_0) = 0$, $\forall [v_0, v_1] \prec \sigma^n \in K$.

Strictly Positive. If $d(v_0, v_1) = 0$, then $v_0 = v_1$, $\forall [v_0, v_1] \prec \sigma^n \in K$.

Symmetry. $d(v_0, v_1) = d(v_1, v_0)$, $\forall [v_0, v_1] \prec \sigma^n \in K$.

Triangle Inequality. $d(v_0, v_2) \leq d(v_0, v_1) + d(v_1, v_2)$, $\forall [v_0, v_1, v_2] \prec \sigma^n \in K$.

This allows us to embed each n-simplex locally into $\mathbb{R}^n$, and thereby compute all the necessary metric dependent quantities in our formulation. For example, the volume of a k-dual cell will be computed as the sum of the k-volumes of the dual cell restricted to each n-simplex in its local embedding into $\mathbb{R}^n$.

This notion of local metrics and local embeddings is consistent with the point of view that exterior calculus is a local theory with operators that operate on objects in the tangent and cotangent space of a fixed point. The issue of comparing objects in different tangent spaces is addressed in the discrete theory of connections on principal bundles in Leok et al. [2003] and Chapter 4.

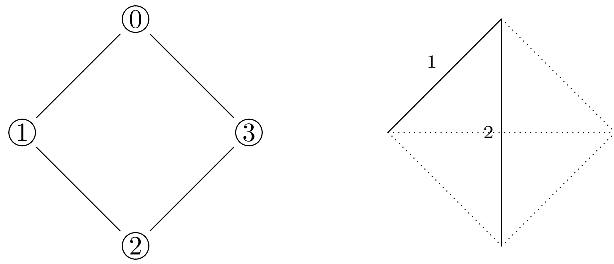
This also provides us with a criterion for evaluating a global embedding. The embedding should be such that the metric of the ambient space $\mathbb{R}^N$ restricted to the vertices of the complex, thought of as points in $\mathbb{R}^N$, agrees with the local metric imposed on the abstract simplicial complex. A global embedding that satisfies this condition will produce the same numerical results in discrete exterior calculus as that obtained using the local embedding method.

It is essential that the metric condition we impose is local, since the notion of distances between points in a manifold which are far away is not a well-defined concept, nor is it particularly useful for embeddings. As the simple example below illustrates, there may not exist any global embeddings into Euclidean space that satisfies a metric constraint imposed for all possible pairs of vertices.

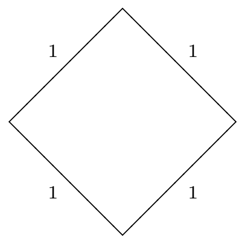
Example 3.4. *Consider a circle, with the distance between two points given by the minimal arc length. Consider a discretization given by 4 equidistant points on the circle, labelled* $v_0, \ldots, v_3$*, with the metric distances as follows,*

$$d(v_i, v_{i+1}) = 1, d(v_i, v_{i+2}) = 2,$$

where the indices are evaluated modulo 4, and this distance function is extended to a metric on all pairs of vertices by symmetry. It is easy to verify that this distance function is indeed a metric on *vertices.*



If we only use the local metric constraint, then we only require that adjacent vertices are separated by 1*, and the following is an embedding of the simplicial complex into* $\mathbb{R}^2$*,*



If, however, we use the metric defined on all possible pairs of vertices, by considering v_0, v_1, v_2*, we have that* $d(v_0, v_1) + d(v_1, v_2) = d(v_0, v_2)$*. Since we are embedding these points into a Euclidean space, it follows that* v_0, v_1, v_2 *are collinear.*

Similarly, by considering v_0, v_2, v_3*, we conclude that they are collinear as well, and that* v_1, v_3 *are coincident, which contradicts* $d(v_1, v_3) = 2$*. Thus, we find that there does not exist a global embedding of the circle into Euclidean space if we require that the embedding is consistent with the metric on vertices defined for all possible pairs of vertices.*

3.5 Differential Forms and Exterior Derivative

We will now define discrete differential forms. We will use some terms (which we will define) from algebraic topology, but it will become clear by looking at the examples that one can gain a clear and working notion of what a discrete form is without any algebraic topology. We start with a few definitions for which more details can be found on page 26 and 27 of Munkres [1984].

Definition 3.10. *Let* K *be a simplicial complex. We denote the free abelian group generated by a basis consisting of oriented* k*-simplices by* $C_k(K;\mathbb{Z})$*. This is the space of finite formal sums of the* k*-simplices, with coefficients in* $\mathbb{Z}$*. Elements of* $C_k(K;\mathbb{Z})$ *are called* k***-chains****.*

Example 3.5. *Figure 3.3 shows examples of* 1*-chains and* 2*-chains.*

Figure 3.3: Examples of chains.

We view discrete k-forms as maps from the space of k-chains to $\mathbb{R}$. Recalling that the space of k-chains is a group, we require that these maps be homomorphisms into the additive group $\mathbb{R}$. Thus, discrete forms are what are called cochains in algebraic topology. We will define cochains below in the definition of forms but for more context and more details readers can refer to any algebraic topology text, for example, page 251 of Munkres [1984].

This point of view of forms as cochains is not new. The idea of defining forms as cochains appears, for example, in the works of Adams [1996], Dezin [1995], Hiptmair [1999], and Sen et al. [2000]. Our point of departure is that the other authors go on to develop a theory of discrete exterior calculus of forms only by introducing interpolation of forms, which we will be able to avoid. The formal definition of discrete forms follows.

Definition 3.11. *A **primal discrete k-form** α is a homomorphism from the chain group $C_k(K;\mathbb{Z})$ to the additive group $\mathbb{R}$. Thus, a discrete k-form is an element of $\mathrm{Hom}(C_k(K),\mathbb{R})$, the space of **cochains**. This space becomes an abelian group if we add two homomorphisms by adding their values in $\mathbb{R}$. The standard notation for $\mathrm{Hom}(C_k(K),\mathbb{R})$ in algebraic topology is $C^k(K;\mathbb{R})$. But we will often use the notation $\Omega^k_d(K)$ for this space as a reminder that this is the space of discrete (hence the d subscript) k-forms on the simplicial complex K. Thus,*

$$\Omega^k_d(K) := C^k(K;\mathbb{R}) = \mathrm{Hom}(C_k(K),\mathbb{R})\,.$$

Note that, by the above definition, given a k-chain $\sum_i a_i c_i^k$ (where $a_i \in \mathbb{Z}$) and a discrete k-form α, we have that

$$\alpha\left(\sum_i a_i c_i^k\right) = \sum_i a_i \alpha(c_i^k)\,,$$

and for two discrete k-forms $\alpha, \beta \in \Omega^k_d(K)$ and a k-chain $c \in C_k(K;\mathbb{Z})$,

$$(\alpha+\beta)(c) = \alpha(c) + \beta(c)\,.$$

In the usual exterior calculus on smooth manifolds integration of k-forms on a k-dimensional manifold is defined in terms of the familiar integration in $\mathbb{R}^k$. This is done roughly speaking by doing the integration in local coordinates, and showing that the value is independent of the choice of coordinates, due to the change of variables theorem in $\mathbb{R}^k$. For details on this, see the first few pages of Chapter 7 of Abraham et al. [1988]. We will not try to introduce the notion of integration of discrete forms on a simplicial complex. Instead the fundamental quantity that we will work with is the natural bilinear pairing of cochains and chains, defined by evaluation. More formally, we have the following definition.

Definition 3.12. *The* ***natural pairing*** *of a k-form α and a k-chain c is defined as the bilinear pairing*

$$\langle \alpha, c \rangle = \alpha(c).$$

As mentioned above, in discrete exterior calculus, this natural pairing plays the role that integration of forms on chains plays in the usual exterior calculus on smooth manifolds. The two are related by a procedure done at the time of discretization. Indeed, consider a simplicial triangulation K of a polyhedron in $\mathbb{R}^n$, i.e., consider a "flat" discrete manifold. If we are discretizing a continuous problem, we will have some smooth forms defined in the space $|K| \subset \mathbb{R}^n$. Consider such a smooth k-form α^k. In order to define the discrete form α_d^k corresponding to α^k, one would integrate α^k on all the k-simplices in K. Then, the evaluation of α_d^k on a k-simplex σ^k is defined by $\alpha_d^k(\sigma^k) := \int_{\sigma^k} \alpha^k$. Thus, discretization is the only place where integration plays a role in our discrete exterior calculus.

In the case of a non-flat manifold, the situation is somewhat complicated by the fact that the smooth manifold, and the simplicial complex, as geometric sets embedded in the ambient space do not coincide. A smooth differential form on the manifold can be discretized into the cochain representation by identifying the vertices of the simplicial complex with points on the manifold, and then using a local chart to identify k-simplices with k-volumes on the manifold.

There is the possibility of k-volumes overlapping even when their corresponding k-simplices do not intersect, and this introduces a discretization error that scales like the mesh size. One can alternatively construct geodesic boundary surfaces in an inductive fashion, which yields a partition of the manifold, but this can be computationally prohibitive to compute.

Now we can define the discrete exterior derivative which we will call $\mathbf{d}$, as in the usual exterior calculus. The discrete exterior derivative will be defined as the dual, with respect to the natural pairing defined above, of the boundary operator, which is defined below.

Definition 3.13. *The* ***boundary*** *operator $\partial_k : C_k(K;\mathbb{Z}) \to C_{k-1}(K;\mathbb{Z})$ is a homomorphism defined by its action on a simplex $\sigma^k = [v_0, \ldots, v_k]$,*

$$\partial_k \sigma^k = \partial_k([v_0, \ldots, v_k]) = \sum_{i=0}^{k} (-1)^i [v_0, \ldots, \hat{v}_i, \ldots, v_k]\,,$$

where $[v_0, \ldots, \hat{v}_i, \ldots, v_k]$ *is the* $(k-1)$*-simplex obtained by omitting the vertex* v_i*. Note that* $\partial_k \circ \partial_{k+1} = 0$*.*

Example 3.6. *Given an oriented triangle* $[v_0, v_1, v_2]$ *the boundary, by the above definition, is the chain* $[v_1, v_2] - [v_0, v_2] + [v_0, v_1]$*, which are the three boundary edges of the triangle.*

Definition 3.14. *On a simplicial complex of dimension* n*, a* ***chain complex*** *is a collection of chain groups and homomorphisms* ∂_k*, such that,*

$$0 \longrightarrow C_n(K) \xrightarrow{\partial_n} \cdots \xrightarrow{\partial_{k+1}} C_k(K) \xrightarrow{\partial_k} \cdots \xrightarrow{\partial_1} C_0(K) \longrightarrow 0\,,$$

and $\partial_k \circ \partial_{k+1} = 0$*.*

Definition 3.15. *The* ***coboundary operator****,* $\delta^k : C^k(K) \to C^{K+1}(K)$*, is defined by duality to the boundary operator, with respect to the natural bilinear pairing between discrete forms and chains. Specifically, for a discrete form* $\alpha^k \in \Omega_d^k(K)$*, and a chain* $c_{k+1} \in C_{k+1}(K;\mathbb{Z})$*, we define* δ^k *by*

$$\left\langle \delta^k \alpha^k, c_{k+1} \right\rangle = \left\langle \alpha^k, \partial_{k+1} c_{k+1} \right\rangle . \tag{3.5.1}$$

That is to say

$$\delta^k(\alpha^k) = \alpha^k \circ \partial_{k+1} .$$

This definition of the coboundary operator induces the ***cochain complex****,*

$$0 \longleftarrow C^n(K) \xleftarrow{\delta^{n-1}} \cdots \xleftarrow{\delta^k} C^k(K) \xleftarrow{\delta^{k-1}} \cdots \xleftarrow{\delta^0} C^0(K) \longleftarrow 0\,,$$

where it is easy to see that $\delta^{k+1} \circ \delta^k = 0$*.*

Definition 3.16. *The* ***discrete exterior derivative*** *denoted by* $\mathbf{d} : \Omega_d^k(K) \to \Omega_d^{k+1}(K)$ *is defined to be the coboundary operator* δ^k*.*

Remark 3.1. *With the above definition of the exterior derivative,* $\mathbf{d} : \Omega_d^k(K) \to \Omega_d^{k+1}(K)$*, and the relationship between the natural pairing and integration, one can regard equation 3.5.1 as a discrete* ***generalized Stokes' theorem****. Thus, given a* k*-chain* c*, and a discrete* k*-form* α*, the discrete Stokes' theorem, which is true by definition, states that*

$$\langle \mathbf{d}\alpha, c \rangle = \langle \alpha, \partial c \rangle .$$

Furthermore, it also follows immediately that $\mathbf{d}^{k+1}\mathbf{d}^k = 0$*.*

Dual Discrete Forms. Everything we have said above in terms of simplices and the simplicial complex K can be said in terms of the cells that are duals of simplices and elements of the dual complex $\star K$. One just has to be a little more careful in the definition of the boundary operator, and the definition we construct below is well-defined on the dual cell complex. This gives us the notion of cochains of cells in the dual complex and these are the ***dual discrete forms***.

Definition 3.17. *The* ***dual boundary*** *operator,* $\partial_k : C_k(\star K;\mathbb{Z}) \to C_{k-1}(\star K;\mathbb{Z})$*, is a homomorphism defined by its action on a dual cell* $\hat{\sigma}^k = \star\sigma^{n-k} = \star[v_0, \ldots, v_{n-k}]$*,*

$$\begin{aligned}\partial\hat{\sigma}^k &= \partial \star [v_0, ..., v_{n-k}] \\ &= \sum_{\sigma^{n-k+1} \succ \sigma^{n-k}} \star\sigma^{n-k+1} \,,\end{aligned}$$

where σ^{n-k+1} *is oriented so that it is consistent with the induced orientation on* σ^{n-k}*.*

3.6 Hodge Star and Codifferential

In the exterior calculus for smooth manifolds, the Hodge star, denoted $*$, is an isomorphism between the space of k-forms and $(n-k)$-forms. The Hodge star is useful in defining the adjoint of the exterior derivative and this is adjoint is called the codifferential. The Hodge star, $* : \Omega^k(M) \to \Omega^{n-k}(M)$, is in the smooth case uniquely defined by the identity,

$$\langle\!\langle \alpha^k, \beta^k \rangle\!\rangle \mathbf{v} = \alpha^k \wedge *\beta^k \,,$$

where $\langle\!\langle\, , \,\rangle\!\rangle$ is a metric on differential forms, and $\mathbf{v}$ is the volume-form. For a more in-depth discussion, see, for example, page 411 of Abraham et al. [1988].

The appearance of k and $(n-k)$ in the definition of Hodge star may be taken to be a hint that primal and dual meshes will play some role in the definition of a discrete Hodge star, since the dual of a k-simplex is an $(n-k)$-cell. Indeed, this is the case.

Definition 3.18. *The* ***discrete Hodge Star*** *is a map* $* : \Omega_d^k(K) \to \Omega_d^{n-k}(\star K)$*, defined by its action on simplices. For a* k*-simplex* σ^k*, and a discrete* k*-form* α^k*,*

$$\frac{1}{|\sigma^k|}\langle \alpha^k, \sigma^k \rangle = \frac{1}{|\star\sigma^k|}\langle *\alpha^k, \star\sigma^k \rangle.$$

The idea that the discrete Hodge star maps primal discrete forms to dual forms, and vice versa, is well-known. See, for example, Sen et al. [2000]. However, notice we now make use of the volume of these primal and dual meshes. But the definition we have given above does appear in the work of Hiptmair [2002].

The definition implies that the primal and dual *averages* must be equal. This idea has already been introduced, not in the context of exterior calculus, but in an attempt at defining discrete differential geometry operators, see Meyer et al. [2002].

Remark 3.2. *Although we have defined the discrete Hodge star above, we will show in Remark 3.8 of §3.12 that if an appropriate discrete wedge product and metric on discrete k-forms is defined, then the expression for the discrete Hodge star operator follows from the smooth definition.*

Lemma 3.1. *For a k-form* α^k,

$$* * \alpha^k = (-1)^{k(n-k)} \alpha^k \, .$$

Proof. The proof is a simple calculation using the property that for a simplex or a cell σ^k, $\star\star(\sigma^k) = (-1)^{k(n-k)}\sigma^k$ (Equation 3.3.1). □

Definition 3.19. *Given a simplicial or a dual cell complex K the **discrete codifferential operator**, $\boldsymbol{\delta} : \Omega_d^{k+1}(K) \to \Omega_d^k(K)$, is defined by $\boldsymbol{\delta}(\Omega_d^0(K)) = 0$ and on discrete $(k+1)$-forms to be*

$$\boldsymbol{\delta}\beta = (-1)^{nk+1} * \mathbf{d} * \beta \, .$$

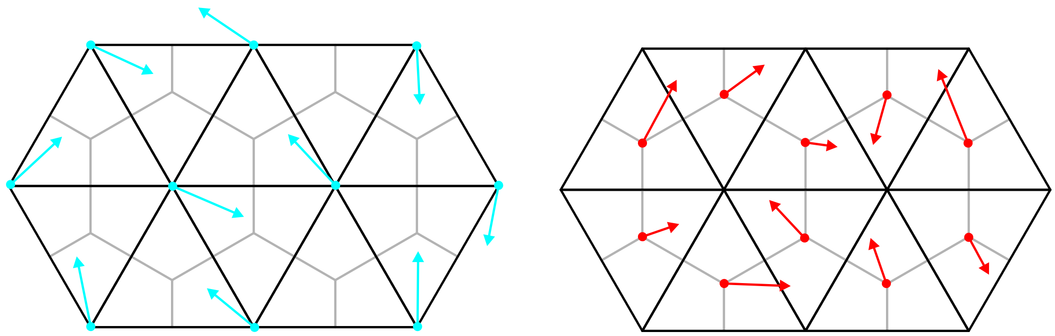
With the discrete forms, Hodge star, $\mathbf{d}$ and $\boldsymbol{\delta}$ defined so far, we already have enough to do an interesting calculation involving the Laplace–Beltrami operator. But, we will show this calculation in §3.9 after we have introduced discrete divergence operator.

3.7 Maps between 1-Forms and Vector Fields

Just as discrete forms come in two flavors, primal and dual (being linear functionals on primal chains or chains made up of dual cells), discrete vector fields also come in two flavors. Before formally defining primal and dual discrete vector fields, consider the examples illustrated in Figure 3.4. The distinction lies in the choice of basepoints, be they primal or dual vertices, to which we assign vectors.

Definition 3.20. *Let K be a flat simplicial complex, that is, the dimension of K is the same as that of the embedding space. A **primal discrete vector field** X on a flat simplicial complex K is a map from the zero-dimensional primal subcomplex $K^{(0)}$ (i.e., the primal vertices) to $\mathbb{R}^N$. We will denote the space of such vector fields by $\mathfrak{X}_d(K)$. The value of such a vector field is piecewise constant on the dual n-cells of $\star K$. Thus, we could just as well have called such vector fields dual and defined them as functions on the n-cells of $\star K$.*

Definition 3.21. *A **dual discrete vector field** X on a simplicial complex K is a map from the zero-dimensional dual subcomplex $(\star K)^{(0)}$ (i.e, the circumcenters of the primal n simplices) to $\mathbb{R}^N$*



(a) Primal vector field (b) Dual vector field

Figure 3.4: Discrete vector fields.

such that its value on each dual vertex is tangential to the corresponding primal n-simplex. We will denote the space of such vector fields by $\mathfrak{X}_d(\star K)$. The value of such a vector field is piecewise constant on the n-simplices of K. Thus, we could just as well have called such vector fields primal and defined them as functions on the n-simplices of K.

Remark 3.3. *In this paper we have defined the primal vector fields only for flat meshes. We will address the issue of non-flat meshes in separate work.*

As in the smooth exterior calculus, we want to define the flat ($\flat$) and sharp ($\sharp$) operators that relate forms to vector fields. This allows one to write various vector calculus identities in terms of exterior calculus.

Definition 3.22. *Given a simplicial complex K of dimension n, the* ***discrete flat operator on a dual vector field****, $\flat : \mathfrak{X}_d(\star K) \to \Omega^d(K)$, is defined by its evaluation on a primal 1 simplex σ^1,*

$$\langle X^\flat, \sigma^1 \rangle = \sum_{\sigma^n \succ \sigma^1} \frac{|\star \sigma^1 \cap \sigma^n|}{|\star \sigma^1|} X \cdot \vec{\sigma}^1 \,,$$

where $X \cdot \vec{\sigma}^1$ is the usual dot product of vectors in $\mathbb{R}^N$, and $\vec{\sigma}^1$ stands for the vector corresponding to σ^1, and with the same orientation. The sum is over all σ^n containing the edge σ^1. The volume factors are in dimension n.

Definition 3.23. *Given a simplicial complex K of dimension n, the* ***discrete sharp operator on a primal 1-form****, $\sharp : \Omega^d(K) \to \mathfrak{X}_d(\star K)$, is defined by its evaluation on a given vertex v,*

$$\alpha^\sharp(v) = \sum_{[v,\sigma^0]} \langle \alpha, [v, \sigma^0] \rangle \sum_{\sigma^n \succ [v,\sigma^0]} \frac{|\star v \cap \sigma^n|}{|\sigma^n|} \hat{n}_{[v,\sigma^0]} \,,$$

where the outer sum is over all 1*-simplices containing the vertex* v*, and the inner sum is over all* n*-simplices containing the* 1*-simplex* $[v, \sigma^0]$*. The volume factors are in dimension* n*, and the vector* $\hat{n}_{[v,\sigma^0]}$ *is the normal vector to the simplex* $[v, \sigma^0]$*, pointing into the* n*-simplex* σ^n*.*

For a discussion of the proliferation of discrete sharp and flat operators that arise from considering the interpolation of differential forms and vector fields, please see Hirani [2003].

3.8 Wedge Product

As in the smooth case, the wedge product we will construct is a way to build higher degree forms from lower degree ones. For information about the smooth case, see the first few pages of Chapter 6 of Abraham et al. [1988].

Definition 3.24. *Given a primal discrete* k*-form* $\alpha^k \in \Omega_d^k(K)$*, and a primal discrete* l*-form* $\beta^l \in \Omega_d^l(K)$*, the* ***discrete primal-primal wedge product****,* $\wedge : \Omega_d^k(K) \times \Omega_d^l(K) \to \Omega_d^{k+l}(K)$*, defined by the evaluation on a* $(k+l)$*-simplex* $\sigma^{k+l} = [v_0, \ldots, v_{k+l}]$ *is given by*

$$\langle \alpha^k \wedge \beta^l, \sigma^{k+l} \rangle = \frac{1}{(k+l)!} \sum_{\tau \in S_{k+l+1}} \operatorname{sign}(\tau) \frac{|\sigma^{k+l} \cap \star v_{\tau(k)}|}{|\sigma^{k+l}|} \alpha \smile \beta(\tau(\sigma^{k+l})) \,,$$

where S_{k+l+1} *is the permutation group, and its elements are thought of as permutations of the numbers* $0, \ldots, k+l+1$*. The notation* $\tau(\sigma^{k+l})$ *stands for the simplex* $[v_{\tau(0)}, \ldots, v_{\tau(k+l)}]$*. Finally, the notation* $\alpha \smile \beta(\tau(\sigma^{k+l}))$ *is borrowed from algebraic topology (see, for example, page 206 of Hatcher [2001]) and is defined as*

$$\alpha \smile \beta(\tau(\sigma^{k+l})) := \langle \alpha, \left[v_{\tau(0)}, \ldots, v_{\tau(k)}\right] \rangle \langle \beta, \left[v_{\tau(k)}, \ldots, v_{\tau(k+l)}\right] \rangle \,.$$

Example 3.7. *When we take the wedge product of two discrete* 1*-forms, we obtain terms in the sum that are graphically represented in Figure 3.5.*

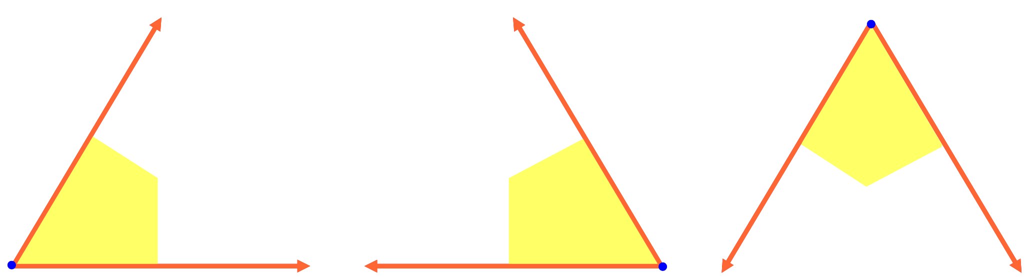


Figure 3.5: Terms in the wedge product of two discrete 1-forms.

Definition 3.25. *Given a dual discrete k-form $\hat{\alpha}^k \in \Omega_d^k(\star K)$, and a primal discrete l-form $\hat{\beta}^l \in \Omega_d^l(\star K)$, the **discrete dual-dual wedge product**, $\wedge : \Omega_d^k(\star K) \times \Omega_d^l(\star K) \to \Omega_d^{k+l}(\star K)$, defined by the evaluation on a $(k+l)$-cell $\hat{\sigma}^{k+l} = \star\sigma^{n-k-l}$, is given by*

$$\begin{aligned}\langle \hat{\alpha}^k \wedge \hat{\beta}^l, \hat{\sigma}^{k+l}\rangle =& \langle \hat{\alpha}^k \wedge \hat{\beta}^l, \star\sigma^{n-k-l}\rangle \\ &= \sum_{\sigma^n \succ \sigma^{n-k-l}} \operatorname{sign}(\sigma^{n-k-l}, [v_{k+l}, \dots, v_n]) \sum_{\tau \in S_{k+l}} \operatorname{sign}(\tau) \\ &\quad \cdot \langle \hat{\alpha}^k, \star[v_{\tau(0)}, \dots, v_{\tau(l-1)}, v_{k+l}, \dots, v_n]\rangle \langle \hat{\beta}^l, \star[v_{\tau(l)}, \dots, v_{\tau(k+l-1)}, v_{k+l}, \dots, v_n]\rangle\end{aligned}$$

where $\sigma^n = [v_0, \dots, v_n]$, and, without loss of generality, assumed that $\sigma^{n-k-l} = \pm[v_{k+l}, \dots, v_n]$.

Anti-Commutativity of the Wedge Product.

Lemma 3.2. *The discrete wedge product, $\wedge : C^k(K) \times C^l(K) \to C^{k+l}(K)$, is anti-commutative, i.e.,*

$$\alpha^k \wedge \beta^k = (-1)^{kl} \beta^l \wedge \alpha^k .$$

Proof. We first rewrite the expression for the discrete wedge product using the following computation,

$$\begin{aligned}&\sum_{\bar{\tau} \in S_{k+l+1}} \operatorname{sign}(\bar{\tau}) |\sigma^{k+l} \cap \star v_{\bar{\tau}(k)}| \langle \alpha^k, \bar{\tau}[v_0, \dots, v_k]\rangle \beta^l, \bar{\tau}[v_k, \dots, v_{k+l}]\rangle \\ &\quad = \sum_{\bar{\tau} \in S_{k+l+1}} (-1)^{k-1} \operatorname{sign}(\bar{\tau}) |\sigma^{k+l} \cap \star v_{\bar{\tau}(k)}| \ \langle \alpha^k, \bar{\tau}[v_1, \dots, v_0, v_k]\rangle \langle \beta^l, \bar{\tau}[v_k, \dots, v_{k+l}]\rangle \\ &\quad = \sum_{\bar{\tau} \in S_{k+l+1}} (-1)^{k-1} \operatorname{sign}(\bar{\tau}) |\sigma^{k+l} \cap \star v_{\bar{\tau}\rho(0)}| \langle \alpha^k, \bar{\tau}\rho[v_1, \dots, v_k, v_0]\rangle \langle \beta^l, \bar{\tau}\rho[v_0, v_{k+1}, \dots, v_{k+l}]\rangle \\ &\quad = \sum_{\bar{\tau} \in S_{k+l+1}} (-1)^{k-1}(-1)^k \operatorname{sign}(\bar{\tau}) |\sigma^{k+l} \cap \star v_{\bar{\tau}\rho(0)}| \langle \alpha^k, \bar{\tau}\rho[v_0, \dots, v_k]\rangle \langle \beta^l, \bar{\tau}\rho[v_0, v_{k+1}, \dots, v_{k+l}]\rangle \\ &\quad = \sum_{\bar{\tau}\rho \in S_{k+l+1}\rho} (-1)^{k-1}(-1)^k(-1) \operatorname{sign}(\bar{\tau}\rho) |\sigma^{k+l} \cap \star v_{\bar{\tau}\rho(0)}| \\ &\qquad\qquad \cdot \langle \alpha^k, \bar{\tau}\rho[v_0, \dots, v_k]\rangle \langle \beta^l, \bar{\tau}\rho[v_0, v_{k+1}, \dots, v_{k+l}]\rangle \\ &\quad = \sum_{\tau \in S_{k+l+1}} \operatorname{sign}(\tau) |\sigma^{k+l} \cap \star v_{\tau(0)}| \langle \alpha^k, \tau[v_0, \dots, v_k]\rangle \langle \beta^l, \tau[v_0, v_{k+1}, \dots, v_{k+l}]\rangle .\end{aligned}$$

Here, we used the elementary fact, from permutation group theory, that a $k+1$ cycle can be written as the product of k transpositions, which accounts for the $(-1)^k$ factors. Also, ρ is a transposition of 0 and k. Then, the discrete wedge product can be rewritten as

$$\langle \alpha^k \wedge \beta^l, \sigma^{k+l} \rangle = \frac{1}{(k+l)!} \sum_{\tau \in S_{k+l+1}} \operatorname{sign}(\tau) \frac{|\sigma^{k+l} \cap \star v_{\tau(0)}|}{|\sigma^{k+l}|} \cdot \langle \alpha^k, [v_{\tau(0)}, \ldots, v_{\tau(k)}] \rangle \langle \beta^l, [v_{\tau(0),\tau(k+1)}, \ldots, v_{\tau(k+l)}] \rangle.$$

For ease of notation, we denote $[v_0, \ldots, v_k]$ by σ^k, and $[v_0, v_{k+1}, \ldots, v_{k+l}]$ by σ^l. Then, we have

$$\langle \alpha^k \wedge \beta^l, \sigma^{k+l} \rangle = \frac{1}{(k+l)!} \sum_{\tau \in S_{k+l+1}} \operatorname{sign}(\tau) \frac{|\sigma^{k+l} \cap \star v_{\tau(0)}|}{|\sigma^{k+l}|} \langle \alpha^k, \tau(\sigma^k) \rangle \langle \beta^l, \tau(\sigma^l) \rangle.$$

Furthermore, we denote $[v_0, v_{l+1} \ldots, v_{k+l}]$ by $\bar{\sigma}^k$, and $[v_0, v_1, \ldots, v_l]$ by $\bar{\sigma}^l$. Then,

$$\langle \beta^l \wedge \alpha^k, \sigma^{k+l} \rangle = \frac{1}{(k+l)!} \sum_{\bar{\tau} \in S_{k+l+1}} \operatorname{sign}(\bar{\tau}) \frac{|\sigma^{k+l} \cap \star v_{\bar{\tau}(0)}|}{|\sigma^{k+l}|} \langle \alpha^k, \bar{\tau}(\bar{\sigma}^k) \rangle \langle \beta^l, \bar{\tau}(\bar{\sigma}^l) \rangle.$$

Consider the permutation $\theta \in S_{k+l+1}$, given by

$$\theta = \begin{pmatrix} 0 & 1 & \ldots & k & k+1 & \ldots & k+l \\ 0 & l+1 & \ldots & k+l & 1 & \ldots & l \end{pmatrix},$$

which has the property that

$$\begin{aligned} \bar{\sigma}^k &= \theta(\sigma^k), \\ \bar{\sigma}^l &= \theta(\sigma^l). \end{aligned}$$

Then, we have

$$\begin{aligned} \langle \beta^l \wedge \alpha^k, \sigma^{k+l} \rangle &= \frac{1}{(k+l)!} \sum_{\bar{\tau} \in S_{k+l+1}} \operatorname{sign}(\bar{\tau}) \frac{|\sigma^{k+l} \cap \star v_{\bar{\tau}(0)}|}{|\sigma^{k+l}|} \langle \alpha^k, \bar{\tau}(\bar{\sigma}^k) \rangle \langle \beta^l, \bar{\tau}(\bar{\sigma}^l) \rangle \\ &= \frac{1}{(k+l)!} \sum_{\bar{\tau} \in S_{k+l+1}} \operatorname{sign}(\bar{\tau}) \frac{|\sigma^{k+l} \cap \star v_{\bar{\tau}\theta(0)}|}{|\sigma^{k+l}|} \langle \alpha^k, \bar{\tau}\theta(\sigma^k) \rangle \langle \beta^l \bar{\tau}\theta(\sigma^l) \rangle \\ &= \frac{1}{(k+l)!} \sum_{\bar{\tau}\theta \in S_{k+l+1}\theta} \operatorname{sign}(\bar{\tau}\theta) \operatorname{sign}(\theta) \frac{|\sigma^{k+l} \cap \star v_{\bar{\tau}\theta(0)}|}{|\sigma^{k+l}|} \langle \alpha^k, \bar{\tau}\theta(\sigma^k) \rangle \langle \beta^l, \bar{\tau}\theta(\sigma^l) \rangle. \end{aligned}$$

By making the substitution, $\tau = \bar{\tau}\theta$, and noting that $S_{k+l+1}\theta = S_{k+l+1}$, we obtain

$$\begin{aligned} \langle \beta^l \wedge \alpha^k, \sigma^{k+l} \rangle &= \operatorname{sign}(\theta) \frac{1}{(k+l)!} \sum_{\tau \in S_{k+l+1}} \operatorname{sign}(\tau) \frac{|\sigma^{k+l} \cap \star v_{\tau(0)}|}{|\sigma^{k+l}|} \langle \alpha^k, \tau(\sigma^k) \rangle \langle \beta^l, \tau(\sigma^l) \rangle \\ &= \operatorname{sign}(\theta) \langle \alpha^k \wedge \beta^l, \sigma^{k+l} \rangle. \end{aligned}$$

To obtain the desired result, we simply need to compute the sign of θ, which is given by

$$\operatorname{sign}(\theta) = (-1)^{kl}.$$

This follows from the observation that in order to move each of the last l vertices of σ^{k+l} forward, we require k transpositions with $v_1, \ldots, v_k$. Therefore, we obtain

$$\langle \beta^l \wedge \alpha^k, \sigma^{k+l} \rangle = \operatorname{sign}(\theta) \langle \alpha^k \wedge \beta^l, \sigma^{k+l} \rangle = (-1)^{kl} \langle \alpha^k \wedge \beta^l, \sigma^{k+l} \rangle,$$

and

$$\alpha^k \wedge \beta^l = (-1)^{kl} \beta^l \wedge \alpha^k. \qquad \square$$

Leibniz Rule for the Wedge Product.

Lemma 3.3. *The discrete wedge product satisfies the Leibniz rule,*

$$\mathbf{d}(\alpha^k \wedge \beta^l) = (\mathbf{d}\alpha^k) \wedge \beta^l + (-1)^k \alpha^k \wedge (\mathbf{d}\beta^l).$$

Proof. The proof of the Leibniz rule for discrete wedge products is directly analogous to the proof of the coboundary formula for the simplicial cup product on cochains, which can be found on page 206 of Hatcher [2001]. This is because the discrete exterior derivative is precisely the coboundary operator, and the wedge product is constructed out of weighted sums of cup products.

The cup product satisfies the Leibniz rule for an given partial ordering of the vertices, and the permutations in the signed sum in the discrete wedge product correspond to different choices of partial ordering. We then obtain the Leibniz rule for the discrete wedge product by applying it term-wise for each choice of permutation.

Consider

$$\begin{aligned}\langle (\mathbf{d}\alpha^k) \wedge \beta^l, \sigma^{k+l+1} \rangle = \sum_{i=0}^{k+1} (-1)^i \frac{1}{(k+l)!} \sum_{\tau \in S_{k+l+1}} \operatorname{sign}(\tau) \frac{|\sigma^{k+l} \cap \star v_{\tau(0)}|}{|\sigma^{k+l}|} \\ \cdot \langle \alpha^k, [v_{\tau(0)}, \ldots, \hat{v}_i, \ldots, v_{\tau(k+1)}] \rangle \langle \beta^l, [v_{\tau(k+1)}, \ldots, v_{\tau(k+l+1)}] \rangle,\end{aligned}$$

and

$$\begin{aligned}(-1)^k \langle \alpha^k \wedge (\mathbf{d}\beta^l), \sigma^{k+l+1} \rangle = (-1)^k \sum_{i=k}^{k+l+1} (-1)^{i-k} \frac{1}{(k+l)!} \sum_{\tau \in S_{k+l+1}} \operatorname{sign}(\tau) \frac{|\sigma^{k+l} \cap \star v_{\tau(0)}|}{|\sigma^{k+l}|} \\ \cdot \langle \alpha^k, [v_{\tau(0)}, \ldots, v_{\tau(k)}] \rangle \langle \beta^l, [v_{\tau(k)}, \ldots, \hat{v}_i, \ldots, v_{\tau(k+l+1)}] \rangle.\end{aligned}$$

The last set of terms, $i = k+1$, of the first expression cancels the first set of terms, $i = k$, of the second expression, and what remains is simply $\langle \alpha^k \wedge \beta^l, \partial\sigma^{k+l+1}\rangle$. Therefore, we can conclude that

$$\langle (\mathbf{d}\alpha^k) \wedge \beta^l, \sigma^{k+l+1}\rangle + (-1)^k \langle \alpha^k \wedge (\mathbf{d}\beta^l), \sigma^{k+l+1}\rangle = \langle \alpha^k \wedge \beta^l, \partial\sigma^{k+l+1}\rangle = \langle \mathbf{d}(\alpha^k \wedge \beta^l), \sigma^{k+l+1}\rangle,$$

or simply that the Leibniz rule for discrete differential forms holds,

$$\mathbf{d}(\alpha^k \wedge \beta^l) = (\mathbf{d}\alpha^k) \wedge \beta^l + (-1)^k \alpha^k \wedge (\mathbf{d}\beta^l). \qquad \square$$

Associativity for the Wedge Product. The discrete wedge product which we have introduced is not associative in general. This is a consequence of the fact that the stencil for the two possible triple wedge products are not the same. In the expression for $\langle \alpha^k \wedge (\beta^l \wedge \gamma^m), \sigma^{k+l+m}\rangle$, each term in the double summation consists of a geometric factor multiplied by $\langle \alpha^k, \sigma^k\rangle\langle \beta^l, \sigma^l\rangle\langle \gamma^m, \sigma^m\rangle$ for some k, l, m simplices $\sigma^k, \sigma^l, \sigma^m$.

Since β^l and γ^m are wedged together first, σ^l and σ^m will always share a common vertex, but σ^k could have a vertex in common with only σ^l, or only σ^m, or both. We can represent this in a graph, where the nodes denote the three simplices, which are connected by an edge if, and only if, they share a common vertex. The graphical representation of the terms which arise in the two possible triple wedge products are given in Figure 3.6.

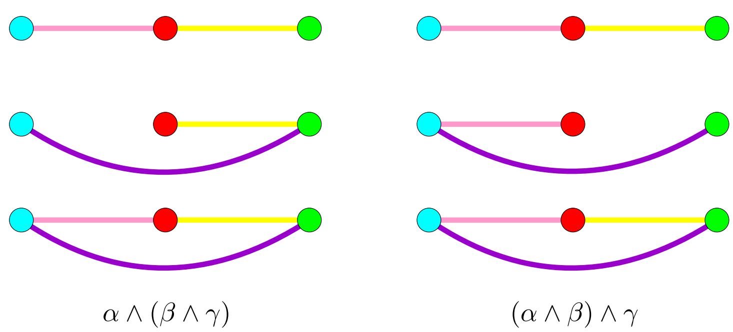


Figure 3.6: Stencils arising in the double summation for the two triple wedge products.

For the wedge product to be associative for all forms, the two stencils must agree. Since the stencils for the two possible triple wedge products differ, the wedge product is not associative in general. However, in the case of closed forms, we can rewrite the terms in the sum so that all the discrete forms are evaluated on triples of simplices that share a common vertex. This is illustrated graphically in Figure 3.7.

This result is proved rigorously in the follow lemma.

Lemma 3.4. *The discrete wedge product is associative for closed forms. That is to say, for* $\alpha^k \in$

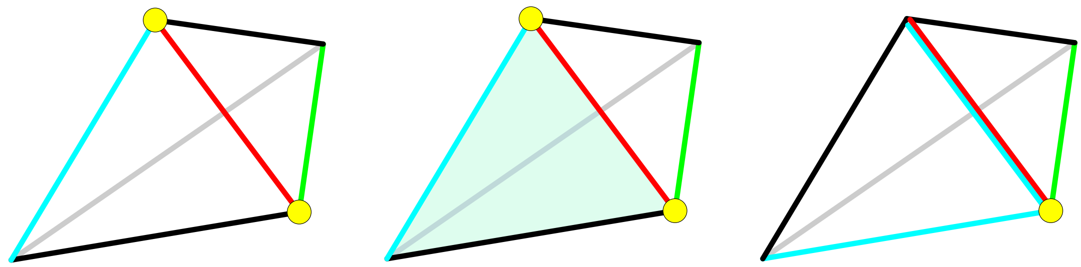


Figure 3.7: Associativity for closed forms.

$C^k(K)$, $\beta^l \in C^l(K)$, $\gamma^m \in C^m(K)$, *such that* $\mathbf{d}\alpha^k = 0$, $\mathbf{d}\beta^l = 0$, $\mathbf{d}\gamma^m = 0$, *we have that*

$$(\alpha^k \wedge \beta^l) \wedge \gamma^m = \alpha^k \wedge (\beta^l \wedge \gamma^m).$$

Proof.

$$\begin{aligned}
&\langle (\alpha^k \wedge \beta^l) \wedge \gamma^m, \sigma^{k+l+m} \rangle \\
&\quad = \sum_{\tau \in S_{k+l+m+1}} \operatorname{sign}(\tau) \langle \alpha^k \wedge \beta^l, \tau[v_0, \ldots, v_{k+l}] \rangle \langle \gamma^m, \tau[v_{k+l}, \ldots, v_{k+l+m}] \rangle \\
&\quad = \sum_{\tau \in S_{k+l+m+1}} \sum_{\rho \in S_{k+l+1}} \operatorname{sign}(\tau) \operatorname{sign}(\rho) \langle \alpha^k, \rho\tau[v_0, \ldots, v_k] \rangle \\
&\qquad\qquad \cdot \langle \beta^l, \rho\tau[v_k, \ldots, v_{k+l}] \rangle \langle \gamma^m, \tau[v_{k+l}, \ldots, v_{k+l+m}] \rangle
\end{aligned}$$

Here, either $\rho\tau(k) = \tau(k+l)$, in which case all three permuted simplices share $v_{\tau(k+l)}$ as a common vertex, or we need to rewrite either $\langle \alpha^k, \rho\tau[v_0, \ldots, v_k] \rangle$ or $\langle \beta^l, \rho\tau[v_k, \ldots, v_{k+l}] \rangle$, using the fact that α^k and β^l are closed forms.

If $v_{\tau(k+l)} \notin \rho\tau[v_0, \ldots, v_k]$, then we need to rewrite $\langle \alpha^k, \rho\tau[v_0, \ldots, v_k] \rangle$ by considering the simplex obtained by adding the vertex $v_{\tau(k+l)}$ to $\rho\tau[v_0, \ldots, v_k]$, which is $[v_{\tau(k+l)}, v_{\rho\tau(0)}, \ldots, v_{\rho\tau(k)}]$. Then, since α^k is closed, we have that

$$\begin{aligned}
0 &= \langle \mathbf{d}\alpha^k, [v_{\tau(k+l)}, v_{\rho\tau(0)}, \ldots, v_{\rho\tau(k)}] \rangle \\
&= \langle \alpha^k, \partial[v_{\tau(k+l)}, v_{\rho\tau(0)}, \ldots, v_{\rho\tau(k)}] \rangle \\
&= \langle \alpha^k, [v_{\rho\tau(0)}, \ldots, v_{\rho\tau(k)}] \rangle - \sum_{i=0}^{k} (-1)^i \langle \alpha^k, [v_{\tau(k+l)}, v_{\rho\tau(0)}, \ldots, \hat{v}_{\rho\tau(i)}, \ldots, v_{\rho\tau(k)}] \rangle
\end{aligned}$$

or equivalently,

$$\langle \alpha^k, [v_{\rho\tau(0)}, \ldots, v_{\rho\tau(k)}] \rangle = \sum_{i=0}^{k} (-1)^i \langle \alpha^k, [v_{\tau(k+l)}, v_{\rho\tau(0)}, \ldots, \hat{v}_{\rho\tau(i)}, \ldots, v_{\rho\tau(k)}] \rangle.$$

Notice that all the simplices in the sum, with the exception of the last one, will share two vertices, $v_{\tau(k+l)}$ and $v_{\rho\tau(k)}$ with $\rho\tau[v_k, \ldots, v_{k+l}]$, and so their contribution in the triple wedge product will vanish due to the anti-symmetrized sum.

Similarly, if $v_{\tau(k+l)} \notin \rho\tau[v_k, \ldots, v_{k+l}]$, using the fact that β^l is closed yields

$$\langle \alpha^k, [v_{\rho\tau(k)}, \ldots, v_{\rho\tau(k+l)}] \rangle = \sum_{i=k}^{k+l} (-1)^{(i-k)} \langle \alpha^k, [v_{\tau(k+l)}, v_{\rho\tau(k)}, \ldots, \hat{v}_{\rho\tau(i)}, \ldots, v_{\rho\tau(k+l)}] \rangle.$$

As before, all the simplices in the sum, with the exception of the last one, will share two vertices, $v_{\tau(k+l)}$ and $v_{\rho\tau(k)}$ with $\rho\tau[v_0, \ldots, v_k]$, and so their contribution in the triple wedge product will vanish due to the anti-symmetrized sum.

This allows us to rewrite the triple wedge product in the case of closed forms as

$$\begin{aligned}\langle (\alpha^k \wedge \beta^l) \wedge \gamma^m, \sigma^{k+l+m} \rangle = \sum_{i=0}^{k+l+m} \sum_{\tau \in S_{k+l+m}} & \operatorname{sign}(\rho_i \tau) \langle \alpha^k, \rho_i \tau[v_0, \ldots, v_k] \rangle \langle \beta^l, \rho_i \tau[v_0, v_{k+1}, \ldots, v_{k+l}] \rangle \\ & \cdot \langle \gamma^m, \rho_i \tau[v_0, v_{k+l+1}, \ldots, v_{k+l+m}] \rangle,\end{aligned}$$

where $\tau \in S_{k+l+m}$ is thought of as acting on the set $\{1, \ldots, k+l+m\}$, and ρ_i is a transposition of 0 and i. A similar argument allows us to write $\alpha^k \wedge (\beta^l \wedge \gamma^m)$ in the same form, and therefore, the wedge product is associative for closed forms. □

Remark 3.4. *This lemma is significant, since if we think of a constant smooth differential form, and discretize it to obtain a discrete differential form, this discrete form will be closed. As such, this lemma states that in the infinitesimal limit, the discrete wedge product we have defined will be associative.*

In practice, if we have a mesh with characteristic length Δx, then we will have that

$$\frac{1}{|\sigma^{k+l+m}|} \langle \alpha^k \wedge (\beta^l \wedge \gamma^m) - (\alpha^k \wedge \beta^l) \wedge \gamma^m, \sigma^{k+l+m} \rangle = \mathcal{O}(\Delta x),$$

which is to say that the average of the associativity defect is of the order of the mesh size, and therefore vanishes in the infinitesimal limit.

3.9 Divergence and Laplace–Beltrami

In this section, we will illustrate the application of some of the DEC operations we have previously defined to the construction of new discrete operators such as the divergence and Laplace–Beltrami operators.

Divergence. The divergence of a vector field is given in terms of the Lie derivative of the volume-form, by the expression, $(\mathrm{div}(\mathbf{X})\mu = \pounds_{\mathbf{X}}\mu$. Physically, this corresponds to the net flow per unit volume of an infinitesimal volume about a point.

We will define the discrete divergence by using the formulas defining them in the smooth exterior calculus. The divergence definition will be valid for arbitrary dimensions. The resulting expressions involve operators that we have already defined and so we can actually perform some calculations to express these quantities in terms of geometric quantities. We will show that the resulting expression in terms of geometric quantities is the same as that derived by variational means in Tong et al. [2003].

Definition 3.26. *For a discrete dual vector field X the divergence* $\mathrm{div}(X)$ *is defined to be*

$$\mathrm{div}(\mathbf{X}) = -\boldsymbol{\delta} X^\flat .$$

Remark 3.5. *The above definition is a theorem in smooth exterior calculus. See, for example, page 458 of Abraham et al. [1988].*

As an example, we will now compute the divergence of a discrete dual vector field on a two-dimensional simplicial complex K, as illustrated in Figure 3.8.

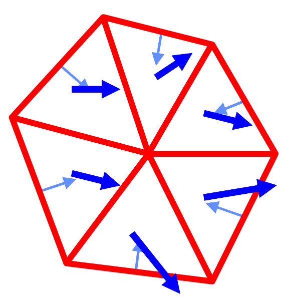


Figure 3.8: Divergence of a discrete dual vector field.

A similar derivation works in higher dimensions, where one needs to be mindful of the sign that arises from applying the Hodge star twice, $**\alpha^k = (-1)^{k(n-k)}\alpha^k$. Since $\mathrm{div}(X) = -\boldsymbol{\delta} X^\flat$, it follows that $\mathrm{div}(X) = *\mathbf{d} * X^\flat$. Since this is a primal 0-form it can be evaluated on a 0-simplex σ^0, and we have that

$$\langle \mathrm{div}(x), \sigma^0 \rangle = \langle *\mathbf{d} * X^\flat, \sigma^0 \rangle .$$

Using the definition of discrete Hodge star, and the discrete generalized Stokes' theorem, we get

$$\begin{aligned}
\frac{1}{|\sigma^0|}\langle \mathrm{div}(X), \sigma^0 \rangle &= \frac{1}{|\star\sigma^0|}\langle * * \mathbf{d} * X^\flat, \star\sigma^0 \rangle \\
&= \frac{1}{|\star\sigma^0|}\langle \mathbf{d} * X^\flat, \star\sigma^0 \rangle \\
&= \frac{1}{|\star\sigma^0|}\langle *X^\flat, \partial(\star\sigma^0) \rangle .
\end{aligned}$$

The second equality is obtained by applying the definition of the Hodge star, and the last equality is obtained by applying the discrete generalized Stokes' theorem. But,

$$\partial(\star\sigma^0) = \sum_{\sigma^1 \succ \sigma^0} \star\sigma^1 ,$$

as given by the expression for the boundary of a dual cell in Equation 3.17. Thus,

$$\begin{aligned}
\frac{1}{|\sigma^0|}\langle \mathrm{div}(X), \sigma^0 \rangle &= \frac{1}{|\star\sigma^0|}\langle *X^\flat, \sum_{\sigma^1 \succ \sigma^0} \star\sigma^1 \rangle \\
&= \frac{1}{|\star\sigma^0|} \sum_{\sigma^1 \succ \sigma^0} \langle *X^\flat, \star\sigma^1 \rangle \\
&= \frac{1}{|\star\sigma^0|} \sum_{\sigma^1 \succ \sigma^0} \frac{|\star\sigma^1|}{|\sigma^1|} \langle X^\flat, \sigma^1 \rangle \\
&= \frac{1}{|\star\sigma^0|} \sum_{\sigma^1 \succ \sigma^0} \frac{|\star\sigma^1|}{|\sigma^1|} \sum_{\sigma^2 \succ \sigma^1} \frac{|\star\sigma^1 \cap \sigma^2|}{|\star\sigma^1|} X \cdot \vec{\sigma}^1 \\
&= \frac{1}{|\star\sigma^0|} \sum_{\sigma^1 \succ \sigma^0} \sum_{\sigma^2 \succ \sigma^1} \frac{|\star\sigma^1 \cap \sigma^2|}{|\sigma^1|} X \cdot \vec{\sigma}^1 \\
&= \frac{1}{|\star\sigma^0|} \sum_{\sigma^1 \succ \sigma^0} |\star\sigma^1 \cap \sigma^2| \, (X \cdot \frac{\vec{\sigma}^1}{|\sigma^1|}) .
\end{aligned}$$

This expression has the nice property that the divergence theorem holds on any dual n-chain, which, as a set, is a simply connected subset of $|K|$. Furthermore, the coefficients we computed for the discrete divergence operator are the unique ones for which a discrete divergence theorem holds.

Laplace–Beltrami. The Laplace–Beltrami operator is the generalization of the Laplacian to curved spaces. In the smooth case the Laplace–Beltrami operator on smooth functions is defined to be $\nabla^2 = \mathrm{div} \circ \mathrm{curl} = \boldsymbol{\delta} d$. See, for example, page 459 of Abraham et al. [1988]. Thus, in the smooth case, the Laplace–Beltrami on functions is a special case of the more general Laplace–deRham operator, $\Delta : \Omega^k(M) \to \Omega^k(M)$, defined by $\Delta = \mathbf{d}\boldsymbol{\delta} + \boldsymbol{\delta}\mathbf{d}$.

As an example, we compute Δf on a primal vertex σ^0, where $f \in \Omega_d^0(K)$, and K is a (not necessarily flat) triangle mesh in $\mathbb{R}^3$, as illustrated in Figure 3.9.

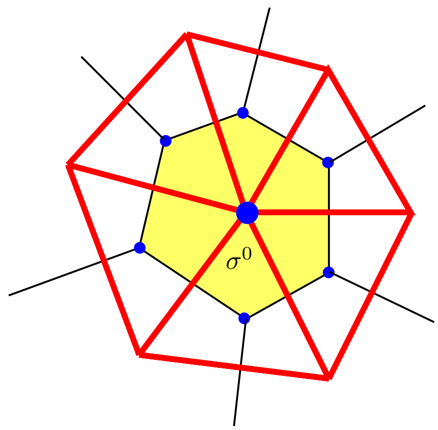


Figure 3.9: Laplace–Beltrami of a discrete function.

This calculation is done below.

$$
\begin{aligned}
\frac{1}{|\sigma^0|}\langle \Delta f, \sigma^0\rangle &= \langle \boldsymbol{\delta}\mathbf{d} f, \sigma^0\rangle \\
&= -\langle * \mathbf{d} * \mathbf{d} f, \sigma^0\rangle \\
&= -\frac{1}{|\star\sigma^0|}\langle \mathbf{d} * \mathbf{d} f, \star\sigma^0\rangle \\
&= -\frac{1}{|\star\sigma^0|}\langle * \mathbf{d} f, \partial(\star\sigma^0)\rangle \\
&= -\frac{1}{|\star\sigma^0|}\langle * \mathbf{d} f, \sum_{\sigma^1 \succ \sigma^0} \star\sigma^1\rangle \\
&= -\frac{1}{|\star\sigma^0|}\sum_{\sigma^1 \succ \sigma^0}\langle * \mathbf{d} f, \star\sigma^1\rangle \\
&= -\frac{1}{|\star\sigma^0|}\sum_{\sigma^1 \succ \sigma^0}\frac{|\star\sigma^1|}{|\sigma^1|}\langle \mathbf{d} f, \sigma^1\rangle \\
&= -\frac{1}{|\star\sigma^0|}\sum_{\sigma^1 \succ \sigma^0}\frac{|\star\sigma^1|}{|\sigma^1|}\left(f(v) - f(\sigma^0)\right),
\end{aligned}
$$

where $\partial\sigma^1 = v - \sigma^0$. But, the above is the same as the formula involving cotangents found by Meyer et al. [2002] without using discrete exterior calculus.

Another interesting aspect, which will be discussed in §3.12, is that the characterization of harmonic functions as those functions which vanish when the Laplace–Beltrami operator is applied is equivalent to that obtained from a discrete variational principle using DEC as the means of discretizing the Lagrangian.

3.10 Contraction and Lie Derivative

In this section we will discuss some more operators that involve vector fields, namely contraction, and Lie derivatives.

For contraction, we will first define the usual smooth contraction algebraically, by relating it to Hodge star and wedge products. This yields one potential approach to defining discrete contraction. However, since in the discrete theory we are only concerned with integrals of forms, we can use the interesting notion of extrusion of a manifold by the flow of a vector field to define the integral of a contracted discrete differential form.

We learned about this definition of contraction via extrusion from Bossavit [2002b], who goes on to define discrete extrusion in his paper. Thus, he is able to obtain a definition of discrete contraction. Extrusion turns out to be a very nice way to define integrals of operators involving vector fields, and we will show how to define integrals of Lie derivatives via extrusion, which will yield discrete Lie derivatives.

Definition 3.27. *Given a manifold M, and S, a k-dimensional submanifold of M, and a vector field $X \in \mathfrak{X}(M)$, we call the manifold obtained by sweeping S along the flow of X for time t as the* ***extrusion*** *of S by X for time t, and denote it by $E_X^t(S)$. The manifold S carried by the* ***flow*** *for time t will be denoted $\varphi_X^t(S)$.*

Example 3.8. *Figure 3.10 illustrates the 2-simplex that arises from the extrusion of a 1-simplex by a discrete vector field that is interpolated using a linear shape function.*

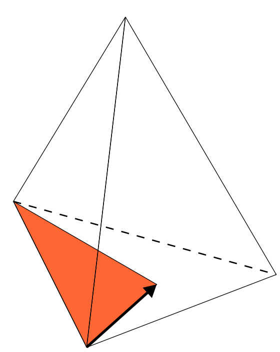


Figure 3.10: Extrusion of 1-simplex by a discrete vector field.

Contraction (Extrusion). We first establish an integral property of the contraction operator.

Lemma 3.5.

$$\int_S \mathbf{i}_X \beta = \left.\frac{d}{dt}\right|_{t=0} \int_{E_X^t(S)} \beta$$

Proof. Prove instead that

$$\int_0^t \left[\int_{S_\tau} \mathbf{i}_X \beta \right] d\tau = \int_{E_X^t(S)} \beta \, .$$

Then, by first fundamental theorem of calculus, the desired result will follow. To prove the above, simply take coordinates on S and carry them along with the flow and define the transversal coordinate to be the flow of X. This proof is sketched in Bossavit [2002b]. □

This lemma allows us to interpret contraction as being the dual, under the integration pairing between k-forms and k-volumes, to the geometric operation of extrusion. The discrete contraction operator is then given by

$$\langle \mathbf{i}_X \alpha^{k+1}, \sigma^k \rangle = \left.\frac{d}{dt}\right|_{t=0} \langle \alpha^{k+1}, E_X^t(\sigma^k) \rangle,$$

where the evaluation of the RHS will typically require that the discrete differential form and the discrete vector field are appropriately interpolated.

Remark 3.6. *Since the dynamic definition of the contraction operator only depends on the derivative of pairing of the differential form with the extruded region, it will only depend on the vector field in the region S, and not on its extension into the rest of the domain.*

In addition, if the interpolation for the discrete vector field satisfies a superposition principle, then the discrete contraction operator will satisfy a corresponding superposition principle.

Contraction (Algebraic). Contraction is an operator that allows one to combine vector fields and forms. For a smooth manifold M, the contraction of a vector field $X \in \mathfrak{X}(M)$ with a $(k+1)$-form $\alpha \in \Omega^{k+1}(M)$ is written as $\mathbf{i}_X \alpha$, and for vector fields $X_1, \ldots, X_k \in \mathfrak{X}(M)$, the contraction in smooth exterior calculus is defined by

$$\mathbf{i}_X \alpha(X_1, \ldots, X_k) = \alpha(X, X_1, \ldots, X_k) \, .$$

We define contraction by using an identity that is true in smooth exterior calculus. This identity originally appeared in Hirani [2003], and we state it here with proof.

Lemma 3.6 (Hirani [2003]). *Given a smooth manifold M of dimension n, a vector field $X \in \mathfrak{X}(M)$, and a k-form $\alpha \in \Omega^k(M)$, we have that*

$$\mathbf{i}_X \alpha = (-1)^{k(n-k)} * (*\alpha \wedge X^\flat) \, .$$

Proof. Recall that for a smooth function $f \in \Omega^0(M)$, we have that $\mathbf{i}_X\alpha = f\mathbf{i}_X\alpha$. This, and the multilinearity of α, implies that it is enough to show the result in terms of basis elements. In particular, let $\tau \in S_n$ be a permutation of the numbers $1,\ldots n$, such that $\tau(1) < \ldots < \tau(k)$, and $\tau(k+1) < \ldots < \tau(n)$. Let $X = e_{\tau(j)}$, for some $j \in 1,\ldots,n$. Then, we have to show that

$$\mathbf{i}_{e_{\tau(j)}} e^{\tau(1)} \wedge \ldots \wedge e^{\tau(k)} = (-1)^{k(n-k)} * (*(e^{\tau(1)} \wedge \ldots \wedge e^{\tau(k)}) \wedge e^{\tau(j)}) .$$

It is easy to see that the LHS is 0 if $j > k$, and it is

$$(-1)^{j-1}(e^{\tau(1)} \wedge \ldots \wedge \widehat{e^{\tau(j)}} \ldots \wedge e^{\sigma(k)}) ,$$

otherwise, where $\widehat{e^{\tau(j)}}$ means that $e^{\tau(j)}$ is omitted from the wedge product. Now, on the RHS of Equation 3.6, we have that

$$*(e^{\tau(1)} \wedge \ldots \wedge e^{\tau(k)}) = \operatorname{sign}(\tau)(e^{\tau(k+1)} \wedge \ldots \wedge e^{\tau(n)}) .$$

Thus, the RHS is equal to

$$(-1)^{k(n-k)} \operatorname{sign}(\tau) * (e^{\tau(k+1)} \wedge \ldots \wedge e^{\tau(n)} \wedge e^{\tau(j)}) ,$$

which is 0 as required if $j > k$. So, assume that $1 \leq j \leq k$. We need to compute

$$*(e^{\tau(k+1)} \wedge \ldots \wedge e^{\tau(n)} \wedge e^{\tau(j)}) ,$$

which is given by

$$s\, e^{\tau(1)} \wedge \ldots \widehat{e^{\tau(j)}} \wedge \ldots \wedge e^{\tau(k)} ,$$

where the sign $s = \pm 1$, such that the equation,

$$s\, e^{\tau(k+1)} \wedge \ldots \wedge e^{\tau(n)} \wedge e^{\tau(j)} \wedge e^{\tau(1)} \wedge \ldots \wedge \widehat{e^{\tau(j)}} \wedge \ldots \wedge e^{\tau(k)} = \mu ,$$

holds for the standard volume-form, $\mu = e^1 \wedge \ldots \wedge e^n$. This implies that

$$s = (-1)^{j-1}(-1)^{k(n-k)} \operatorname{sign}(\tau) .$$

Then, RHS = LHS as required. ∎

Since we have expressions for the discrete Hodge star ($*$), wedge product ($\wedge$), and flat ($\flat$), we have the necessary ingredients to use the algebraic expression proved in the above lemma to construct a discrete contraction operator.

One has to note, however, that the wedge product is only associative for closed forms, and as a consequence, the Leibniz rule for the resulting contraction operator will only hold for closed forms as well. This is, however, sufficient to establish that the Leibniz rule for the discrete contraction will hold in the limit as the mesh is refined.

Lie Derivative (Extrusion). As was the case with contraction, we will establish a integral identity that allows the Lie derivative to be interpreted as the dual of a geometric operation on a volume. This involves the flow of a volume by a vector field, and it is illustrated in the following example.

Example 3.9. *Figure 3.11 illustrates the flow of a* 1*-simplex by a discrete vector field interpolated using a linear shape function.*

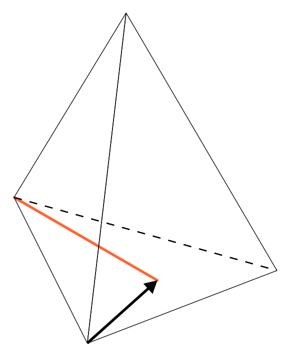


Figure 3.11: Flow of a 1-simplex by a discrete vector field.

Lemma 3.7.

$$\int_S \pounds_X \beta = \left.\frac{d}{dt}\right|_{t=0} \int_{\varphi_X^t(S)} \beta\,.$$

Proof.

$$\begin{aligned} F_t^*(\pounds_X \beta) &= \frac{d}{dt} F_t^* \beta \\ \int_0^t F_\tau^*(\pounds_X \beta) d\tau &= F_t^* \beta - \beta \\ \int_S \int_0^t F_\tau^*(\pounds_X \beta) d\tau &= \int_S F_t^* \beta - \int_S \beta \\ \int_0^t \int_{\varphi_X^\tau(S)} \pounds_X \beta d\tau &= \int_{\varphi_X^t(S)} \beta - \int_S \beta\,. \end{aligned}$$

□

This lemma allows us to define a discrete Lie derivative as follows,

$$\langle \pounds_X \beta^k, \sigma^k \rangle = \left.\frac{d}{dt}\right|_{t=0} \langle \beta^k, \varphi_X^t(\sigma^k) \rangle \,,$$

where, as before, evaluating the RHS will require the discrete differential form and discrete vector field to be appropriately interpolated.

Lie Derivative (Algebraic). Alternatively, as we have expressions for the discrete contraction operator ($\mathbf{i}_X$), and exterior derivative ($\mathbf{d}$), we can construct a discrete Lie derivative using the Cartan magic formula,

$$\pounds_X \omega = \mathbf{i}_X \mathbf{d} \omega + \mathbf{d} \mathbf{i}_X \omega.$$

As is the case with the algebraic definition of the discrete contraction, the discrete Lie derivative will only satisfy a Leibniz rule for closed forms. As before, this is sufficient to establish that the Leibniz rule will hold in the limit as the mesh is refined.

3.11 Discrete Poincaré Lemma

In this section, we will prove the discrete Poincaré lemma by constructing a homotopy operator though a generalized cocone construction. This section is based on the work in Desbrun et al. [2003b].

The standard cocone construction fails at the discrete level, since the cone of a simplex is not, in general, expressible as a chain in the simplicial complex. As such, the standard cocone does not necessarily map k-cochains to $(k-1)$-cochains.

An example of how the standard cone construction fails to map chains to chains is illustrated in Figure 3.12. Given the simplicial complex on the left, consisting of triangles, edges and nodes, we wish, in the center figure, to consider the cone of the bold edge with respect to the top most node. Clearly, the resulting cone in the right figure, which is shaded grey, cannot be expressed as a combination of the triangles in the original complex.

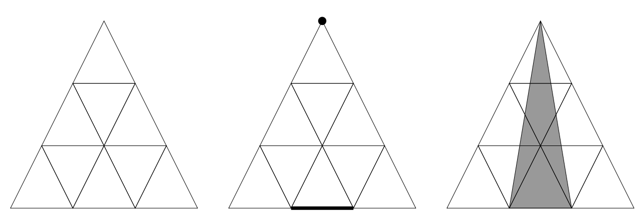


Figure 3.12: The cone of a simplex is, in general, not expressible as a chain.

In this subsection, a generalized cone operator that is valid for chains is developed which has the essential homotopy properties to yield a discrete analogue of the Poincaré lemma.

We will first consider the case of trivially star-shaped complexes, followed by logically star-shaped complexes, before generalizing the result to contractible complexes.

Definition 3.28. *Given a k-simplex $\sigma^k = [v_0, \ldots, v_k]$ we construct the **cone** with vertex w and base σ^k, as follows,*

$$w \diamond \sigma^k = [w, v_0, \ldots, v_k].$$

Lemma 3.8. *The geometric cone operator satisfies the following property,*

$$\partial(w \diamond \sigma^k) + w \diamond (\partial \sigma^k) = \sigma^k.$$

Proof. This is a standard result from simplicial algebraic topology. □

Trivially Star-Shaped Complexes.

Definition 3.29. *A complex K is called **trivially star-shaped** if there exists a vertex $w \in K^{(0)}$, such that for all $\sigma^k \in K$, the cone with vertex w and base σ^k is expressible as a chain in K. That is to say,*

$$\exists w \in K^{(0)} \mid \forall \sigma^k \in K, w \diamond \sigma^k \in C_{k+1}(K).$$

We can then denote the cone operation with respect to w as $p : C_k(K) \to C_{k+1}(K)$.

Lemma 3.9. *In trivially star-shaped complexes, the cone operator, $p : C_k(K) \to C_{k+1}(K)$, satisfies the following identity,*

$$p\partial + \partial p = I,$$

at the level of chains.

Proof. Follows immediately from the identity for cones, and noting that the cone is well-defined at the level of chains on trivially star-shaped complexes. □

Definition 3.30. *The **cocone** operator, $H : C^k(K) \to C^{k-1}(K)$, is defined by*

$$\langle H\alpha^k, \sigma^{k-1} \rangle = \langle \alpha^k, p(\sigma^{k-1}) \rangle.$$

This operator is well-defined on trivially star-shaped simplicial complexes.

Lemma 3.10. *The cocone operator, $H : C^k(K) \to C^{k-1}(K)$, satisfies the following identity,*

$$H\mathbf{d} + \mathbf{d}H = I,$$

at the level of cochains.

Proof. A simple duality argument applied to the cone identity,

$$p\partial + \partial p = I,$$

yields the following,

$$\begin{aligned}\langle \alpha^k, \sigma^k \rangle &= \langle \alpha^k, (p\partial + \partial p)\sigma^k \rangle \\ &= \langle \alpha^k, p\partial\sigma^k \rangle + \langle \alpha^k, \partial p\sigma^k \rangle \\ &= \langle H\alpha^k, \partial\sigma^k \rangle + \langle \mathbf{d}\alpha^k, p\sigma^k \rangle \\ &= \langle (\mathbf{d}H\alpha^k, \sigma^k \rangle + \langle H\mathbf{d}\alpha^k, \sigma^k \rangle \\ &= \langle (\mathbf{d}H + H\mathbf{d})\alpha^k, \sigma^k \rangle.\end{aligned}$$

Therefore,

$$H\mathbf{d} + \mathbf{d}H = I,$$

at the level of cochains. □

Corollary 3.11 (Discrete Poincaré Lemma for Trivially Star-shaped Complexes). *Given a closed cochain α^k, that is to say, $\mathbf{d}\alpha^k = 0$, there exists a cochain β^{k-1}, such that, $\mathbf{d}\beta^{k-1} = \alpha^k$.*

Proof. Applying the identity for cochains,

$$H\mathbf{d} + \mathbf{d}H = I,$$

we have,

$$\langle \alpha^k, \sigma^k \rangle = \langle (H\mathbf{d} + \mathbf{d}H)\alpha^k, \sigma^k \rangle,$$

but, $\mathbf{d}\alpha^k = 0$, so,

$$\langle \alpha^k, \sigma^k \rangle = \langle \mathbf{d}(H\alpha^k), \sigma^k \rangle.$$

Therefore, $\beta^{k-1} = H\alpha^k$ is such that $\mathbf{d}\beta^{k-1} = \alpha^k$ at the level of cochains. □

Example 3.10. *We demonstrate the construction of the tetrahedralization of the cone of a $(n-1)$-simplex over the origin.*

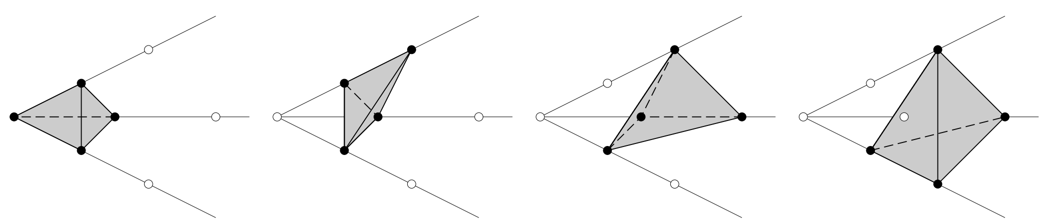
If we denote by v_i^k, the projection of the v_i vertex to the k-th concentric sphere, where the 0-th concentric sphere is simply the central point, then we fill up the cone $[c, v_1, ...v_n]$ with simplices as follows,

$$[v_1^0, v_1^1, \dots, v_n^1], [v_1^2, v_1^1, \dots, v_n^1], [v_1^2, v_2^2, v_2^1, \dots, v_n^1], \dots, [v_1^2, \dots, v_n^2, v_n^1].$$

Since S^{n-1} is orientable, we can use a consistent triangulation of S^{n-1} and these n-cones to consistently triangulate B^n such that the resulting triangulation is star-shaped.

This fills up the region to the 1st concentric sphere, and we repeat the process by leapfrogging at the last vertex to add $[v_1^2, ..., v_n^2, v_n^3]$, and continuing the construction, to fill up the annulus between the 1st and 2nd concentric sphere. Thus, we can keep adding concentric shells to create an arbitrarily dense triangulation of a n-ball about the origin.

In three dimensions, these simplices are given by



$[c, v_1^1, v_2^1, v_3^1]$, $[v_1^2, v_1^1, v_2^1, v_3^1]$, $[v_1^2, v_2^2, v_2^1, v_3^1]$, $[v_1^2, v_2^2, v_3^2, v_3^1]$.

Putting them together, we obtain Figure 3.13.

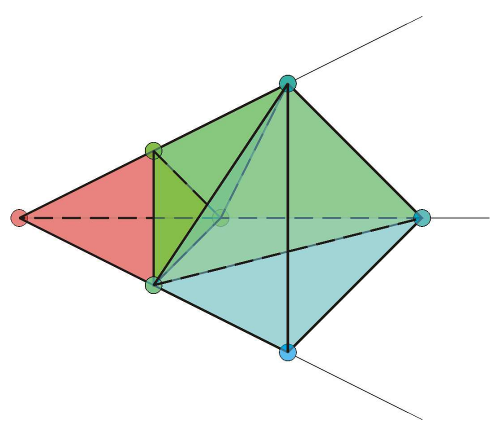


Figure 3.13: Triangulation of a three-dimensional cone.

This example is significant, since we have demonstrated that for any n-dimensional ball about a point, we can construct a trivially star-shaped triangulation of the ball, with arbitrarily high resolution. This allows us to recover the smooth Poincaré lemma in the limit of an infinitely fine mesh, using the discrete Poincaré lemma for trivially star-shaped complexes.

Logically Star-Shaped Complexes.

Definition 3.31. *A simplicial complex L is* ***logically star-shaped*** *if it is isomorphic, at the level of an abstract simplicial complex, to a trivially star-shaped complex K.*

Example 3.11. *We see two simplicial complexes, in Figure 3.14, which are clearly isomorphic as abstract simplicial complexes.*

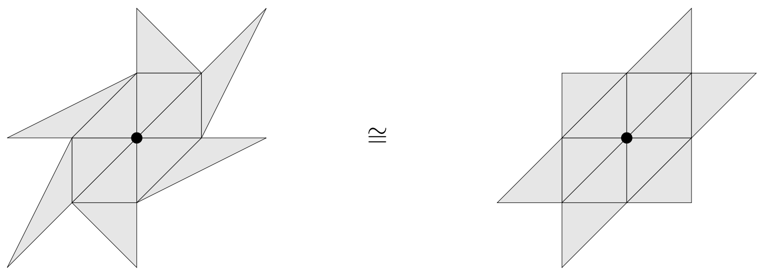


Figure 3.14: Trivially star-shaped complex (left); Logically star-shaped complex (right).

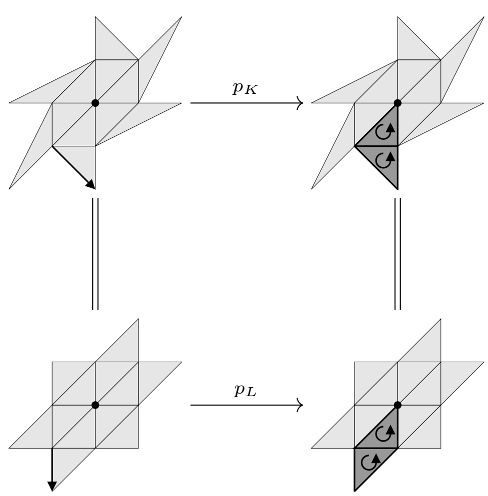
Definition 3.32. *The* ***logical cone*** *operator $p : C^k(L) \to C^{k+1}(L)$ is defined by making the following diagram commute,*

$$\begin{array}{ccc} C^k(K) & \xrightarrow{p_K} & C^{k+1}(K) \\ \| & & \| \\ C^k(L) & \xrightarrow{p_L} & C^{k+1}(L) \end{array}$$

Which is to say that, given the isomorphism $\varphi : K \to L$, we define

$$p_L = \varphi \circ p_K \circ \varphi^{-1}.$$

Example 3.12. *We show an example of the construction of the logical cone operator.*



This definition of the logical cone operator results in identities for the cone and cocone operator that follow from the trivially star-shaped case, and we record the results as follows.

Lemma 3.12. *In logically star-shaped complexes, the logical cone operator satisfies the following identity,*

$$p\partial + \partial p = I,$$

at the level of chains.

Proof. Follows immediately by pushing forward the result for trivially star-shaped complexes using the isomorphism. □

Lemma 3.13. *In logically star-shaped complexes, the logical cocone operator satisfies the following identity,*

$$H\mathbf{d} + \mathbf{d}H = I,$$

at the level of cochains.

Proof. Follows immediately by pushing forward the result for trivially star-shaped complexes using the isomorphism. □

Similarly, we have a Discrete Poincaré Lemma for logically star-shaped complexes.

Corollary 3.14 (Discrete Poincaré Lemma for Logically Star-shaped Complexes). *Given a closed cochain α^k, that is to say, $\mathbf{d}\alpha^k = 0$, there exists a cochain β^{k-1}, such that, $\mathbf{d}\beta^{k-1} = \alpha^k$.*

Proof. Follows from the above lemma using the proof for the trivially star-shaped case. □

Contractible Complexes. For arbitrary contractible complexes, we construct a generalized cone operator such that it satisfies the identity,

$$p\partial + \partial p = I,$$

which is the crucial property of the cone operator, from the point of view of proving the discrete Poincaré lemma.

The trivial cone construction gives a clue as to how to proceed in the construction of a ***generalized cone operator***. Notice that if a σ^{k+1} is a term in $p(\sigma^k)$, then $p(\sigma^{k+1}) = \emptyset$. This suggests how we can use the cone identity to inductively construct the generalized cone operator.

To define $p(\sigma^k)$, we consider $\sigma^{k+1} \succ \sigma^k$, such that, σ^{k+1} and σ^k are consistently oriented. We apply $p\partial + \partial p$ to σ^{k+1}. Then, we have

$$\sigma^{k+1} = p(\sigma^k) + p(\partial\sigma^{k+1} - \sigma^k) + \partial p(\sigma^{k+1}).$$

If we set $p(\sigma^{k+1}) = \varnothing$,

$$\begin{aligned}\sigma^{k+1} &= p(\sigma^k) + p(\partial\sigma^{k+1} - \sigma^k) + \partial(\varnothing) \\ &= p(\sigma^k) + p(\partial\sigma^{k+1} - \sigma^k).\end{aligned}$$

Rearranging, we have

$$p(\sigma^k) = \sigma^{k+1} - p(\partial\sigma^{k+1} - \sigma^k),$$

and

$$p(\sigma^{k+1}) = \varnothing.$$

We are done, so long as the simplices in the chain $\partial\sigma^{k+1} - \sigma^k$ already have p defined on it. This then reduces to enumerating the simplices in such a way that in the right hand side of the equation, we never evoke terms that are undefined.

We now introduce a method of augmenting a complex so that the enumeration condition is always satisfied.

Definition 3.33. *Given a n-complex K, consider a $(n-1)$-chain c_{n-1} that is contained on the boundary of K, and is included in the one-ring of some vertex on ∂K. Then, the **one-ring cone augmentation** of K is the complex obtained by adding the n-cone $w \diamond c_{n-1}$, and all its faces to the complex.*

Definition 3.34. *A complex is **generalized star-shaped** if it can be constructed by repeatedly applying the one-ring augmentation procedure.*

We will explicitly show in Examples 3.13, and 3.16, how to enumerate the vertices in two and three dimensions. And in Examples 3.15, and 3.17, we will introduce regular triangulations of $\mathbb{R}^2$ and $\mathbb{R}^3$ that can be constructed by inductive one-ring cone augmentation.

Remark 3.7. *Notice that a non-contractible complex cannot be constructed by inductive one-ring cone augmentation, since it will involve adding a cone to a vertex that has two disjoint base chains. This prevents us from enumerating the simplices in such as way that all the terms in $\partial\sigma^{k+1} - \sigma^k$ have had p defined on them, and we see in Example 3.18 how this causes the cone identity, and hence the discrete Poincaré lemma to break.*

Example 3.13. *In two dimensions, the one-ring condition implies that the base of the cone consists of either one or two 1-simplices. To aid in visualization, consider Figure 3.15.*

In the case of one 1-simplex, $[v_0, v_1]$, when we augment using the cone construction with the new

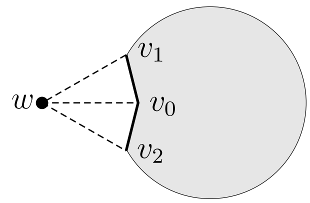


Figure 3.15: One-ring cone augmentation of a complex in two dimensions.

vertex w, we define,

$$p([w]) = [v_0, w] + p([v_0]), \qquad p([v_0, w]) = \varnothing,$$
$$p([v_1, w]) = [v_0, v_1, w] - p([v_0, v_1]), \qquad p([v_0, v_1, w]) = \varnothing.$$

In the case of two 1*-simplices,* $[v_0, v_1]$, $[v_0, v_2]$, *we have,*

$$p([w]) = [v_0, w] + p([v_0]), \qquad p([v_0, w]) = \varnothing,$$
$$p([v_1, w]) = [v_0, v_1, w] - p([v_0, v_1]), \qquad p([v_0, v_1, w]) = \varnothing,$$
$$p([v_2, w]) = [v_0, v_2, w] - p([v_0, v_2]), \qquad p([v_0, v_2, w]) = \varnothing.$$

Example 3.14. *We will now explicitly utilize the one-ring cone augmentation procedure to compute the generalized cone operator for part of a regular two-dimensional triangulation that is not logically star-shaped.*

As a preliminary, we shall consider a logically star-shaped complex, and augment with a new vertex, as seen in Figure 3.16.

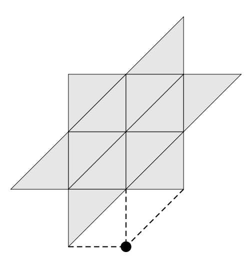
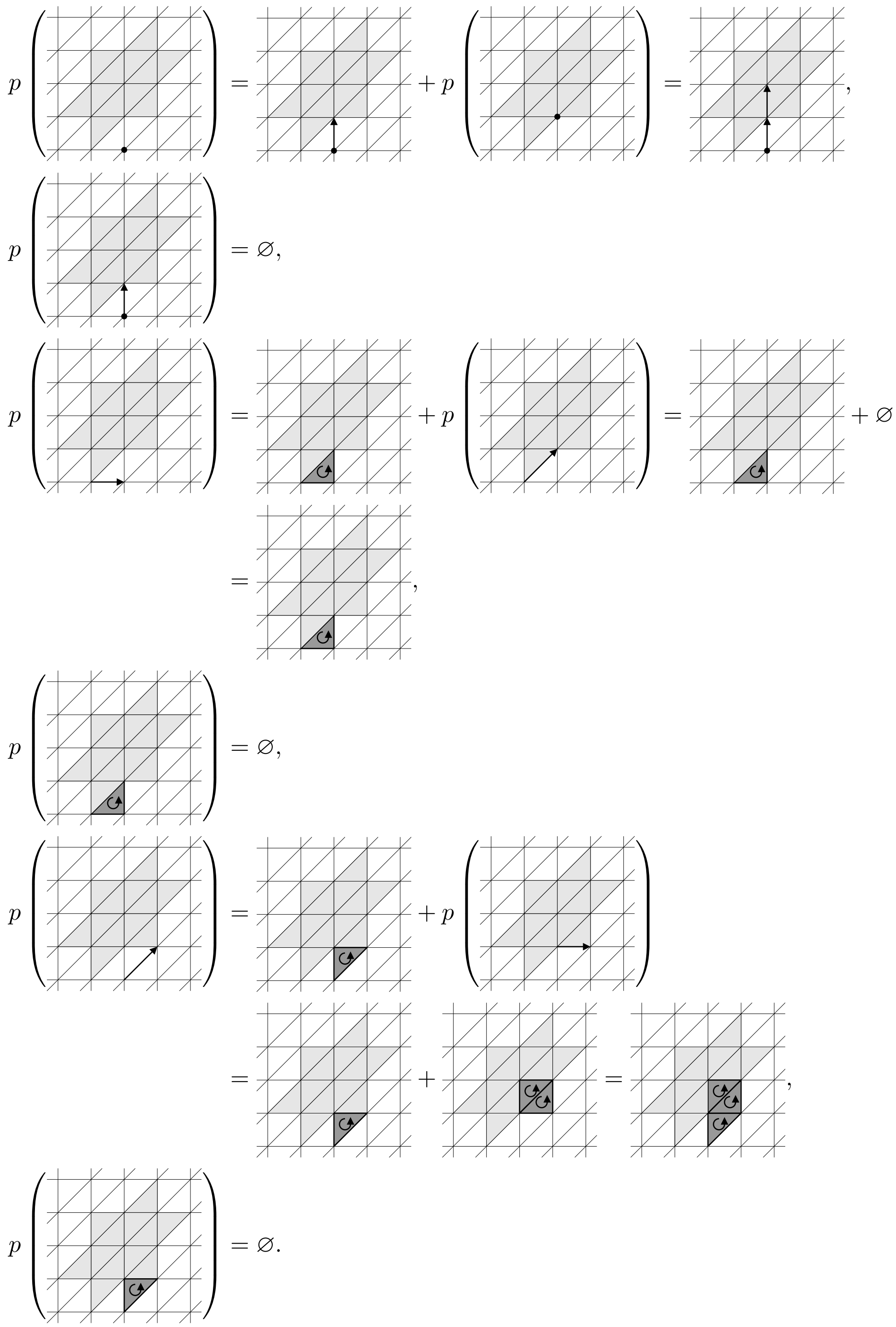


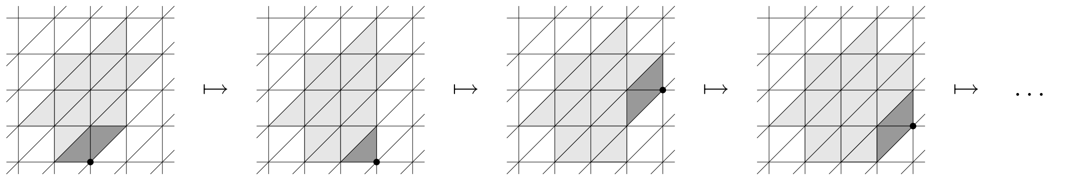
Figure 3.16: Logically star-shaped complex augmented by cone.

We use the logical cone operator for the subcomplex that is logically star-shaped, and the aug-

mentation rules in the example above for the newly introduced simplices. This yields,



Example 3.15. *Clearly, the regular two-dimensional triangulation can be obtained by the successive application of the one-ring cone augmentation procedure, as the following sequence illustrates,*



which means that the discrete Poincaré lemma can be extended to the entire regular triangulation of the plane.

Example 3.16. *We consider the case of augmentation in three dimensions. Denote by v_0, the center of the one-ring on the two-surface, to which we are augmenting the new vertex w. The other vertices of the one-ring are enumerated in order, $v_1, \ldots, v_m$. To aid in visualization, consider Figure 3.17.*

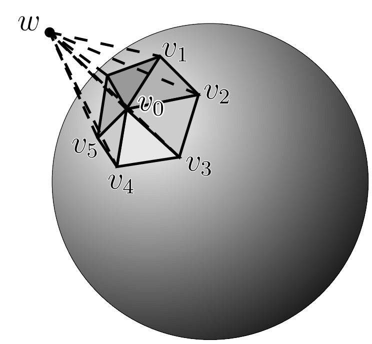


Figure 3.17: One-ring cone augmentation of a complex in three dimensions.

If the one-ring does not go completely around v_0, we shall denote the missing term by $[v_0, v_1, v_m]$. The generalized cone operators are given as follows.

k=0,

$$p([w]) = [v_0, w] + p([v_0]), \qquad p([v_0, w]) = \varnothing,$$

k=1,

$$p([v_1, w]) = [v_0, v_1, w] - p([v_0, v_1]), \qquad p([v_0, v_1, w]) = \varnothing,$$
$$p([v_m, w]) = [v_0, v_m, w] - p([v_0, v_m]), \qquad p([v_0, v_m, w]) = \varnothing,$$

k=2,

$$p([v_1, v_2, w]) = [v_0, v_1, v_2, w] + p([v_0, v_1, v_2]), \qquad p([v_1, v_2, w]) = \varnothing,$$

$$p([v_{m-1}, v_m, w]) = [v_0, v_{m-1}, v_m, w] + p([v_0, v_{m-1}, v_m]), \qquad p([v_{m-1}, v_m, w]) = \varnothing.$$

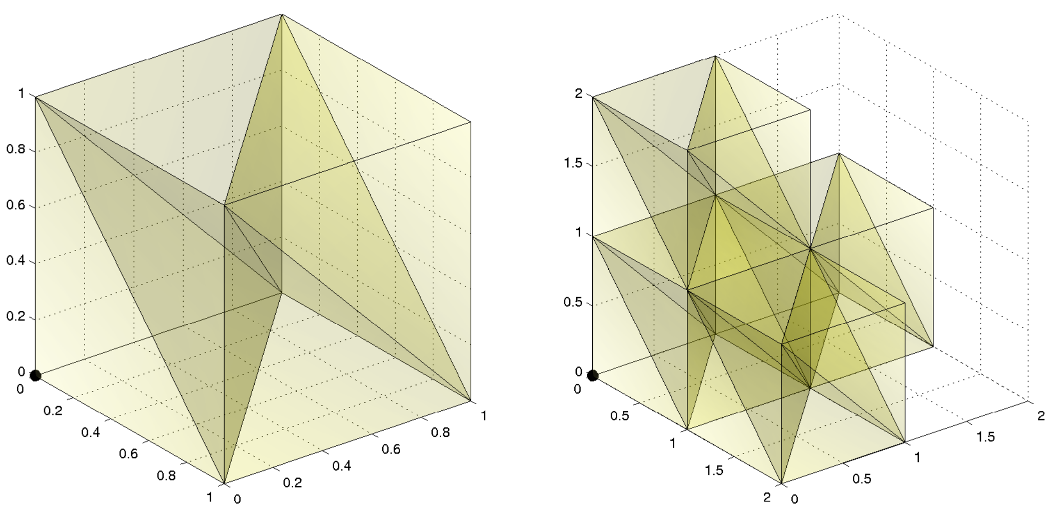
If it does go around completely,

$$p([v_m, v_1, w]) = [v_0, v_m, v_1, w] + p([v_0, v_m, v_1]), \qquad p([v_0, v_m, v_1, w]) = \varnothing.$$

Example 3.17. *We provide a tetrahedralization of the unit cube that can be tiled to yield a regular tetrahedralization of* $\mathbb{R}^3$*. The* 3*-simplices are as follows,*

$$[v_{000}, v_{001}, v_{010}, v_{10}], [v_{001}, v_{010}, v_{100}, v_{101}], [v_{001}, v_{010}, v_{011}, v_{101}],$$
$$[v_{010}, v_{100}, v_{101}, v_{110}], [v_{010}, v_{011}, v_{101}, v_{110}], [v_{011}, v_{101}, v_{110}, v_{111}].$$

The tetrahedralization of the unit cube can be seen in Figure 3.18.



(a) Tileable tetrahedralization of the unit cube

(b) Partial tiling of $\mathbb{R}^3$

Figure 3.18: Regular tiling of $\mathbb{R}^3$ that admits a generalized cone operator.

Since this regular tetrahedralization can be constructed by the successive application of the one-ring cone augmentation procedure, the Discrete Poincaré lemma can be extended to the entire regular tetrahedralization of $\mathbb{R}^3$*.*

In higher dimensions, we can extend the construction of the generalized cone operator inductively using the one-ring cone augmentation by choosing an appropriate enumeration of the base chain. Topologically, the base chain will be the cone of S^{n-2} (with possibly an open $(n-2)$-ball removed) with respect to the central point.

By spiraling around S^{n-2}, starting from around the boundary of the $n-2$ ball, and covering the rest of S^{n-2}, as in Figure 3.19, we obtain the higher-dimensional generalization of the procedure we have taken in Examples 3.13, and 3.16.

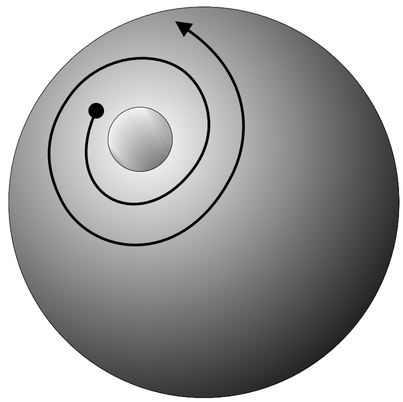


Figure 3.19: Spiral enumeration of S^{n-2}, $n = 4$.

Notice that $n = 2$ is distinguished, since $S^{2-2} = S^0$ is disjoint, which is why in the two-dimensional case, we were not able to use the spiraling technique to enumerate the simplices.

Since we have constructed the generalized cone operator such that the cone identity holds, we have,

Lemma 3.15. *In generalized star-shaped complexes, the generalized cone operator satisfies the following identity,*

$$p\partial + \partial p = I,$$

at the level of chains.

Proof. By construction. □

Lemma 3.16. *In generalized star-shaped complexes, the generalized cocone operator satisfies the following identity,*

$$H\mathbf{d} + \mathbf{d}H = I,$$

at the level of cochains.

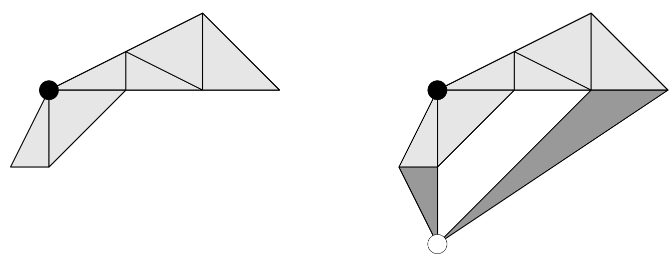
Proof. Follows immediately from applying the proof in the trivially star-shaped case, and using the identity in the previous lemma. □

Similarly, we have a discrete Poincaré lemma for generalized star-shaped complexes.

Corollary 3.17 (Discrete Poincaré Lemma for Generalized Star-shaped Complexes). *Given a closed cochain α^k, that is to say, $\mathbf{d}\alpha^k = 0$, there exists a cochain β^{k-1}, such that, $\mathbf{d}\beta^{k-1} = \alpha^k$.*

Proof. Follows from the above lemma using the proof for the trivially star-shaped case. □

Example 3.18. *We will consider an example of how the Poincaré lemma fails in the case when the complex is not contractible. Consider the following trivially star-shaped complex, and augment by one vertex so as to make the region non-contractible, as show in Figure 3.20.*



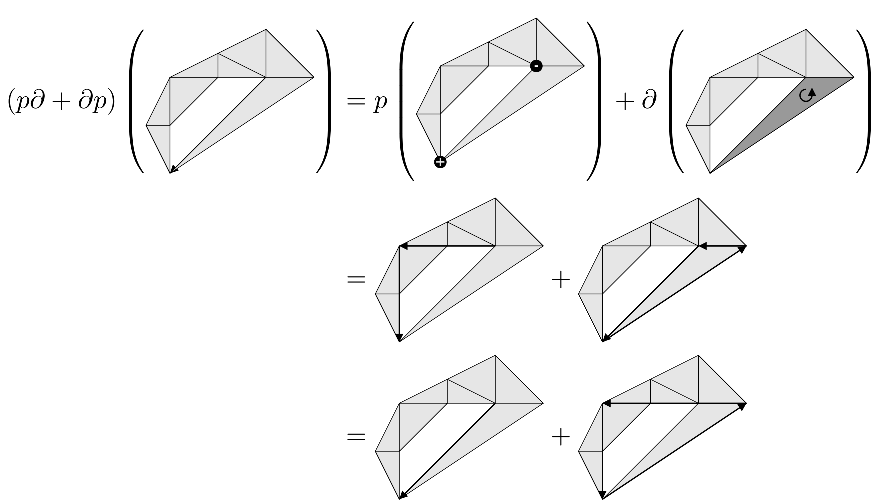
(a) Trivially star-shaped complex (b) Non-contractible complex

Figure 3.20: Counter-example for the discrete Poincaré lemma for a non-contractible complex.

Now we attempt to verify the identity,

$$p\partial + \partial p = I,$$

and we will see how this is only true up to a chain that is homotopic to the inner boundary.



Since the second term cannot be expressed as the boundary of a 2-chain, it will contribute a non-trivial effect, even on closed discrete forms, and therefore the discrete Poincaré lemma does not hold for non-contractible complexes, as expected.

3.12 Discrete Variational Mechanics and DEC

We recall that discrete variational mechanics is based on a discrete analogue of Hamilton's principle, and they yield the discrete Euler–Lagrange equations. A particularly interesting property of DEC arises when it is used to construct the discrete Lagrangian for harmonic functions, and Maxwell's equations.

In particular, for these examples, the following diagram commutes,

$$\begin{array}{ccc} \textbf{Lagrangian} & & \textbf{Discrete Lagrangian} \\ L : TQ \to \mathbb{R} & \xrightarrow{\quad DEC \quad} & L_d : Q \times Q \to \mathbb{R} \\ \downarrow & & \downarrow \\ \textbf{Euler–Lagrange} & & \textbf{Discrete Euler–Lagrange} \\ \mathcal{EL} : T^2Q \to T^*Q & \xrightarrow{\quad DEC \quad} & \mathcal{EL}_d : Q^3 \to T^*Q \end{array}$$

Which is to say that directly discretizing the differential equations for harmonic functions, and Maxwell's equations using DEC results in the same expressions as the discrete Euler–Lagrange equations associated with a discrete Lagrangian which is discretized from the corresponding continuous Lagrangian by using DEC as the discretization scheme.

This is significant, since it implies that when DEC is used to discretize these equations, the corresponding numerical scheme which is obtained is variational, and consequently exhibits excellent structure-preserving properties.

In the variational principles for both harmonic functions and Maxwell's equations, we require the L^2 norm obtained from the L^2 inner product on $\Omega^k(M)$, which is given by

$$\langle \alpha^k, \beta^k \rangle = \int_M \alpha \wedge *\beta \, .$$

The discrete analogue of this requires a primal-dual wedge product, which is given below for forms of complementary dimension.

Definition 3.35. *Given a primal discrete k-form $\alpha^k \in \Omega_d^k(K)$, and a dual discrete $(n-k)$-form*

*$\hat{\beta}^{n-k} \in \Omega_d^{n-k}(\star K)$, the **discrete primal-dual wedge product** is defined as follows,*

$$\begin{aligned}\langle \alpha^k \wedge \hat{\beta}^{n-k}, V_{\sigma^k} \rangle &= \frac{|V_{\sigma^k}|}{|\sigma^k||\star\sigma^k|} \langle \alpha^k, \sigma^k \rangle \langle \hat{\beta}^{n-k}, \star\sigma^k \rangle \\ &= \frac{1}{n} \langle \alpha^k, \sigma^k \rangle \langle \hat{\beta}^{n-k}, \star\sigma^k \rangle \,,\end{aligned}$$

where V_{σ^k} is the n-dimensional support volume obtained by taking the convex hull of the simplex σ^k and its dual cell $\star\sigma^k$.

The corresponding L^2 inner product is as follows.

Definition 3.36. *Given two primal discrete k-forms, $\alpha^k, \beta^k \in \Omega_d^k(K)$, their **discrete L^2 inner product**, $\langle \alpha^k, \beta^k \rangle_d$, is given by*

$$\begin{aligned}\langle \alpha^k, \beta^k \rangle_d &= \sum_{\sigma^k \in K} \frac{|V_{\sigma^k}|}{|\sigma^k||\star\sigma^k|} \langle \alpha^k, \sigma^k \rangle \langle *\beta, \star\sigma^k \rangle \\ &= \frac{1}{n} \sum_{\sigma^k \in K} \langle \alpha^k, \sigma^k \rangle \langle *\beta, \star\sigma^k \rangle \,.\end{aligned}$$

Remark 3.8. *Notice that it would have been quite natural from the smooth theory to propose the following metric tensor $\langle\!\langle \, , \, \rangle\!\rangle$ for differential forms,*

$$\langle \, \langle\!\langle \alpha^k, \beta^k \rangle\!\rangle \mathbf{v}, V_{\sigma^k} \rangle = |V_{\sigma^k}| \frac{\langle \alpha^k, \sigma^k \rangle}{|\sigma^k|} \frac{\langle \beta^k, \sigma^k \rangle}{|\sigma^k|} \,,$$

where the $|V_{\sigma^k}|$ is the factor arising from integrating the volume-form over V_{σ^k}, and

$$\frac{\langle \alpha^k, \sigma^k \rangle}{|\sigma^k|} \frac{\langle \beta^k, \sigma^k \rangle}{|\sigma^k|}$$

is what we would expect for $\langle\!\langle \alpha^k, \beta^k \rangle\!\rangle$, if the forms α^k and β^k were constant on σ^k, which is the product of the average values of α^k, and β^k.

If we adopt this as our definition of the metric tensor for forms, we can recover the definition we obtained in §3.6 for the Hodge star operator. Starting from the definition from the smooth theory,

$$\int \langle\!\langle \alpha^k, \beta^k \rangle\!\rangle \mathbf{v} = \int \alpha^k \wedge *\beta^k \,,$$

and expanding this in terms of the metric tensor for discrete forms, and the primal-dual wedge operator, we obtain

$$\langle \, \langle\!\langle \alpha^k, \beta^k \rangle\!\rangle \mathbf{v}, V_{\sigma^k} \rangle = \langle \alpha^k \wedge *\beta^k, V_{\sigma^k} \rangle \,,$$

$$|V_{\sigma^k}|\frac{\langle\alpha^k,\sigma^k\rangle}{|\sigma^k|}\frac{\langle\beta^k,\sigma^k\rangle}{|\sigma^k|} = \frac{|V_{\sigma^k}|}{|\sigma^k||\star\sigma^k|}\langle\alpha^k,\sigma^k\rangle\langle*\beta^k,\star\sigma^k\rangle\,.$$

When we eliminate common factors from both sides, we obtain the expression,

$$\frac{1}{|\sigma^k|}\langle\beta^k,\sigma^k\rangle = \frac{1}{|\star\sigma^k|}\langle*\beta^k,\star\sigma^k\rangle\,,$$

which is the expression we previously obtained in Definition 3.18 of §3.6.

The L^2 norm for discrete differential forms is given below.

Definition 3.37. *Given a primal discrete k-form $\alpha^k \in \Omega_d^k(K)$, its **discrete L^2 norm** is given by*

$$\begin{aligned}\|\alpha^k\|_d^2 &= \langle\alpha^k,\alpha^k\rangle_d \\ &= \frac{1}{n}\sum_{\sigma^k\in K}\langle\alpha^k,\sigma^k\rangle\langle*\alpha^k,\star\sigma^k\rangle \\ &= \frac{1}{n}\sum_{\sigma^k\in K}\frac{|\star\sigma^k|}{|\sigma^k|}\langle\alpha^k,\sigma^k\rangle^2\,.\end{aligned}$$

Given these definitions, we can now reproduce some computations that were originally shown in Castrillón-López [2003].

Harmonic Functions. Harmonic functions $\phi : M \to \mathbb{R}$ can be characterized in a variational fashion as extremals of the following action functional,

$$\mathcal{S}(\phi) = \frac{1}{2}\int_M \|\mathbf{d}\phi\|^2\mathbf{v},$$

where $\mathbf{v}$ is a Riemannian volume-form in M. The corresponding Euler–Lagrange equation is given by

$$*\mathbf{d} * \mathbf{d}\phi = -\Delta\phi = 0,$$

which is the familiar characterization of harmonic functions in terms of the Laplace–Beltrami operator.

The discrete action functional can be expressed in terms of the L^2 norm we introduced above for discrete forms,

$$\begin{aligned}\mathcal{S}_d(\phi) &= \frac{1}{2}\|\mathbf{d}\phi\|_d^2 \\ &= \frac{1}{2n}\sum_{\sigma^1\in K}\frac{|\star\sigma^1|}{|\sigma^1|}\langle\mathbf{d}\phi,\sigma^1\rangle^2.\end{aligned}$$

The basic variations needed for the determination of the discrete Euler–Lagrange operator are obtained from variations that vary the value of the function ϕ at a given vertex v_0, leaving the other values fixed. These variations have the form,

$$\phi_\varepsilon = \phi + \varepsilon\tilde{\eta},$$

where $\tilde{\eta} \in \Omega^0(M;\mathbb{R})$ is such that $\langle\tilde{\eta}, v_0\rangle = 1$, and $\langle\tilde{\eta}, v\rangle = 0$, for any $v \in K^{(0)} - \{v_0\}$. This family of variations is enough to establish the variational principle. That is, we have

$$\begin{aligned} 0 &= \left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} \mathcal{S}_d(\phi_\varepsilon) \\ &= \frac{1}{n}\sum_{\sigma^1\in K} \frac{|\star\sigma^1|}{|\sigma^1|}\langle\mathbf{d}\phi, \sigma^1\rangle\langle\mathbf{d}\tilde{\eta}, \sigma^1\rangle \\ &= \frac{1}{n}\sum_{v_0\prec\sigma^1} \frac{|\star\sigma^1|}{|\sigma^1|}\langle\mathbf{d}\phi, \sigma^1\rangle \operatorname{sgn}(\sigma^1; v_0), \end{aligned} \tag{3.12.1}$$

where $\operatorname{sgn}(\sigma^1; v)$ stands for the sign of σ^1 with respect to v. Which is to say, $\operatorname{sgn}(\sigma^1; v) = 1$ if $\sigma^1 = [v', v]$, and $\operatorname{sgn}(\sigma^1; v) = -1$ if $\sigma^1 = [v, v']$. On the other hand,

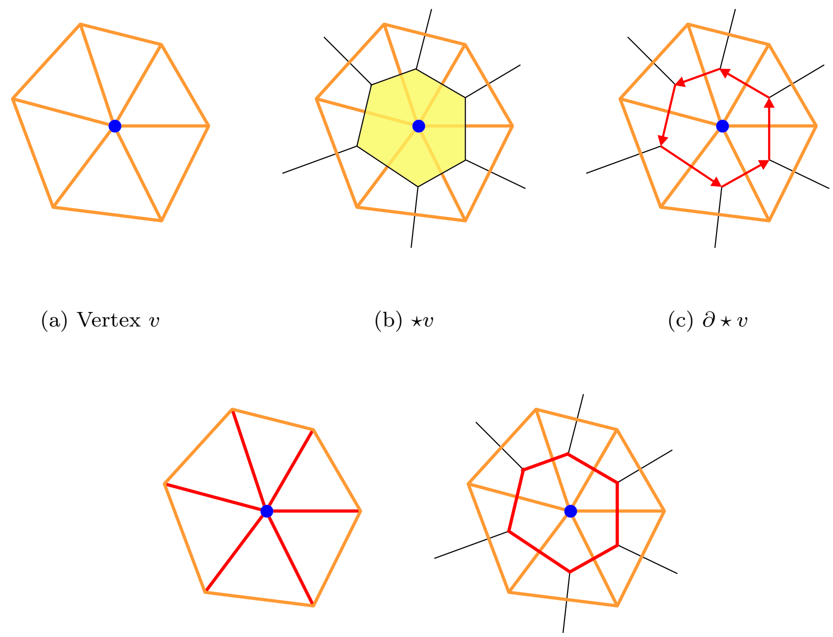
$$\begin{aligned} \langle *\mathbf{d} * \mathbf{d}\phi, v_0\rangle &= \frac{1}{|\star v_0|}\langle\mathbf{d} * \mathbf{d}\phi, \star v_0\rangle \\ &= \frac{1}{|\star v_0|}\langle *\mathbf{d}\phi, \partial \star v_0\rangle \\ &= \frac{1}{|\star v_0|}\sum_{v_0\prec\sigma^1}\langle *\mathbf{d}\phi, \star\sigma^1\rangle \operatorname{sgn}(\sigma^1; v_0) \\ &= \frac{1}{|\star v_0|}\sum_{v_0\prec\sigma^1}\frac{|\star\sigma^1|}{|\sigma^1|}\langle\mathbf{d}\phi, \sigma^1\rangle \operatorname{sgn}(\sigma^1; v_0), \end{aligned}$$

where in the second to last equality, one has to note that the border of the dual cell of a vertex v_0 consists, up to orientation, in the dual of all the 1-simplices starting from v_0. This is illustrated in Figure 3.21, and follows from a general expression for the boundary of a dual cell that was given in Definition 3.17.

The sign factor comes from the relation between the orientation of the dual of the 1-simplices and that of $\partial * v_0$. From this, we conclude that the variational discrete equation, given in Equation 3.12.1, is equivalent to the vanishing of the discrete Laplace–Beltrami operator,

$$*\mathbf{d} * \mathbf{d}\phi = -\Delta = 0.$$

Maxwell Equations. We can formulate the Maxwell equations of electromagnetism in a covariant fashion by considering the 1-form A (the potential) as our fundamental variable in a Lorentzian



(a) Vertex v (b) $\star v$ (c) $\partial \star v$

(d) $\sigma^1 \succ v$ (e) $\star \sigma^1$

Figure 3.21: Boundary of a dual cell.

manifold X. The action functional for a Lagrangian formulation of electromagnetism is given by,

$$\mathcal{S}(A) = \frac{1}{2} \int_X \|\mathbf{d}A\|^2 \mathbf{v}\,,$$

where $\| \cdot \|$ is the norm on forms induced by the Lorentzian metric on X, and $\mathbf{v}$ is the pseudo-Riemannian volume-form. The 1-form A is related to the 4-vector potential encountered in the relativistic formulation of electromagnetism (see, for example Jackson [1998]).

The Euler–Lagrange equation corresponding to this action functional is given by

$$*\mathbf{d} * \mathbf{d}A = 0\,.$$

In terms of the field strength, $F = \mathbf{d}A$, the last equation is usually rewritten as

$$\mathbf{d}F = 0\,, \qquad *\mathbf{d} * F = 0\,,$$

which is the geometric formulation of the Maxwell equations.

For the purposes of simplicity of exposition, we consider the special case where the Lorentzian manifold decomposes into $X = M \times \mathbb{R}$, where (M, g) is a compact Riemannian 3-manifold. In formulating the discrete version of this variational problem, we need to generalize the notion of a discrete Hodge dual to take into account the pseudo-Riemannian metric structure. This can be subtle in practice, and to overcome this, we consider a special family of complexes instead.

Let K' be a simplicial complex modelling M. For the sake of simplicity we consider $M = \mathbb{R}^3$ although this is not strictly necessary. We now consider a discretization $\{t_n\}_{n\in\mathbb{Z}}$ of $\mathbb{R}$. We define the complex K, modelling $X = \mathbb{R}^4$, the cells of which are the sets $\sigma = \sigma' \times \{t_n\} \subset \mathbb{R}^3 \times \mathbb{R}$, and $\sigma = \sigma' \times (t_n, t_{n+1}) \subset \mathbb{R}^3 \times \mathbb{R}$ for any $\sigma' \in K'$ and $n \in \mathbb{Z}$. Of course, this is not a simplicial complex but rather a "prismal" complex, as shown in Figure 3.22.

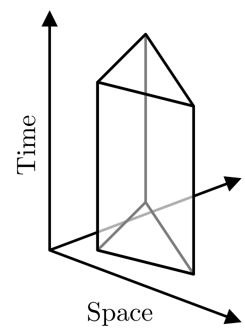


Figure 3.22: Prismal cell complex decomposition of space-time.

The advantage of these cell complexes is the existence of the Voronoi dual. More precisely, given any prismal cells $\sigma' \times \{t_n\} \in K$ and $\sigma' \times (t_n, t_{n+1}) \in K$, the Lorentz orthonormal to any of its edges coincide with the Euclidean one in $\mathbb{R}^4$ and the existence of the circumcenter is thus guaranteed. In other words, the Lorentz circumcentric dual $\star K$ to K is the same as the Euclidean one in $\mathbb{R}^4$.

Remark 3.9. *Much of the construction above can be carried out more generally by considering arbitrary cell complexes in $\mathbb{R}^4$ that are not necessarily prismal, as long as none of its 1-cells are lightlike. This causality condition is necessary to ensure that the circumcentric dual complex is well-behaved. However, it is sufficient for computational purposes that the complex is well-centered, in the sense that the Lorentzian circumcenter of each cell is contained inside the cell. These issues will be addressed in future work.*

Recall that the Hodge star $*$ is uniquely defined by satisfying the following expression,

$$\alpha \wedge *\beta = \langle\langle \alpha, \beta \rangle\rangle \mathbf{v}\,,$$

for all $\alpha, \beta \in \Omega^k(X)$. The upshot of this is that the Hodge star operator depends on the metric, and since we have a pseudo-Riemannian metric, there is a sign that is introduced in our expression for the discrete Hodge star (Definition 3.18) that depends on whether the cell it is applied to is either spacelike or timelike. The discrete Hodge star for prismal complexes in Lorentzian space is given below.

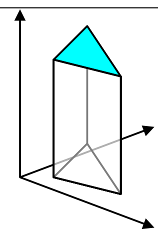
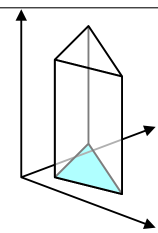
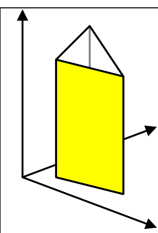
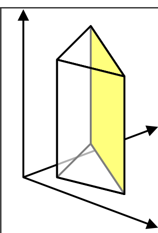
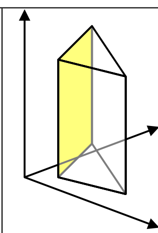
Definition 3.38. *The* ***discrete Hodge star for prismal complexes in Lorentzian space*** *is a map* $* : \Omega_d^k(K) \to \Omega_d^k(*K)$ *defined by giving its action on cells in a prismal complex as follows,*

$$\frac{1}{|\star \sigma^k|}\langle *\alpha^k, \star\sigma^k\rangle = \kappa(\sigma^k)\frac{1}{|\sigma^k|}\langle \alpha^k, \sigma^k\rangle,$$

where $|\cdot|$ *stands for the volume and the* ***causality sign*** $\kappa(\sigma^k)$ *is defined to be* $+1$ *if all the edges of* σ^k *are spacelike, and* -1 *otherwise.*

The causality sign of 2-cells in a $(2+1)$-space-time is summarized in Table 3.4. We should note that the causality sign for a 0-simplex, $\kappa(\sigma^0)$, is always 1. This is because a 0-simplex has no edges, and as such the statement that *all* of its edges are spacelike is trivially true.

Table 3.4: Causality sign of 2-cells in a $(2+1)$-space-time.

σ^2					
$\kappa(\sigma^2)$	$+1$	$+1$	-1	-1	-1

This causality term in the discrete Hodge star has consequences for the expression for the discrete norm (Definition 3.37), which is now given.

Definition 3.39. *Given a primal discrete* k*-form* $\alpha^k \in \Omega_d^k(K)$*, its* ***discrete*** L^2 ***Lorentzian norm*** *is given by,*

$$\begin{aligned}\|\alpha^k\|^2_{\mathrm{Lor},d} &= \frac{1}{n}\sum_{\sigma^k \in K}\langle \alpha^k, \sigma^k\rangle\langle *\alpha^k, \star\sigma^k\rangle \\ &= \frac{1}{n}\sum_{\sigma^k \in K}\kappa(\sigma^k)\frac{|\star\sigma^k|}{|\sigma^k|}\langle \alpha^k, \sigma^k\rangle^2 .\end{aligned}$$

Having defined the discrete Lorentzian norm, we can express the discrete action as

$$\mathcal{S}_d(A) = \frac{1}{2}\|\mathbf{d}A\|^2_{\mathrm{Lor},d}$$

$$= \frac{1}{8} \sum_{\sigma^2 \in K} \langle \mathbf{d}A, \sigma^2 \rangle \langle * \mathbf{d}A, \star \sigma^2 \rangle$$
$$= \frac{1}{8} \sum_{\sigma^2 \in K} \kappa(\sigma^2) \frac{|\star \sigma^2|}{|\sigma^2|} \langle \mathbf{d}A, \sigma^2 \rangle^2 .$$

The basic variations needed to determine the discrete Euler–Lagrange operator are obtained from variations that vary the value of the 1-form A at a given 1-simplex σ_0^1, leaving the other values fixed. These variations have the form,

$$A_\varepsilon = A_\varepsilon + \varepsilon \tilde{\eta},$$

where $\tilde{\eta} \in \Omega_d^1(K)$ is given by $\langle \tilde{\eta}, \sigma_0^1 \rangle = 1$ for a fixed interior $\sigma_0^1 \in K$ and $\langle \tilde{\eta}, \sigma^1 \rangle = 0$ for $\sigma^1 \neq \sigma_0^1$. The derivation of the variational principle gives

$$\left. \frac{d}{d\varepsilon} \right|_{\varepsilon=0} \mathcal{S}_d(A_\varepsilon) = \frac{1}{4} \sum_{\sigma^2 \in K} \frac{|\star \sigma^2|}{|\sigma^2|} \kappa(\sigma^2) \langle \mathbf{d}A, \sigma^2 \rangle \langle \mathbf{d}\tilde{\eta}, \sigma^2 \rangle$$
$$= \frac{1}{4} \sum_{\sigma_0^1 \prec \sigma^2} \frac{|\star \sigma^2|}{|\sigma^2|} \kappa(\sigma^2) \langle \mathbf{d}A, \sigma^2 \rangle \langle \mathbf{d}\tilde{\eta}, \sigma^2 \rangle$$
$$= \frac{1}{4} \sum_{\sigma_0^1 \prec \sigma^2} \frac{|\star \sigma^2|}{|\sigma^2|} \kappa(\sigma^2) \langle \mathbf{d}A, \sigma^2 \rangle \operatorname{sgn}(\sigma^2, \sigma_0^1),$$

which vanishes for all the basic variations above. On the other hand, we now expand the discrete 1-form $* \mathbf{d} * \mathbf{d}A$. For any $\sigma_0^1 \in K$, we have that

$$\langle * \mathbf{d} * \mathbf{d}A, \sigma_0^1 \rangle = \frac{|\sigma_0^1|}{|\star \sigma_0^1|} \kappa(\sigma_0^1) \langle \mathbf{d} * \mathbf{d}A, \star \sigma_0^1 \rangle$$
$$= \frac{|\sigma_0^1|}{|\star \sigma_0^1|} \kappa(\sigma_0^1) \langle * \mathbf{d}A, \partial \star \sigma_0^1 \rangle$$
$$= \frac{|\sigma_0^1|}{|\star \sigma_0^1|} \kappa(\sigma_0^1) \sum_{\sigma_0^1 \prec \sigma^2} \operatorname{sgn}(\sigma^2, \sigma_0^1) \langle * \mathbf{d}A, \star \sigma^2 \rangle$$
$$= \frac{|\sigma_0^1|}{|\star \sigma_0^1|} \kappa(\sigma_0^1) \sum_{\sigma_0^1 \prec \sigma^2} \frac{|\star \sigma^2|}{|\sigma^2|} \kappa(\sigma^2) \langle \mathbf{d}A, \sigma^2 \rangle \operatorname{sgn}(\sigma^2, \sigma_0^1),$$

where the sign $\operatorname{sgn}(\sigma^2, \sigma^1)$ stands for the relative orientation between σ^2 and σ^1. Which is to say, $\operatorname{sgn}(\sigma^2, \sigma^1) = 1$ if the orientation induced by σ^2 on σ^1 coincides with the orientation of σ^1, and $\operatorname{sgn}(\sigma^2, \sigma^1) = -1$ otherwise. For the second to last equality, one has to note that the border of the dual cell of an edge σ_0^1 consists, conveniently oriented with the sgn operator, of the union of the duals of all the 2-simplices containing σ_0^1. This statement is the content of Definition 3.17, which gives the expression for the boundary of a dual cell, and was illustrated in Figure 3.21 for the case of n-dimensional dual cells.

By comparing the two computations, we find that for an arbitrary choice of $\sigma_0^1 \in K$, $\langle * \mathbf{d} * \mathbf{d}A, \sigma_0^1 \rangle$

is equal (up to a non-zero constant) to $\delta\mathcal{S}_d(A)$, which always vanishes. It follows that the variational discrete equations obtained above is equivalent to the discrete Maxwell equations,

$$*\mathbf{d} * \mathbf{d}A = 0.$$

3.13 Extensions to Dynamic Problems

It is desirable to leverage the exactness properties of the operators of discrete exterior calculus to construct numerical algorithms with discrete conservation properties. For these purposes, it is appropriate to extend the scope of DEC to incorporate dynamical behavior, by addressing the issue of discrete diffeomorphisms and flows.

As discussed in the previous section, DEC and discrete mechanics have interesting synergistic properties, and in this section we will explore a groupoid interpretation of discrete mechanics that is particularly appropriate to formulating the notion of pull-back and push-forward of discrete differential forms.

3.13.1 Groupoid Interpretation of Discrete Variational Mechanics

The groupoid formulation of discrete mechanics is particularly fruitful and natural, and it serves as a unifying tool for understanding the variational formulation of discrete Lagrangian mechanics, and discrete Euler–Poincaré reduction, as discussed in the work of Weinstein [1996] and Marsden et al. [1999, 2000a].

The groupoid interpretation of discrete mechanics is most clearly illustrated if we consider the discretization of trajectories on TQ in two stages. Given a curve $\gamma : \mathbb{R}^+ \to TQ$, we consider a discrete sampling given by

$$g_i = \gamma(ih) \in TQ.$$

We then approximate TQ by $Q \times Q$, and associate to g_i two elements in Q. We denote this by

$$g_i \mapsto (q_i^0, q_i^1).$$

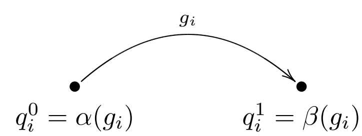
Or equivalently, in the language of groupoids, see Cannas da Silva and Weinstein [1999]; Weinstein [2001], we have

$$\begin{array}{c} G \\ \alpha \downarrow \; \downarrow \beta \\ Q \end{array}$$

where α is the ***source*** map, and β is the ***target*** map. Then,

$$g_i \mapsto (\alpha(g_i), \beta(g_i)) = (q_i^0, q_i^1).$$

This can be visualized as



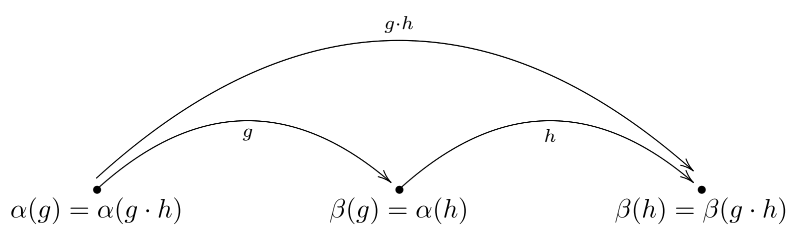
A product $\cdot : G^{(2)} \to G$ is defined on the set of composable pairs,

$$G^{(2)} := \{(g, h) \in G \times G \mid \beta(g) = \alpha(h)\}.$$

The ***groupoid composition*** $g \cdot h$ is defined by

$$\alpha(g \cdot h) = \alpha(g),$$
$$\beta(g \cdot h) = \beta(h).$$

This can be represented graphically as follows,



The set of composable pairs is the discrete analogue of the set of second-order curves on TQ. A curve $\gamma : \mathbb{R}^+ \to TQ$ is said to be second-order if there exists a curve $q : \mathbb{R}^+ \to Q$, such that,

$$\gamma(t) = (q(t), \dot{q}(t)).$$

The corresponding condition for discrete curves is that given a sequence of points in $Q \times Q$, $(q_1^0, q_1^1), \ldots, (q_p^0, q_p^1)$, we require that

$$q_i^1 = q_{i+1}^0.$$

This implies that the discrete curve on $Q \times Q$ is derived from a $(p+1)$-pointed curve $(q_0, \ldots, q_p)$ on

Q, where

$$q_i = \begin{cases} q^0_{i+1}, & \text{if } 0 \le i < p; \\ q^1_i, & \text{if } i = p. \end{cases}$$

This condition has a direct equivalent in groupoids,

$$\beta(g_i) = q^1_i = q^0_{i+1} = \alpha(g_{i+1}).$$

Which is to say that the sequence of points in $Q \times Q$ are composable. In general, this hierarchy of sets is denoted by

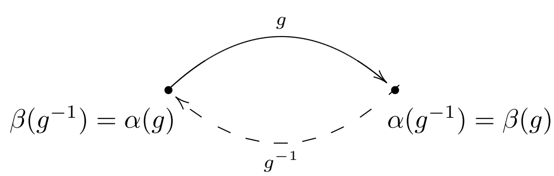
$$G^{(p)} := \{(g_1, \dots, g_p) \in G^p \mid \beta(g_i) = \alpha(g_{i+1})\},$$

where $G^{(0)} \simeq Q$.

In addition, the ***groupoid inverse*** is defined by the following,

$$\alpha(g^{-1}) = \beta(g),$$
$$\beta(g^{-1}) = \alpha(g).$$

This is represented as follows,



Visualizing Groupoids. In summary, composition of groupoid elements, and the inverse of groupoid elements can be illustrated by Figure 3.23. As we will see in the next subsection, representing discrete diffeomorphisms as pair groupoids is the natural method of ensuring that the mesh remains nondegenerate.

3.13.2 Discrete Diffeomorphisms and Discrete Flows

We will adopt the point of view of representing a discrete diffeomorphism as a groupoid, which was first introduced in Pekarsky and West [2003], and appropriately modify it to reflect the simplicial nature of our mesh. In addition, we will address the induced action of a discrete diffeomorphism on the dual mesh.

Definition 3.40. *Given a complex K embedded in V, and its corresponding abstract simplicial complex M, a* ***discrete diffeomorphism****, $\varphi \in \mathrm{Diff}_d(M)$, is a pair of simplicial complexes K_1, K_2,*

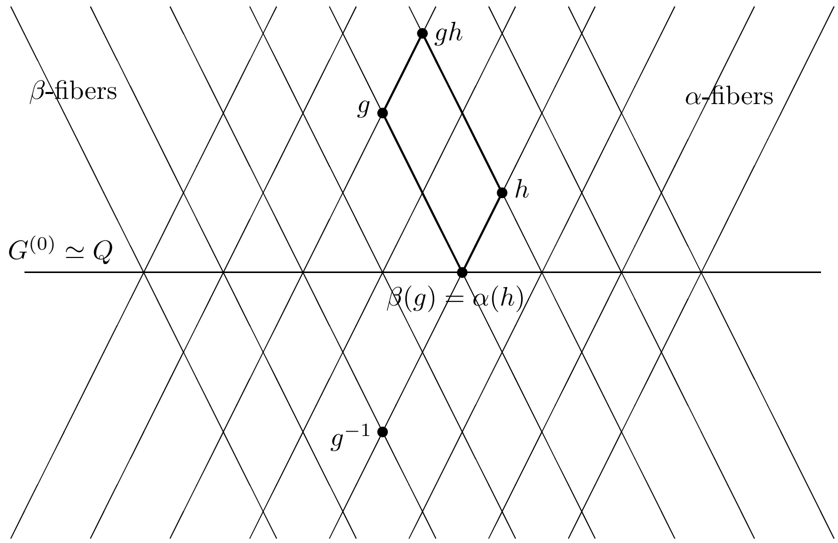


Figure 3.23: Groupoid composition and inverses.

which are realizations of M in the ambient space V. This is denoted by $\varphi(M) = (K_1, K_2)$.

Definition 3.41. *A* ***one-parameter family of discrete diffeomorphisms*** *is a map $\varphi : I \to \text{Diff}_d(M)$, such that,*

$$\pi_1(\varphi(t)) = \pi_1(\varphi(s)), \qquad \forall s, t \in I.$$

Since we are concerned with evolving equations represented by these discrete diffeomorphisms, and mesh degeneracy causes the numerics to fail, we introduce the notion of non-degenerate discrete diffeomorphisms,

Definition 3.42. *A* ***non-degenerate discrete diffeomorphism*** *$\varphi = (K_1, K_2)$ is such that K_1 and K_2 are non-degenerate realizations of the abstract simplicial complex M in the ambient space V.*

Notice that it is sufficient to define the discrete diffeomorphism on the vertices of the abstract complex M, since we can extend it to the entire complex by the relation

$$\varphi([v_0, ..., v_k]) = ([\pi_1\varphi(v_0), ..., \pi_1\varphi(v_k)], [\pi_2\varphi(v_0), ..., \pi_2\varphi(v_k)]).$$

If $X \in K^{(0)}$ is a material vertex of the manifold, corresponding to the abstract vertex w, that is to say, $\pi_1\varphi_t(w) = X, \forall t \in I$, the corresponding trajectory followed by X in space is $x = \pi_2\varphi_t(w)$. Then, the ***material velocity*** $V(X,t)$ is given by

$$V(\pi_1(w), t) = \left.\frac{\partial \pi_2 \varphi_s(w)}{\partial s}\right|_{s=t},$$

and the ***spatial velocity*** $v(x,t)$ is given by

$$v(\pi_2(w),t) = V(\pi_1(w),t) = \left.\frac{\partial \varphi_s(\varphi_t^{-1}(x))}{\partial s}\right|_{s=t}.$$

The distinction between the spatial and material representation is illustrated in Figure 3.24.

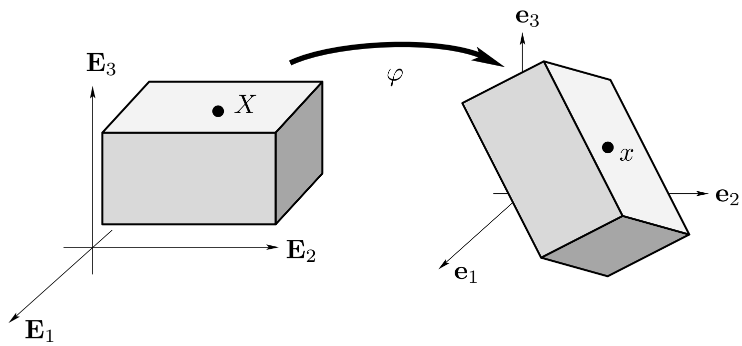


Figure 3.24: Spatial and material representations.

The material velocity field can be thought of as a discrete vector field with the vectors based at the vertices of K, which is to say that $T\varphi_t \in \mathfrak{X}_d(K)$, is a discrete primal vector field. Notice that φ_t on K induces a map $\star\varphi_t$ on the vertices of the dual $\star K$, by the following,

$$\star\varphi_t(c[v_0,\ldots,v_n]) = (c[\pi_1\varphi_t(v_0),\ldots,\pi_1\varphi_t(v_n)], c[\pi_2\varphi_t(v_0),\ldots,\pi_2\varphi_t(v_n)]).$$

Similarly then, $T\star\varphi_t \in \mathfrak{X}_d(\star K)$ is a discrete dual vector field.

Comparison with Interpolatory Methods. At first glance, the groupoid formulation seems like a cumbersome way to define a one-parameter family of discrete diffeomorphisms, and one may be tempted to think of extending φ_t to the ambient space. We would then be thinking of $\varphi_t : V \to V$. This is undesirable since given φ_t and ψ_s which are non-degenerate flows, their composition $\varphi_t \circ \psi_s$, which is defined, may result in a degenerate mesh when applied to K. Thus, non-degenerate flows are not closed under this notion of composition.

If we adopt groupoid composition instead at the level of vertices, we can always be sure that if we compose two nondegenerate discrete diffeomorphisms, they will remain a nondegenerate discrete diffeomorphism.

Discrete Diffeomorphisms as Pair Groupoids. The space of discrete diffeomorphisms naturally has the structure of a pair groupoid. The discrete analogue of $T\,\mathrm{Diff}(M)$ from the point of view of temporal discretization is the pair groupoid $\mathrm{Diff}(M) \times \mathrm{Diff}(M)$. In addition, we discretize

Diff(M) using Diff$_d(M)$, which is in turn a pair groupoid involving realizations of an abstract simplicial complex in an ambient space.

3.13.3 Push-Forward and Pull-Back of Discrete Vector Fields and Discrete Forms

For us to construct a discrete theory of exterior calculus that admits dynamic problems, it is critical that we introduce the notion of push-forward and pull-back of discrete vector fields and discrete forms under a discrete flow.

Push-Forward and Pull-Back of Discrete Vector Fields. The push-forward of a discrete vector field satisfies the following commutative diagram,

$$\begin{array}{ccccc} K & \xrightarrow{\star} & \star K & \xrightarrow{X} & \mathbb{R}^N \\ \downarrow{\scriptstyle f} & & \downarrow{\scriptstyle \star f} & & \downarrow{\scriptstyle Tf} \\ L & \xrightarrow{\star} & \star L & \xrightarrow{f_* X} & \mathbb{R}^N \end{array}$$

and the pull-back satisfies the following commutative diagram,

$$\begin{array}{ccccc} K & \xrightarrow{\star} & \star K & \xrightarrow{f^* X} & \mathbb{R}^N \\ \downarrow{\scriptstyle f} & & \downarrow{\scriptstyle \star f} & & \downarrow{\scriptstyle Tf} \\ L & \xrightarrow{\star} & \star L & \xrightarrow{X} & \mathbb{R}^N \end{array}$$

By appropriately following the diagram around its boundary, we obtain the following expressions for the push-forward and pull-back of a discrete vector field.

Definition 3.43. *The* ***push-forward of a dual discrete vector field*** $X \in \mathfrak{X}_d(\star K)$*, under the map* $f : K \to L$*, is given by its evaluation on a dual vertex* $\hat{\sigma}_0 = \star\sigma^n \in (\star L)^{(0)}$*,*

$$f_* X(\star\sigma^n) = Tf \cdot X(\star(f^{-1}(\sigma^n))).$$

Definition 3.44. *The* ***pull-back of a dual discrete vector field*** $X \in \mathfrak{X}_d(\star L)$*, under the map* $f : K \to L$*, is given by its evaluation on a dual vertex* $\hat{\sigma}_0 = \star\sigma^n \in (\star K)^{(0)}$*,*

$$f^* X(\star\sigma^n) = (f^{-1})_* X(\star\sigma^n) = T(f^{-1}) \cdot X(\star(f(\sigma^n))).$$

Pull-Back and Push-Forward of Discrete Forms. A natural operation involving exterior calculus in the context of dynamic problems is the pull-back of a differential form by a flow. We define the pull-back of a discrete form as follows.

Definition 3.45. *The* ***pull-back of a discrete form*** $\alpha^k \in \Omega_d^k(L)$*, under the map* $f : K \to L$*, is defined so that the* ***change of variables formula*** *holds,*

$$\langle f^* \alpha^k, \sigma^k \rangle = \langle \alpha^k, f(\sigma^k) \rangle,$$

where $\sigma^k \in K$*.*

We can define the push-forward of a discrete form as its pull-back under the inverse map as follows.

Definition 3.46. *The* ***push-forward of a discrete form*** $\alpha^k \in \Omega_d^k(K)$*, under the map* $f : K \to L$ *is defined by its action on* $\sigma^k \in L$*,*

$$\langle f_* \alpha^k, \sigma^k \rangle = \langle (f^{-1})^* \alpha^k, \sigma^k \rangle = \langle \alpha^k, f^{-1}(\sigma^k) \rangle.$$

Naturality under Pull-Back of Wedge Product. We find that the discrete wedge product we introduced in §3.8 is not natural under pull-back, which is to say that the relation

$$f^*(\alpha \wedge \beta) = f^* \alpha \wedge f^* \beta\,,$$

does not hold in general. However, a metric independent definition that is natural under pull-back was proposed in Castrillón-López [2003].

Definition 3.47 (Castrillón-López [2003]). *Given a primal discrete* k*-form* $\alpha^k \in \Omega_d^k(K)$*, and a primal discrete* l*-form* $\beta^l \in \Omega_d^l(K)$*, the* ***natural discrete primal-primal wedge product****,* $\wedge : \Omega_d^k(K) \times \Omega_d^l(K) \to \Omega_d^{k+l}(K)$*, is defined by its evaluation on a* $(k+l)$*-simplex* $\sigma^{k+l} = [v_0, \dots, v_{k+l}]$*,*

$$\langle \alpha^k \wedge \beta^l, \sigma^{k+l} \rangle = \frac{1}{(k+l+1)!} \sum_{\tau \in S_{k+l+1}} \operatorname{sign}(\tau) \alpha \smile \beta(\tau(\sigma^{k+l}))\,.$$

In contrasting this definition to that given by Definition 3.24, we see that the geometric factor

$$\frac{|\sigma^{k+l} \cap \star v_{\tau(k)}|}{|\sigma^{k+l}|}\,,$$

has been replaced by

$$\frac{1}{k+l+1}$$

in this alternative definition. By replacing the geometric factor which is metric dependent with a constant factor, Definition 3.47 becomes natural under pull-back.

The proofs in §3.8 that the discrete wedge product is anti-commutative, and satisfies a Leibniz rule, remain valid for this alternative discrete wedge product, with only trivial modifications. As for the proof of the associativity of the wedge product for closed forms, we note the following identity,

$$\sum_{\tau \in S_{k+l+1}} \frac{|\sigma^{k+l} \cap \star v_{\tau(k)}|}{|\sigma^{k+l}|} = \sum_{\tau \in S_{k+l+1}} \frac{1}{k+l+1} = (k+l)!\,,$$

which is a crucial observation for the original proof to apply to the alternative wedge product.

3.14 Remeshing Cochains and Multigrid Extensions

It is sometimes desirable, particularly in the context of multigrid, multiscale, and multiresolution computations, to be able to represent a discrete differential form which is given as a cochain on a prescribed mesh, as one which is supported on a new mesh. Given a differential form $\omega^k \in \Omega^k(K)$, and a new mesh M such that $|K| = |M|$, we can define it at the level of cosimplices,

$$\forall \tau^k \in M^{(k)}, \qquad \langle \omega^k, \tau^k \rangle = \sum_{\sigma^k \in K^{(k)}} \operatorname{sgn}(\tau^k, \sigma^k) \frac{|V_{\tau^k} \cap V_{\sigma^k}|}{|V_{\sigma^k}|} \langle \omega^k, \sigma^k \rangle,$$

and extend this by linearity to cochains. Here, $\operatorname{sgn}(\tau^k, \sigma^k)$ is $+1$ if the orientation of τ^k and σ^k are consistent, and -1 otherwise. Since k-skeletons of meshes that are not related by subdivision may not have nontrivial intersections, intersections of support volumes are used in the remeshing formula, as opposed to intersections of the k-simplices.

We denote this transformation at the level of cochains as, $T_{K,M} : C^k(K) \to C^k(M)$. This has the natural property that if we have a k-volume U^k that can be represented as a chain in either the complex K or the complex M, that is to say, $U^k = \sigma_1^k + \ldots + \sigma_l^k = \tau_1^k + \ldots + \tau_l^k$, then we have

$$\begin{aligned}
\langle \omega^k, \tau_1^k + \ldots + \tau_m^k \rangle &= \sum_{i=1}^m \langle \omega, \tau_i^k \rangle = \sum_{i=1}^m \sum_{\sigma^k \in K^{(k)}} \operatorname{sgn}(\tau_i^k, \sigma^k) \frac{|V_{\tau_i^k} \cap V_{\sigma^k}|}{|V_{\sigma^k}|} \langle \omega^k, \sigma^k \rangle \\
&= \sum_{i=1}^m \sum_{j=1}^l \operatorname{sgn}(\tau_i^k, \sigma_j^k) \frac{|V_{\tau_i^k} \cap V_{\sigma_j^k}|}{|V_{\sigma_j^k}|} \langle \omega^k, \sigma_j^k \rangle \\
&= \sum_{j=1}^l \sum_{i=1}^m \operatorname{sgn}(\tau_i^k, \sigma_j^k) \frac{|V_{\tau_i^k} \cap V_{\sigma_j^k}|}{|V_{\sigma_j^k}|} \langle \omega^k, \sigma_j^k \rangle \\
&= \sum_{j=1}^l \langle \omega^k, \sigma_j^k \rangle = \langle \omega^k, \sigma_1^k + \ldots + \sigma_l^k \rangle.
\end{aligned}$$

Which is to say that the integral of the differential form over U^k is well-defined, and independent of the representation of the differential form.

Note that, in particular, if we choose to coarsen the mesh, the value the form takes on a cell in the coarser mesh is simply the sum of the values the form takes on the old cells of the fine mesh which make up the new cell in the coarser mesh.

Non-Flat Manifolds. The case of non-flat manifolds presents a challenge in remeshing akin to that encountered in the discretization of differential forms. In particular, if the two meshes represent different discretizations of a non-flat manifold, they will in general correspond to different polyhedral regions in the embedding space, and not have the same support region.

We assume that our discretization of the manifold is sufficiently fine that for every simplex, all its vertices are contained in some chart. Then, by using these local charts, we can identify support volumes in the computational domain with n-volumes in the manifold, and thereby make sense of the remeshing formula.

3.15 Conclusions and Future Work

We have presented a framework for discrete exterior calculus using the cochain representation of discrete differential forms, and introduced combinatorial representations of discrete analogues of differential operators on discrete forms and discrete vector fields. The role of primal and dual cell complexes in the theory are developed in detail. In addition, extensions to dynamic problems and multi-resolution computations are discussed.

In the next few paragraphs, we will describe some of the future directions that emanate from the current work on discrete exterior calculus.

Relation to Computational Algebraic Topology Since we have introduced a discrete Laplace-deRham operator, one can hope to develop a discrete Hodge-deRham theory, and relate the deRham cohomology of a simplicial complex to its simplicial cohomology.

Extensions to Non-Flat Manifolds. The intrinsic notion of what constitutes the discrete tangent space to a node on a non-flat mesh remains an open question. It is possible that this notion is related to a choice of discrete connection on the mesh, and it is an issue that deserves further exploration.

Generalization to Arbitrary Tensors. The discretization of differential forms as cochains is particularly natural, due to the pairing between forms and volumes by integration. When attempting to discretize an arbitrary tensor, the natural discrete analogue is unclear. In particular, while it is possible to expand an arbitrary tensor using the tensor product of covariant and contravariant one-tensors, this would be cumbersome to represent on a mesh. In Chapter 4, which is on discrete connections, we will see Lie group-valued discrete 1-forms, and one possible method of discretizing a (p, q)-tensor that is alternating in the contravariant indices, is to consider it as a $(0, q)$-tensor-valued discrete p-form.

It would be particularly interesting to explore this in the context of the elasticity complex (see, for example, Arnold [2002]),

$$\mathfrak{se}(3) \hookrightarrow C^\infty(\Omega, \mathbb{R}^3) \xrightarrow{\epsilon} C^\infty(\Omega, \mathbb{S}) \xrightarrow{J} C^\infty(\Omega, \mathbb{S}) \xrightarrow{\text{div}} C^\infty(\Omega, \mathbb{R}^3) \longrightarrow 0\,,$$

where $\mathbb{S}$ is the space of 3×3 symmetric matrices. One approach to discretize this was suggested in Arnold [2002], which cites the use of the Bernstein–Gelfand–Gelfand resolution in Eastwood [2000] to derive the elasticity complex from the deRham complex. Alternatively, it might be appropriate in the context of the elasticity complex to consider Lie algebra-valued discrete differential forms.

Convergence and Higher-Order Theories. The natural question from the point of view of numerical analysis would be to carefully analyze the convergence properties of these discrete differential geometric operators. In addition, higher-order analogues of the discrete theory of exterior calculus are desirable from the point of view of computational efficiency, but the cochain representation is attractive due to its conceptual simplicity and the elegance of representing discrete operators as combinatorial operations on the mesh.

It would therefore be desirable to reconcile the two, by ensuring that high-order interpolation and combinatorial operations are consistent. As a low-order example, Whitney forms, which are used to interpolate differential forms on a simplicial mesh, have the nice property that taking the Whitney form associated with the coboundary of a simplicial cochain is equal to taking the exterior derivative of the Whitney form associated with the simplicial cochain. As such, the coboundary operation, which is a combinatorial operation akin to finite differences, is an exact discretization of the exterior derivative, when applied to the degrees of freedom associated to the finite-dimensional function space of Whitney forms.

It would be interesting to apply subdivision surface techniques to construct interpolatory spaces that are compatible with differential geometric operations that are combinatorial operations on the degrees of freedom. This will result in a massively simplified approach to higher-order theories of discrete exterior calculus, by avoiding the use of symbolic computation, which would otherwise be necessary to compute the action of continuous exterior differential operators on the polynomial expansions for differential forms.

Chapter 4

Discrete Connections on Principal Bundles

In collaboration with Jerrold E. Marsden, and Alan D. Weinstein.

Abstract

Connections on principal bundles play a fundamental role in expressing the equations of motion for mechanical systems with symmetry in an intrinsic fashion. A discrete theory of connections on principal bundles is constructed by introducing the discrete analogue of the Atiyah sequence, with a connection corresponding to the choice of a splitting of the short exact sequence. Equivalent representations of a discrete connection are considered, and an extension of the pair groupoid composition, that takes into account the principal bundle structure, is introduced. Computational issues, such as the order of approximation, are also addressed. Discrete connections provide an intrinsic method for introducing coordinates on the reduced space for discrete mechanics, and provide the necessary discrete geometry to introduce more general discrete symmetry reduction. In addition, discrete analogues of the Levi-Civita connection, and its curvature, are introduced by using the machinery of discrete exterior calculus, and discrete connections.

4.1 Introduction

One of the major goals of geometric mechanics is the study of symmetry, and its consequences. An important tool in this regard is the non-singular reduction of mechanical systems under the action of free and proper symmetries, which is naturally formulated in the setting of principal bundles.

The reduction procedure results in the decomposition of the equations of motion into terms involving the shape and group variables, and the coupling between these are represented in terms of a connection on the principal bundle.

Connections and their associated curvature play an important role in the phenomena of geometric phases. A discussion of the history of geometric phases can be found in Berry [1990]. Shapere and Wilczek [1989] is a collection of papers on the theory and application of geometric phases to physics. In the rest of this section, we will survey some of the applications of geometric phases and connections to geometric mechanics and control, some of which were drawn from Marsden [1994, 1997]; Marsden and Ratiu [1999].

The simulation of these phenomena requires the construction of a discrete notion of connections on principal bundles that is compatible with the approach of discrete variational mechanics, and it towards this end that this chapter is dedicated.

Falling Cat. Geometric phases arise in nature, and perhaps the most striking example of this is the falling cat, which is able to reorient itself by 180°, while remaining at *zero* angular momentum, as show in Figure 4.1.

The key to reconciling this with the constancy of the angular momentum is that angular momentum depends on the moment of inertia, which in turn depends on the shape of the cat. When the cat changes it shape by curling up and twisting, its moment of inertia changes, which is in turn compensated by its overall orientation changing to maintain the zero angular momentum condition. The zero angular momentum condition induces a connection on the principal bundle, and the curvature of this connection is what allows the cat to reorient itself.

A similar experiment can be tried on Earth, as described on page 10 of Vedral [2003]. This involves standing on a swivel chair, lifting your arms, and rotating them over your head, which will result in the chair swivelling around slowly.

Holonomy. The sense in which curvature is related to geometric phases is most clearly illustrated by considering the parallel transport of a vector around a curve on the sphere, as shown in Figure 4.2.

Think of the point on the sphere as representing the shape of the cat, and the vector as representing its orientation. The fact that the vector experiences a phase shift when parallel transported around the sphere is an example of ***holonomy***. In general, holonomy refers to a situation in geometry wherein an orthonormal frame that is parallel transported around a closed loop, back to its original position, is rotated with respect to its original orientation.

Curvature of a space is critically related to the presence of holonomy. Indeed, curvature should be thought of as being an infinitesimal version of holonomy, and this interpretation will resurface when considering the discrete analogue of curvature in the context of a discrete exterior calculus.

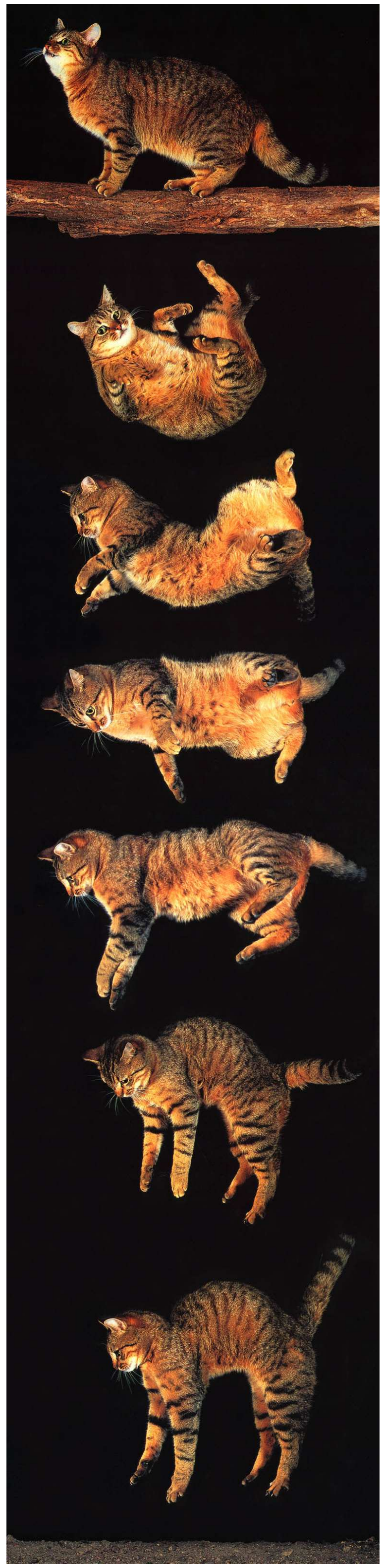


Figure 4.1: Reorientation of a falling cat at zero angular momentum.

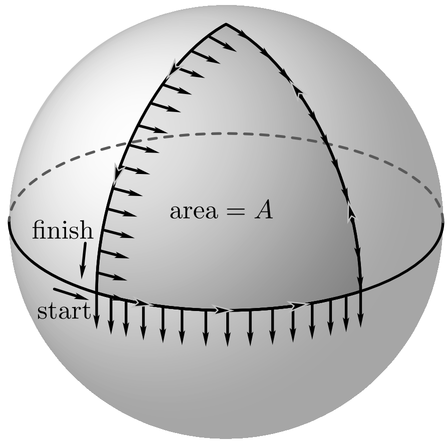


Figure 4.2: A parallel transport of a vector around a spherical triangle produces a phase shift.

Foucault Pendulum. Another example relating geometric phases and holonomy is that of the Foucault pendulum. As the Earth rotates about the Sun, the Foucault pendulum exhibits a phase shift of $\Delta\theta = 2\pi \cos\alpha$ (where α is the co-latitude). This phase shift is geometric in nature, and is a consequence of holonomy. If one parallel transports an orthonormal frame around the line of constant latitude, it exhibits a phase shift that is identical to that of the Foucault pendulum, as illustrated in Figure 4.3.

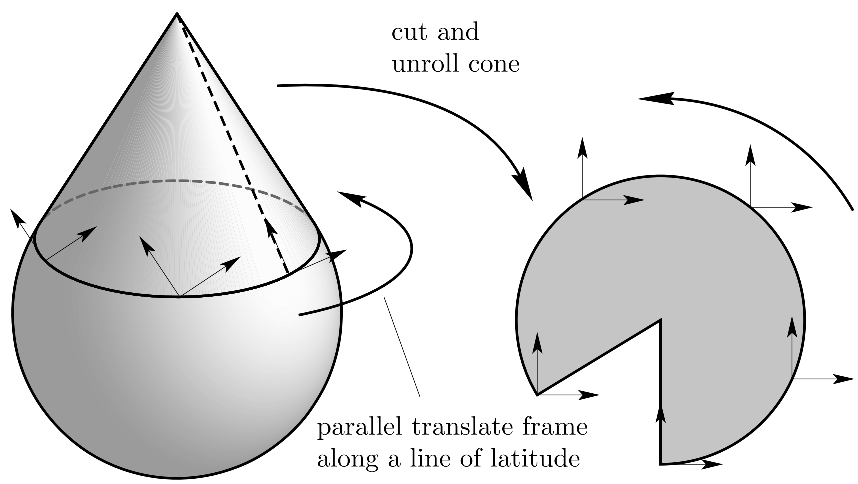


Figure 4.3: Geometric phase of the Foucault pendulum.

True Polar Wander. A particular striking example of the consequences of geometric phases and the conservation of angular momentum is the phenomena of true polar wander, that was studied by

Goldreich and Toomre [1969], and more recently by Leok [1998]. It is thought that some 500 to 600 million years ago, during the Vendian–Cambrian transition, the Earth, over a 15-million-year period, experienced an inertial interchange true polar wander event. This occurred when the intermediate and maximum moments of inertia crossed due to the redistribution of mass anomalies, associated with continental drift and mantle convection, thereby causing a catastrophic shift in the axis of rotation.

This phenomena is illustrated in Figure 4.4, wherein the places corresponding to the North and South poles of the Earth migrate towards the equator as the axis of rotation changes.

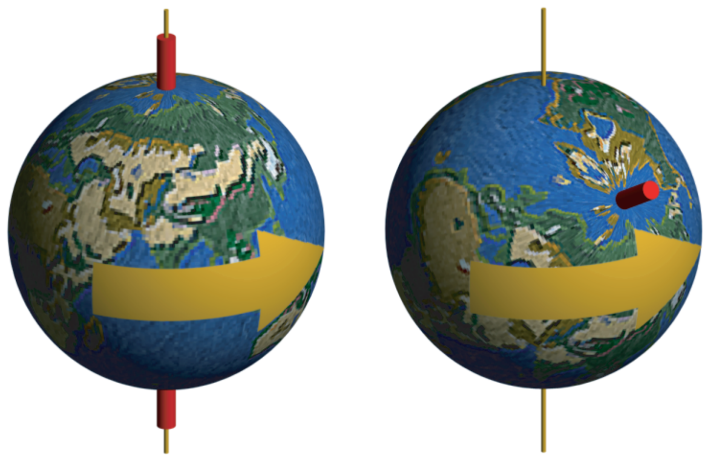


Figure 4.4: True Polar Wander. Red axis corresponds to the original rotational axis, and the gold axis corresponds to the instantaneous rotational axis.

Geometric Control Theory. Geometric phases also have interesting applications and consequences in geometric control theory, and allow, for example, astronauts in free space to reorient themselves by changing their shape. By holding one of their legs straight, swivelling at the hip, and moving their foot in a circle, they are able to change their orientation. Since the reorientation only occurs as the shape is being changed, this allows the reorientation to be done with extremely high precision. Such ideas have been applied to the control of robots and spacecrafts; see, for example, Walsh and Sastry [1993]. The role of connections in geometric control is also addressed in-depth in Marsden [1994, 1997].

One of the theoretical underpinnings of the application of geometric phases to geometric control was developed in Montgomery [1991] and Marsden et al. [1990], in the form of the ***rigid-body phase formula***,

$$\Delta\theta = \frac{1}{\|\mu\|}\left\{\int_D \omega_\mu + 2H_\mu T\right\} = -\Lambda + \frac{2H_\mu T}{\|\mu\|},$$

the geometry of which is illustrated in Figure 4.5.

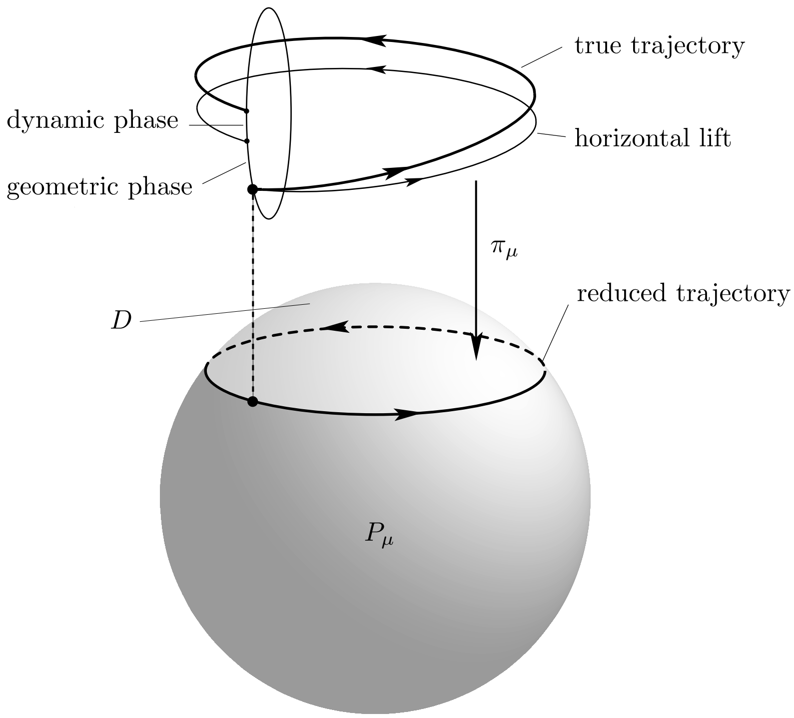


Figure 4.5: Geometry of rigid-body phase.

An example that has been studied extensively is that of the satellite with internal rotors, with a configuration space given by $Q = \mathrm{SE}(3) \times S^1 \times S^1 \times S^1$, and illustrated in Figure 4.6.

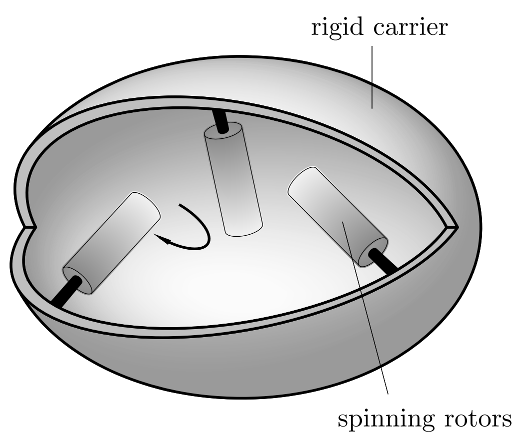


Figure 4.6: Rigid body with internal rotors.

The generalization of the rigid-body phase formula in the presence of feedback control is particularly useful in the study and design of attitude control algorithms.

4.2 General Theory of Bundles

Before considering the discrete analogue of connections on principal bundles, we will review some basic material on the general theory of bundles, fiber bundles, and principal fiber bundles. A more in-depth discussion of fiber bundles can be found in Steenrod [1951] and Kobayashi and Nomizu [1963].

A bundle $\mathcal{Q}$ consists of a triple (Q, S, π), where Q and S are topological spaces, respectively referred to as the ***bundle space*** and the ***base space***, and $\pi : Q \to S$ is a continuous map called the ***projection***. We may assume, without loss of generality, that π is surjective, by considering the bundle over the image $\pi(Q) \subset S$.

The ***fiber over the point*** $x \in S$, denoted F_x, is given by, $F_x = \pi^{-1}(x)$. In most situations of practical interest, the fiber at every point is homeomorphic to a common space F, in which case, F is the ***fiber*** of the bundle, and the bundle is a ***fiber bundle***. The geometry of a fiber bundle is illustrated in Figure 4.7.

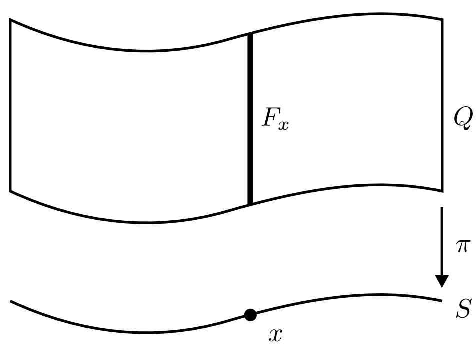


Figure 4.7: Geometry of a fiber bundle.

A bundle (Q, S, π) is a ***G-bundle*** if G acts on Q by left translation, and it is isomorphic to $(Q, Q/G, \pi_{Q/G})$, where Q/G is the orbit space of the G action on Q, and $\pi_{Q/G}$ is the natural projection.

If G acts freely on Q, then (Q, S, π) is called a ***principal G-bundle***, or ***principal bundle***, and G is its ***structure group***. G acting freely on Q implies that each orbit is homeomorphic to G, and therefore, $\mathcal{Q}$ is a fiber bundle with fiber G.

To make the setting for the rest of this chapter more precise, we will adopt the following definition of a principal bundle,

Definition 4.1. *A **principal bundle** is a manifold Q with a free left action, $\rho : G \times Q \to Q$, of a Lie group G, such that the natural projection, $\pi : Q \to Q/G$, is a submersion. The base space Q/G*

*is often referred to as the **shape space** S, which is a terminology originating from reduction theory.*

We will now consider a few standard techniques for combining bundles together to form new bundles. These methods include the fiber product, Whitney sum, and the associated bundle construction.

Fiber Product. Given two bundles with the same base space, we can construct a new bundle, referred to as the ***fiber product***, which has the same base space, and a fiber which is the direct product of the fibers of the original two bundles. More formally, we have,

Definition 4.2. *Given two bundles $\pi_i : Q_i \to S$, $i = 1, 2$, the **fiber product** is the bundle,*

$$\pi_1 \times_S \pi_2 : Q_1 \times_S Q_2 \to S,$$

where $Q_1 \times_S Q_2$ is the set of all elements $(q_1, q_2) \in Q_1 \times Q_2$ such that $\pi_1(q_1) = \pi_2(q_2)$, and the projection $\pi_1 \times_S \pi_2$ is naturally defined by $\pi_1 \times_S \pi_2(q_1, q_2) = \pi_1(q_1) = \pi_2(q_2)$. The fiber is given by $(\pi_1 \times_Q \pi_2)^{-1}(x) = \pi_1^{-1}(x) \times \pi_2^{-1}(x)$.

Whitney Sum. The ***Whitney sum*** combines two vector bundles using the fiber product construction.

Definition 4.3. *Given two vector bundles $\tau_i : V_i \to Q$, $i = 1, 2$, with the same base, their **Whitney sum** is their fiber product, and it is a vector bundle over Q, and is denoted $V_1 \oplus V_2$. This bundle is obtained by taking the fiberwise direct sum of the fibers of V_1 and V_2.*

Associated Bundle. Given a principal bundle, $\pi : Q \to Q/G$, and a left action, $\rho : G \times M \to M$, of the Lie group G on a manifold M, we can construct the associated bundle.

Definition 4.4. *An **associated bundle** $\tilde{M}$ with standard fiber M is,*

$$\tilde{M} = Q \times_G M = (Q \times M)/G,$$

where the action of G on $Q \times M$ is given by $g(q, m) = (gq, gm)$. The class (or orbit) of (q, m) is denoted $[q, m]_G$ or simply $[q, m]$. The projection $\pi_M : Q \times_G M \to Q/G$ is given by,

$$\pi_M : ([q, m]_G) = \pi(q)\,,$$

and it is easy to check that it is well-defined and is a surjective submersion.

4.3 Connections and Bundles

Before formally introducing the precise definition of a connection, we will attempt to develop some intuition and motivation for the concept. As alluded to in the introduction to this chapter, a connection describes the curvature of a space. In the classical Riemannian setting used by Einstein in his theory of general relativity, the curvature of the space is constructed out of the connection, in terms of the Christoffel symbols that encode the connection in coordinates.

In the context of principal bundles, the connection provides a means of decomposing the tangent space to the bundle into complementary spaces, as show in Figure 4.8. Directions in the bundle that project to zero on the base space are called ***vertical directions***, and a ***connection*** specifies a set of directions, called ***horizontal directions***, at each point, which complements the space of vertical directions.

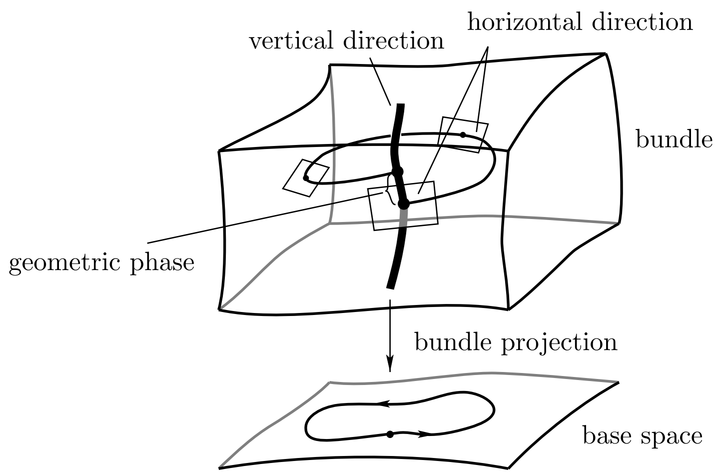


Figure 4.8: Geometric phase and connections.

In the rest of this section, we will formally define connections on principal bundles, and in the next section, discrete connections will be introduced in a parallel fashion.

Short Exact Sequence. This decomposition of the tangent space TQ into horizontal and vertical subspaces yields the following short exact sequence of vector bundles over Q,

$$0 \longrightarrow VQ \longrightarrow TQ \xrightarrow{\pi_*} \pi^* TS \longrightarrow 0\,,$$

where VQ is the vertical subspace of TQ, and $\pi^* TS$ is the pull-back of TS by the projection $\pi : Q \to S$.

Atiyah Sequence. When the short exact sequence above is quotiented modulo G, we obtain an exact sequence of vector bundles over S,

$$0 \longrightarrow \tilde{\mathfrak{g}} \xrightarrow{\ i\ } TQ/G \xrightarrow{\ \pi_*\ } TS \longrightarrow 0\,,$$

which is called the ***Atiyah sequence*** (see, for example Atiyah [1957]; Almeida and Molino [1985]; Mackenzie [1995]). Here, $\tilde{\mathfrak{g}}$ is the ***adjoint bundle***, which is a special case of an associated bundle (see Definition 4.4). In particular,

$$\tilde{\mathfrak{g}} = Q \times_G \mathfrak{g} = (Q \times \mathfrak{g})/G\,,$$

where the action of G on $Q \times \mathfrak{g}$ is given by $g(q,\xi) = (gq, Ad_g\xi)$, and $\pi_{\mathfrak{g}} : \tilde{\mathfrak{g}} \to S$ is given by $\pi_{\mathfrak{g}}([q,\xi]_G) = \pi(q)$.

The maps in the Atiyah sequence, $i : (Q \times \mathfrak{g})/G \to TQ/G$ and $\pi_* : TQ/G \to TS$, are given by

$$i([q,\xi]_G) = [\xi_Q(q)]_G,$$

and

$$\pi_*([v_q]_G) = T\pi(v_q).$$

Connection 1-form. Given a connection on a principal fiber bundle $\pi : Q \to Q/G$, we can represent this as a Lie algebra-valued ***connection*** 1***-form***, $\mathcal{A} : TQ \to \mathfrak{g}$, constructed as follows (see, for example, Kobayashi and Nomizu [1963]). Given an element of the Lie algebra $\xi \in \mathfrak{g}$, the infinitesimal generator map $\xi \mapsto \xi_Q$ yields a linear isomorphism between $\mathfrak{g}$ and V_qQ for each $q \in Q$. For each $v_q \in T_qQ$, we define $\mathcal{A}(v_q)$ to be the unique $\xi \in \mathfrak{g}$ such that ξ_Q is equal to the vertical component of v_q.

Proposition 4.1. *The connection* 1*-form,* $\mathcal{A} : TQ \to \mathfrak{g}$*, of a connection satisfies the following conditions.*

1. *The* 1*-form is* G*-equivariant, that is,*

$$\mathcal{A} \circ TL_g = \mathrm{Ad}_g \circ \mathcal{A}\,,$$

for every $g \in G$*, where* Ad *denotes the adjoint representation of* G *in* $\mathfrak{g}$*.*

2. *The* 1*-form induces a splitting of the Atiyah sequence, that is,*

$$\mathcal{A}(\xi_Q) = \xi\,,$$

for every $\xi \in \mathfrak{g}$.

Conversely, given a $\mathfrak{g}$-valued 1-form $\mathcal{A}$ on Q satisfying conditions 1 and 2, there is a unique connection in Q whose connection 1-form is $\mathcal{A}$.

Proof. See page 64 of Kobayashi and Nomizu [1963]. □

Horizontal Lift. The ***horizontal lift*** of a vector field $X \in \mathfrak{X}(S)$ is the unique vector field $X^h \in \mathfrak{X}(Q)$ which is horizontal and which projects onto X, that is, $T\pi_q(X^h_q) = X_{\pi(q)}$ for all $q \in Q$. The horizontal lift is in one-to-one correspondence with the choice of a connection on Q, as the following proposition states.

Proposition 4.2. *Given a connection in Q, and a vector field $X \in \mathfrak{X}(S)$, there is a unique horizontal lift X^h of X. The lift X^h is left-invariant under the action of G. Conversely, every horizontal vector field X^h on Q that is left-invariant by G is the lift of a vector field $X \in \mathfrak{X}(S)$.*

Proof. See page 65 of Kobayashi and Nomizu [1963]. □

Connection as a Splitting of the Atiyah Sequence. For a review of the basic concepts of homological algebra, properties of short exact sequences, and splittings, please refer to Appendix A. Consider the continuous Atiyah sequence,

$$0 \longrightarrow \tilde{\mathfrak{g}} \underset{(\pi_1,\mathcal{A})}{\overset{i}{\rightleftarrows}} TQ/G \underset{X^h}{\overset{\pi_*}{\rightleftarrows}} TS \longrightarrow 0$$

We see that the connection 1-form, $\mathcal{A} : TQ \to \mathfrak{g}$, induces a splitting of the continuous Atiyah sequence, since

$$(\pi_1, \mathcal{A}) \circ i([q,\xi]_G) = (\pi_1, \mathcal{A})([\xi_Q(q)]_g) = [q, \mathcal{A}(\xi_Q(q))]_G = [q,\xi]_G, \qquad \text{for all } q \in Q, \xi \in \mathfrak{g},$$

which is to say that $(\pi_1, \mathcal{A}) \circ i = 1_{\tilde{\mathfrak{g}}}$. Conversely, given a splitting of the continuous Atiyah sequence, we can extend the map, by equivariance, to yield a connection 1-form.

The horizontal lift also induces a splitting on the continuous Atiyah sequence, since, by definition, the horizontal lift of a vector field $X \in \mathfrak{X}(S)$ projects onto X, which is to say that $\pi_* \circ X^h = 1_{TS}$. The horizontal lift and the connection are related by the fact that

$$1_{TQ/G} = i \circ (\pi_1, \mathcal{A}) + X^h \circ \pi_*,$$

which is a simple consequence of the fact that the two splittings are part of the following commutative diagram,

$$\begin{array}{ccccccccc}
0 & \longrightarrow & \tilde{\mathfrak{g}} & \underset{(\pi_1,\mathcal{A})}{\overset{i}{\rightleftarrows}} & TQ/G & \underset{X^h}{\overset{\pi_*}{\rightleftarrows}} & TS & \longrightarrow & 0 \\
 & & \Big\| \, 1_{\tilde{\mathfrak{g}}} & & \Big\downarrow \alpha_{\mathcal{A}} & & \Big\| \, 1_{TS} & & \\
0 & \longrightarrow & \tilde{\mathfrak{g}} & \underset{\pi_1}{\overset{i_1}{\rightleftarrows}} & \tilde{\mathfrak{g}} \oplus TS & \underset{i_2}{\overset{\pi_2}{\rightleftarrows}} & TS & \longrightarrow & 0
\end{array}$$

where $\alpha_{\mathcal{A}}$ is an isomorphism (see Appendix A). The isomorphism is given in the following lemma.

Lemma 4.3. *The map $\alpha_{\mathcal{A}} : TQ/G \to \tilde{\mathfrak{g}} \oplus TS$ defined by*

$$\alpha_{\mathcal{A}}([q, \dot{q}]_G) = [q, \mathcal{A}(q, \dot{q})]_G \oplus T\pi(q, \dot{q}),$$

is a well-defined vector bundle isomorphism. The inverse of $\alpha_{\mathcal{A}}$ is given by

$$\alpha_{\mathcal{A}}^{-1}([q, \xi]_G \oplus (x, \dot{x})) = [(x, \dot{x})_q^h + \xi q]_G.$$

Proof. See page 15 of Cendra et al. [2001]. □

This lemma, and its higher-order generalization, that identifies $T^{(2)}Q/G$ with $T^{(2)}S \times_S 2\tilde{\mathfrak{g}}$, is critical in allowing us to construct the Lagrange–Poincaré operator, which is an intrinsic method of expressing the reduced equations arising from Lagrangian reduction.

In the next section, we will develop the theory of discrete connections on principal bundles in a parallel fashion to the way we introduced continuous connections.

4.4 Discrete Connections

Discrete variational mechanics is based on the idea of approximating the tangent bundle TQ of Lagrangian mechanics with the pair groupoid $Q \times Q$. As such, the purpose of a discrete connection is to decompose the subset of $Q \times Q$ that projects to a neighborhood of the diagonal of $S \times S$ into horizontal and vertical spaces.

The reason why we emphasize that the construction is only valid for the subset of $Q \times Q$ that projects to a neighborhood of the diagonal of $S \times S$ is that there are topological obstructions to globalizing the construction to all of $Q \times Q$ except in the case that Q is a trivial bundle.

One of the challenges of dealing with the discrete space modelled by the pair groupoid $Q \times Q$ is that it is not a linear space, in contrast to TQ. As we shall see, the standard pair groupoid composition is not sufficient to make sense of the notion of an element $(q_0, q_1) \in Q \times Q$ being the composition of a horizontal and a vertical element. We will propose a natural notion of composing an element with a vertical element that makes sense of the horizontal and vertical decomposition.

In the subsequent sections, we will use the discrete connection to extend the pair groupoid composition even further, and explore its applications to the notion of curvature in discrete geometry.

Intrinsic Representation of the Tangent Bundle. The intuition underlying our construction of discrete horizontal and vertical spaces is best developed by considering the intrinsic representation of the tangent bundle. This representation is obtained by identifying a tangent vector at a point on the manifold with the equivalence class of curves on the manifold going through the point, such that the tangent to the curve at the point is given by the tangent vector. This notion is illustrated in Figure 4.9.

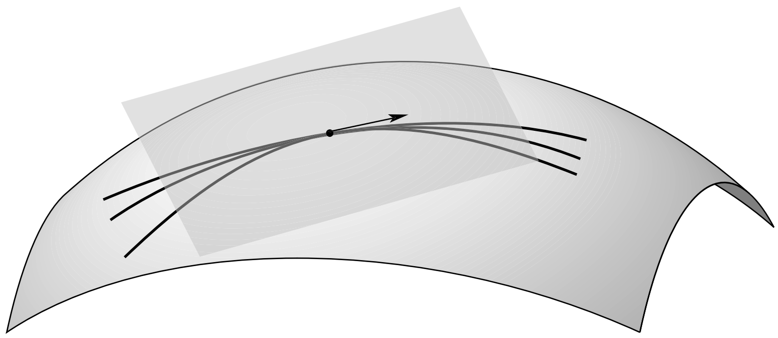


Figure 4.9: Intrinsic representation of the tangent bundle.

Given a vector $v_q \in TQ$, we identify it with the family of curves $q : \mathbb{R} \to Q$, such that $q(0) = q$, and $\dot{q}(0) = v$. The equivalence class $[\,\cdot\,]$ identifies curves with the same basepoint, and the same velocity at the basepoint.

With this representation, it is natural to consider $(q_0, q_1) \in Q \times Q$ to be an approximation of $[q(\cdot)] = v_q \in TQ$, in the sense that,

$$q_0 = q(0), \qquad\qquad q_1 = q(h),$$

for some fixed time step h, and where $q(\cdot)$ is a representative curve corresponding to v_q in the intrinsic representation of the tangent bundle.

4.4.1 Horizontal and Vertical Subspaces of $Q \times Q$

Recall that the vertical subspace at a point q, denoted V_q, is given by

$$V_q = \{v_q \in TQ \mid \pi_*(v_q) = 0\} = \{\xi_Q \mid \xi \in \mathfrak{g}\}.$$

Notice that the vertical space is precisely that subspace of TQ which maps under the lifted projection map to the embedded copy of S in TS. We proceed in an analogous fashion to define a discrete vertical subspace at a point q.

The natural discrete analogue of the lifted projection map π_* is the diagonal action of the projection map on $Q \times Q$, $(\pi, \pi) : Q \times Q \to Q \times Q$, where $(q_0, q_1) \mapsto (\pi q_0, \pi q_1)$. This is because

$$\pi_*(v_q) = \pi_*([q(\cdot)]) = [\pi(q(\cdot))].$$

In the same way that we embed S into TS by the map $x \mapsto [x] = 0_x$, S naturally embeds itself into the diagonal of $S \times S$, $x \mapsto (x, x) = e_{S\times S}$, which we recall is the identity subspace of the pair groupoid.

The alternative description of the vertical space is in terms of the embedding of $Q \times \mathfrak{g}$ into TQ, by $(q, \xi) \mapsto \xi_Q(q)$, using the infinitesimal generator construction,

$$\xi_Q(q) = [\exp(\xi t) q].$$

In an analogous fashion, we construct a ***discrete generator*** map, which is given in the following definition.

Definition 4.5. *The **discrete generator** is the map $i : Q \times G \to Q \times Q$, given by*

$$i(q, g) = (q, gq),$$

which we also denote by $i_q(g) = i(q, g) = (q, gq)$.

Then, we have the following definition of the ***discrete vertical space***.

Definition 4.6. *The **discrete vertical space** is given by*

$$\begin{aligned} \mathrm{Ver}_q &= \{(q, q') \in Q \times Q \mid (\pi, \pi)(q, q') = e_{S\times S}\} \\ &= \{i_q(g) \mid g \in G\}. \end{aligned}$$

This is the discrete analogue of the statement $\mathrm{Ver}_q = \{v_q \in TQ \mid \pi_*(v_q) = 0\} = \{\xi_Q \mid \xi \in \mathfrak{g}\}$.

Since the pair groupoid composition is only defined on the space of composable pairs, we need to extend the composition to make sense of how the discrete horizontal space is complementary to the discrete vertical space. In particular, we define the composition of a vertical element with an arbitrary element of $Q \times Q$ as follows.

Definition 4.7. *The composition of an arbitrary element* $(q_0, q_1) \in Q \times Q$ *with a vertical element is given by*

$$i_{q_0}(g) \cdot (q_0, q_1) = (e, g)(q_0, q_1) = (q_0, gq_1).$$

An elementary consequence of this definition is that it makes the discrete generator map a homomorphism.

Lemma 4.4. *The discrete generator,* i_q*, is a homomorphism. This is a discrete analogue of the statement in the continuous theory that* $(\xi + \chi)_Q = \xi_Q + \chi_Q$*.*

Proof. We compute,

$$\begin{aligned} i_q(g) \cdot i_q(h) &= i_q(g) \cdot (q, hq) \\ &= (e, g)(q, hq) \\ &= (q, ghq) \\ &= i_q(gh). \end{aligned}$$

Therefore, i_q is a homomorphism. □

If we define the G action on $Q \times G$ to be $h(q, g) = (hq, hgh^{-1})$, we find that the composition of a vertical element with an arbitrary element is G-equivariant.

Lemma 4.5. *The composition of a vertical element with an arbitrary element of* $Q \times Q$ *is* G*-equivariant,*

$$i_{hq_0}(hgh^{-1}) \cdot (hq_0, hq_1) = h \cdot i_{q_0}(g) \cdot (q_0, q_1).$$

Proof. Consider the following computation,

$$\begin{aligned} i_{hq_0}(hgh^{-1}) \cdot (hq_0, hq_1) &= (hq_0, hgh^{-1}hq_1) \\ &= (hq_0, hgq_1) \\ &= h(q_0, gq_1) \\ &= h \cdot i_{q_0}(g) \cdot (q_0, q_1). \end{aligned}$$

□

Having made sense of how to compose an arbitrary element of $Q \times Q$ with a vertical element, we are in a position to introduce the notion of a discrete connection.

A ***discrete connection*** is a G-equivariant choice of a subset of $Q \times Q$ called the ***discrete horizontal space***, that is complementary to the discrete vertical space. In particular, given $(q_0, q_1) \in Q \times Q$, a discrete connection decomposes this into the ***horizontal component***, $\mathrm{hor}(q_0, q_1)$, and the ***vertical component***, $\mathrm{ver}(q_0, q_1)$, such that

$$\mathrm{ver}(q_0, q_1) \cdot \mathrm{hor}(q_0, q_1) = (q_0, q_1)\,,$$

in the sense of the composition of a vertical element with an arbitrary element we defined previously. Furthermore, the G-equivariance condition states that

$$\mathrm{hor}(gq_0, gq_1) = g \cdot \mathrm{hor}(q_0, q_1)\,,$$

and

$$\mathrm{ver}(gq_0, gq_1) = g \cdot \mathrm{ver}(q_0, q_1)\,.$$

4.4.2 Discrete Atiyah Sequence

Recall that we obtain a short exact sequence corresponding to the decomposition of TQ into horizontal and vertical spaces. Due to the equivariant nature of the decomposition, quotienting this short exact sequence yields the Atiyah sequence. In this subsection, we will introduce the analogous discrete objects.

Short Exact Sequence. The decomposition of the pair groupoid $Q \times Q$, into discrete horizontal and vertical spaces, yields the following short exact sequence of bundles over Q.

$$0 \longrightarrow \mathrm{Ver}\, Q \xrightarrow{\;i\;} Q \times Q \xrightarrow{(\pi,\pi)} (\pi, \pi)^* S \times S \longrightarrow 0,$$

where $\mathrm{Ver}\, Q$ is the discrete vertical subspace of $Q \times Q$, and $(\pi, \pi)^* S \times S$ is the pull-back of $S \times S$ by the projection $(\pi, \pi) : Q \times Q \to S \times S$.

Discrete Atiyah Sequence. When the short exact sequence above is quotiented modulo G, we obtain an exact sequence of bundles over S,

$$0 \longrightarrow \tilde{G} \xrightarrow{\;i\;} (Q \times Q)/G \xrightarrow{(\pi,\pi)} S \times S \longrightarrow 0\,,$$

which we call the ***discrete Atiyah sequence***. Here, $\tilde{G}$ is an associated bundle (see Definition 4.4). In particular,

$$\tilde{G} = Q \times_G G = (Q \times G)/G\,,$$

where the action of G on $Q \times G$ is given by $g(q,h) = (gq, ghg^{-1})$, which is the natural discrete analogue of the adjoint action of $\mathfrak{g}$ on $Q \times \mathfrak{g}$. Furthermore, $\pi_G : \tilde{G} \to S$ is given by $\pi_G([q,g]_G) = \pi(q)$.

The maps in the discrete Atiyah sequence $i : \tilde{G} \to (Q \times Q)/G$, and $(\pi,\pi) : (Q \times Q)/G] \to S \times S$, are given by

$$i([q,g]_G) = [q, gq]_G = [i_q(g)]_G \,,$$

and

$$(\pi,\pi)([q_0,q_1]_g) = (\pi q_0, \pi q_1) \,.$$

4.4.3 Equivalent Representations of a Discrete Connection

In addition to the discrete connection which arises from a G-equivariant decomposition of the pair groupoid $Q \times Q$ into a discrete horizontal and vertical space, we have equivalent representations in terms of splittings of the discrete Atiyah sequence, as well as maps on the unreduced short exact sequence.

Maps on the Unreduced Short Exact Sequence. These correspond to discrete analogues of the connection 1-form, and the horizontal lift.

- Discrete connection 1-form, $\mathcal{A}_d : Q \times Q \to G$.
- Discrete horizontal lift, $(\cdot,\cdot)^h_q : S \times Q \to Q \times Q$.

Maps That Yield a Splitting of the Discrete Atiyah Sequence.

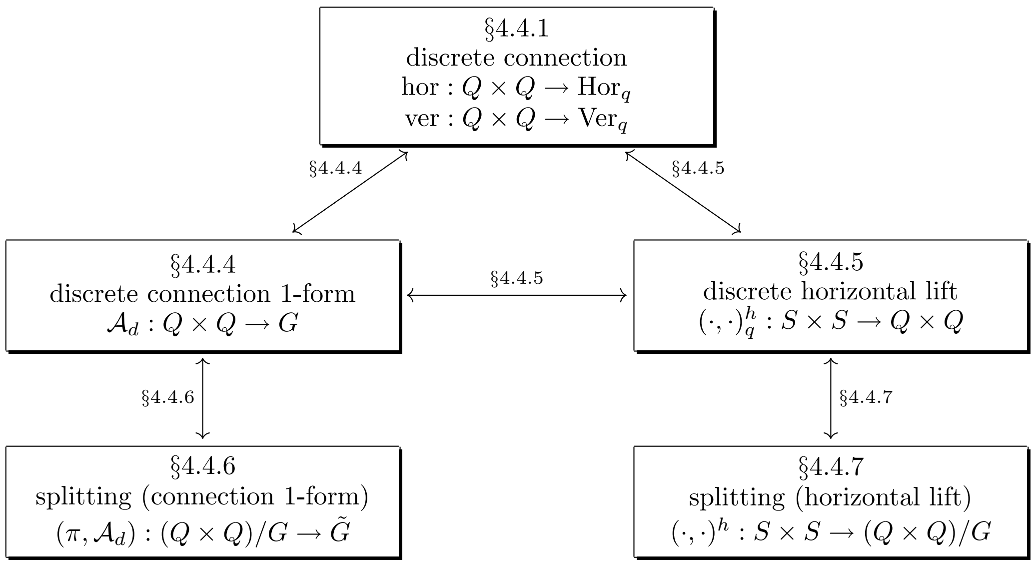
- $(\pi_1, \mathcal{A}_d) : (Q \times Q)/G \to \tilde{G}$, which is related to the discrete connection 1-form.
- $(\cdot,\cdot)^h : S \times S \to (Q \times Q)/G$, which is related to the discrete horizontal lift.

Relating the Two Sets of Representations. These two sets of representations are related in the following way:

- The maps on the unreduced short exact sequence are equivariant, and hence drop to the discrete Atiyah sequence, where they induce splittings of the short exact sequence.
- The maps that yield splittings of the discrete Atiyah sequence can be extended equivariantly to recover the maps on the unreduced short exact sequence.

Furthermore, standard results from homological algebra (see Appendix A) yield an equivalence between the two splittings of the discrete Atiyah sequence.

In the rest of this section, we will also discuss in detail the method of moving between the various representations of the discrete connection. The organization of the rest of the section, and the subsections in which we relate the various representations are given in the following diagram.



4.4.4 Discrete Connection 1-Form

Given a discrete connection on a principal fiber bundle $\pi : Q \to Q/G$, we can represent this as a Lie group-valued ***discrete connection*** 1***-form***, $\mathcal{A}_d : Q \times Q \to G$, which is a natural generalization of the Lie algebra-valued connection 1-form on tangent bundles, $\mathcal{A} : TQ \to \mathfrak{g}$, to the discrete context.

Discrete Connection 1-Forms from Discrete Connections. The discrete connection 1-form is constructed as follows. Given an element of the Lie group $g \in G$, the discrete generator map $g \mapsto i_q(g)$ yields an isomorphism between G and Ver_q for each $q \in Q$. For each $(q_0, q_1) \in Q \times Q$, we define $\mathcal{A}_d(q_0, q_1)$ to be the unique $g \in G$ such that $i_q(g)$ is equal to the vertical component of (q_0, q_1). In particular, this is equivalent to the condition that the following statement holds,

$$(q_0, q_1) = i_{q_0}(\mathcal{A}_d(q_0, q_1)) \cdot \mathrm{hor}(q_0, q_1).$$

Remark 4.1. *It follows from the above identity that the discrete horizontal space can also be expressed as*

$$\begin{aligned}\mathrm{Hor}_{q_0} &= \{(q_0, q_1) \in Q \times Q \mid \mathrm{hor}(q_0, q_1) = (q_0, q_1)\} \\ &= \{(q_0, q_1) \in Q \times Q \mid \mathcal{A}_d(q_0, q_1) = e\}.\end{aligned}$$

We will now establish a few properties of the discrete connection 1-form.

Proposition 4.6. *The **discrete connection** 1**-form**, $\mathcal{A}_d : Q \times Q \to G$, satisfies the following properties.*

1. *The* 1*-form is* G*-equivariant, that is,*

$$\mathcal{A}_d \circ L_g = I_g \circ \mathcal{A}_d,$$

   which is the discrete analogue of the G*-equivariance of the continuous connection,* $\mathcal{A} \circ TL_g = Ad_g \circ \mathcal{A}$.

2. *The* 1*-form induces a splitting of the Discrete Atiyah sequence, that is,*

$$\mathcal{A}_d(i_q(g)) = \mathcal{A}_d(q_0, gq_0) = g,$$

   which is the discrete analogue of $\mathcal{A}(\xi_Q) = \xi$.

Proof. The proof relies on the properties of a discrete connection, and the definition of the discrete connection 1-form.

1. The discrete connection 1-form satisfies the condition

$$(q_0, q_1) = i_{q_0}(\mathcal{A}_d(q_0, q_1)) \cdot \text{hor}(q_0, q_1)\,.$$

   If we denote $\text{hor}(q_0, q_1)$ by $(q_0, \bar{q}_1)$, we have that

$$(q_0, q_1) = (q_0, \mathcal{A}_d(q_0, q_1)\bar{q}_1)\,.$$

   Similarly, we have,

$$\begin{aligned}(gq_0, gq_1) &= i_{gq_0}(\mathcal{A}_d(gq_0, gq_1)) \cdot \text{hor}(gq_0, gq_1) \\ &= i_{gq_0}(\mathcal{A}_d(gq_0, gq_1)) \cdot g \cdot \text{hor}(q_0, q_1) \\ &= (e, \mathcal{A}_d(gq_0, gq_1))(gq_0, g\bar{q}_1) \\ &= (gq_0, \mathcal{A}_d(gq_0, gq_1)g\bar{q}_1)\,,\end{aligned}$$

   where we have used the G-equivariance of the discrete horizontal space. By looking at the expressions for gq_1 and q_1, we conclude that

$$\begin{aligned}\mathcal{A}_d(gq_0, gq_1)g\bar{q}_1 &= gq_1 \\ &= g\mathcal{A}_d(q_0, q_1)\bar{q}_1\,, \\ \mathcal{A}_d(gq_0, gq_1)g &= g\mathcal{A}_d(q_0, q_1)\,, \\ \mathcal{A}_d(gq_0, gq_1) &= g\mathcal{A}_d(q_0, q_1)g^{-1}\,,\end{aligned}$$

which is precisely the statement that $\mathcal{A}_d \circ L_g = I_g \circ \mathcal{A}_d$, that is to say that $\mathcal{A}_d$ is G-equivariant.

2. Recall that $i_q(g)$ is an element of the discrete vertical space. Since the discrete horizontal space is complementary to the discrete vertical space, it follows that $\operatorname{ver}(i_q(g)) = i_q(g)$. Then, by the construction of the discrete connection 1-form, $\mathcal{A}_d(i_q(g))$ is the unique element of G such that

$$i_q(\mathcal{A}_d(i_q(g))) = \operatorname{ver}(i_q(g)) = i_q(g)\,.$$

Since i_q is an isomorphism between G and the discrete vertical space, we conclude that $\mathcal{A}_d(i_q(g)) = g$, as desired. □

The second result is equivalent to the map recovering the discrete Euler–Poincaré connection when restricted to a G-fiber, that is, $\mathcal{A}_d(x, g_0, x, g_1) = g_1 g_0^{-1}$. In particular, it follows that the map is trivial when restricted to the diagonal space, that is, $\mathcal{A}_d(q, q) = e$.

The properties of a discrete connection are discrete analogues of the properties of a continuous connection in the sense that if a discrete connection has a given property, the corresponding continuous connection which is induced in the infinitesimal limit has the analogous continuous property. The precise sense in which a discrete connection induces a continuous connection will be discussed in §4.5.2.

Discrete Connections from Discrete Connection 1-Forms. Having shown how to obtain a discrete connection 1-form from a discrete connection, let us consider the converse case of obtaining a discrete connection from a discrete connection 1-form with the properties above. We do this by constructing the discrete horizontal and vertical components as follows.

Definition 4.8. *Given a discrete connection* 1*-form,* $\mathcal{A}_d : Q \times Q \to G$ *that is* G*-equivariant and induces a splitting of the discrete Atiyah sequence, we define the* ***horizontal component*** *to be*

$$\operatorname{hor}(q_0, q_1) = i_{q_0}((\mathcal{A}_d(q_0, q_1))^{-1}) \cdot (q_0, q_1)\,.$$

*The **vertical component** is given by*

$$\mathrm{ver}(q_0, q_1) = i_{q_0}(\mathcal{A}_d(q_0, q_1))\,.$$

Proposition 4.7. *The discrete connection we obtain from a discrete connection 1-form has the following properties.*

1. *The discrete connection yields a horizontal and vertical decomposition of $Q \times Q$, in the sense that*

   $$(q_0, q_1) = \mathrm{ver}(q_0, q_1) \cdot \mathrm{hor}(q_0, q_1)\,,$$

   for all $(q_0, q_1) \in Q \times Q$.

2. *The discrete connection is G-equivariant, in the sense that*

   $$\mathrm{hor}(gq_0, gq_1) = g \cdot \mathrm{hor}(q_0, q_1)\,,$$

   and

   $$\mathrm{ver}(gq_0, gq_1) = g \cdot \mathrm{ver}(q_0, q_1)\,.$$

Proof. The proof relies on the properties of the discrete connection 1-form, and the definitions of the discrete horizontal and vertical spaces.

1. Consider the following computation,

   $$\begin{aligned}\mathrm{ver}(q_0, q_1) \cdot \mathrm{hor}(q_0, q_1) &= i_{q_0}(\mathcal{A}_d(q_0, q_1)) \cdot i_{q_0}((\mathcal{A}_d(q_0, q_1))^{-1}) \cdot (q_0, q_1)\\ &= i_{q_0}(\mathcal{A}_d(q_0, q_1)(\mathcal{A}_d(q_0, q_1))^{-1}) \cdot (q_0, q_1)\\ &= i_{q_0}(e) \cdot (q_0, q_1)\\ &= (q_0, q_1)\,,\end{aligned}$$

   where we used that i_q is a homomorphism (see Lemma 4.4).

2. We compute,

   $$\begin{aligned}\mathrm{hor}(gq_0, gq_1) &= i_{gq_0}((\mathcal{A}_d(gq_0, gq_1))^{-1}) \cdot (gq_0, gq_1)\\ &= i_{gq_0}(g(\mathcal{A}_d(q_0, q_1))^{-1}g^{-1}) \cdot (gq_0, gq_1)\\ &= (e, g(\mathcal{A}_d(q_0, q_1))^{-1}g^{-1})(gq_0, gq_1)\end{aligned}$$

$$
\begin{aligned}
&= (gq_0, g(\mathcal{A}_d(q_0, q_1))^{-1} q_1) \\
&= g \cdot i_{q_0}((\mathcal{A}_d(q_0, q_1))^{-1}) \cdot (q_0, q_1) \\
&= g \cdot \mathrm{hor}(q_0, q_1)\,,
\end{aligned}
$$

where we have used the fact that the composition of a vertical element with an arbitrary element is G-equivariant (see Lemma 4.5). Similarly, we compute,

$$
\begin{aligned}
\mathrm{ver}(gq_0, gq_1) &= i_{gq_0}(\mathcal{A}_d(gq_0, gq_1)) \\
&= i_{gq_0}(g\mathcal{A}_d(q_0, q_1)g^{-1}) \\
&= (gq_0, g\mathcal{A}_d(q_0, q_1)g^{-1}gq_0) \\
&= g \cdot (q_0, \mathcal{A}_d(q_0, q_1)q_0) \\
&= g \cdot i_{q_0}(\mathcal{A}_d(q_0, q_1)) \\
&= g \cdot \mathrm{ver}(q_0, q_1)\,.
\end{aligned}
$$

□

Local Representation of the Discrete Connection 1-Form. Since the discrete connection 1-form can be thought of as comparing group fiber quantities at different base points, we obtain the natural identity that

$$\mathcal{A}_d(gq_0, hq_1) = h\mathcal{A}_d(q_0, q_1)g^{-1}.$$

In a local trivialization, this corresponds to

$$\mathcal{A}_d(x_0, g_0, x_1, g_1) = g_1\mathcal{A}_d(x_0, e, x_1, e)g_0^{-1}.$$

We define

$$A(x_0, x_1) = \mathcal{A}_d(x_0, e, x_1, e),$$

which yields the local representation of the discrete connection 1-form.

Definition 4.9. *Given a discrete connection* 1*-form,* $\mathcal{A}_d : Q \times Q \to G$*, its* ***local representation*** *is given by*

$$\mathcal{A}_d(x_0, g_0, x_1, g_1) = g_1 A(x_0, x_1) g_0^{-1}\,,$$

where

$$A(x_0, x_1) = \mathcal{A}_d(x_0, e, x_1, e)\,.$$

Lemma 4.8. *The local representation of a discrete connection is* G*-equivariant.*

Proof. Consider the following computation,

$$\begin{aligned}\mathcal{A}_d(g(x_0,g_0),g(x_1,g_1)) &= \mathcal{A}_d((x_0,gg_0),(x_1,gg_1))\\ &= gg_1A(x_0,x_1)(gg_0)^{-1}\\ &= g(g_1A(x_0,x_1)g_0^{-1})g^{-1}\\ &= g\mathcal{A}_d((x_0,g_0),(x_1,g_1))g^{-1}\,,\end{aligned}$$

which shows that the local representation is G-equivariant, as expected. □

Notice also that in the pure group case, where $Q = G$, this recovers the discrete Euler–Poincaré connection, as we would expect, since the shape space is trivial. In particular, $x_0 = x_1 = e$, which implies that $A(x_0, x_1) = \mathcal{A}_d(e, e, e, e) = e$, and $\mathcal{A}_d(g_0, g_1) = g_1g_0^{-1}$.

Example 4.1. *As an example, we construct the natural discrete analogue of the mechanical connection, $\mathcal{A} : TQ \to \mathfrak{g}$, by the following procedure, which yields a discrete connection 1-form, $\mathcal{A}_d : Q \times Q \to G$.*

1. *Given the point $(q_0, q_1) \in Q \times Q$, we construct the geodesic path $q_{01} : [0, 1] \to Q$ with respect to the kinetic energy metric, such that $q_{01}(0) = q_0$, and $q_{01}(1) = q_1$.*

2. *Project the geodesic path to the shape space, $x_{01}(t) \equiv \pi q_{01}(t)$, to obtain the curve x_{01} on S.*

3. *Taking the horizontal lift of x_{01} to Q using the connection $\mathcal{A}$ yields $\tilde{q}_{01}$.*

4. *There is a unique $g \in G$ such that $q_{01}(1) = g \cdot \tilde{q}_{01}(1)$.*

5. *Define $\mathcal{A}_d(q_0, q_1) = g$.*

This discrete connection is consistent with the classical notion of a connection in the limit that q_1 approaches q_0, in the usual sense in which discrete mechanics on $Q \times Q$ converges to continuous Lagrangian mechanics on TQ. As mentioned before, this statement is made more precise in §4.5.2.

4.4.5 Discrete Horizontal Lift

The ***discrete horizontal lift*** of an element $(x_0, x_1) \in S \times S$ is the subset of $Q \times Q$ that are horizontal elements, and project to (x_0, x_1). Once we specify the base point $q \in Q$, the discrete horizontal lift is unique, and we introduce the map $(\cdot, \cdot)^h_q : S \times S \to Q \times Q$.

Discrete Horizontal Lifts from Discrete Connections. The discrete horizontal lift can be constructed once the discrete horizontal space is defined by a choice of discrete connection.

Definition 4.10. *The **discrete horizontal lift** is the unique map* $(\cdot,\cdot)_q^h : S\times S \to Q\times Q$*, such that*

$$(\pi,\pi)\cdot(x_0,x_1)_q^h = (x_0,x_1)\,,$$

and

$$(x_0,x_1)_q^h \in \mathrm{Hor}_q\ .$$

Lemma 4.9. *The discrete horizontal lift is* G*-equivariant, which is to say that*

$$(x_0,x_1)_{gq}^h = g\cdot(x_0,x_1)_q^h\,.$$

Proof. Given $(x_0,x_1)\in S\times S$, denote $(x_0,x_1)_{q_0}^h$ by (q_0,q_1). Then, by the definition of the discrete horizontal lift, we have that

$$(\pi,\pi)\cdot(q_0,q_1) = (x_0,x_1)\,,$$

and it follows that

$$(\pi,\pi)\cdot(gq_0,gq_1) = (x_0,x_1)\,.$$

Also, from the definition of the discrete horizontal lift,

$$(q_0,q_1)\in \mathrm{Hor}_{q_0}\,,$$

and by the G-equivariance of the horizontal space,

$$(gq_0,gq_1)\in g\cdot \mathrm{Hor}_{q_0} = \mathrm{Hor}_{gq_0}\ .$$

This implies that (gq_0,gq_1) satisfies the conditions for being the discrete horizontal lift of (x_0,x_1) with basepoint gq_0. Therefore, $(x_0,x_1)_{gq_0}^h = (gq_0,gq_1) = g\cdot(q_0,q_1) = g\cdot(x_0,x_1)_{q_0}^h$, as desired. □

Discrete Connections from Discrete Horizontal Lifts. Conversely, given a discrete horizontal lift, we can recover a discrete connection.

Definition 4.11. *Given a discrete horizontal lift, we define the **horizontal component** to be*

$$\mathrm{hor}(q_0,q_1) = (\pi(q_0,q_1))_{q_0}^h\,,$$

*and the **vertical component** is given by*

$$\mathrm{ver}(q_0, q_1) = i_{q_0}(g)\,,$$

where g is the unique group element such that

$$(q_0, q_1) = i_{q_0}(g) \cdot \mathrm{hor}(q_0, q_1)\,.$$

The last expression simply states that the discrete horizontal and vertical space are complementary with respect to the composition we defined between a vertical element and an arbitrary element of $Q \times Q$.

Discrete Horizontal Lifts from Discrete Connection 1-Forms. We wish to construct a discrete horizontal lift $(\cdot, \cdot)^h : S \times S \to (Q \times Q)/G$, given a discrete connection $\mathcal{A}_d : Q \times Q \to G$. We state the construction of such a discrete horizontal lift as a proposition.

Proposition 4.10. *Given a discrete connection 1-form, $\mathcal{A}_d : Q \times Q \to G$, the discrete horizontal lift is given by*

$$(x_0, x_1)^h = [\pi^{-1}(x_0, x_1) \cap \mathcal{A}_d^{-1}(e)]_G.$$

Furthermore, the discrete horizontal lift satisfies the following identity,

$$i_{q_0}(\mathcal{A}_d(q_0, q_1)) \cdot (\pi(q_0, q_1))^h_{q_0} = (q_0, q_1),$$

which implies that the discrete connection 1-form and the discrete horizontal lift induces a horizontal and vertical decomposition of $Q \times Q$.

The horizontal lift can be expressed in a local trivialization, where $q_0 = (x_0, g_0)$, using the local expression for the discrete connection,

$$(x_0, x_1)^h_{q_0} = (x_0, g_0, x_1, g_0(A(x_0, x_1))^{-1}).$$

Proof. We will show that this operation is well-defined on the quotient space. Using the local representation of the discrete connection in the local trivialization (see Definition 4.9), we have,

$$\begin{aligned}
&\mathcal{A}_d^{-1}(e) \cap \pi^{-1}(x_0, x_1) \\
&\qquad = \{(\tilde{x}_0, g, \tilde{x}_1, g \cdot (A(\tilde{x}_0, \tilde{x}_1))^{-1}) \mid \tilde{x}_0, \tilde{x}_1 \in S, g \in G\} \\
&\qquad\qquad \cap \{(x_0, h_0, x_1, h_1) \mid h_0, h_1 \in G\} \\
&\qquad = \{(x_0, g, x_1, g \cdot (A(x_0, x_1))^{-1}) \mid h \in G\}
\end{aligned}$$

$$= G \cdot (x_0, e, x_1, (A(x_0, x_1))^{-1}),$$

which is a well-defined element of $(Q \times Q)/G$. Since this is true in a local trivialization, and both the discrete connection and projection operators are globally defined, this inverse coset is globally well-defined as an element of $(Q \times Q)/G$.

In particular, the computation above allows us to obtain a local expression for the discrete horizontal lift in terms of the local representation of the discrete connection. That is,

$$\begin{aligned} (x_0, x_1)^h_{(x_0,e)} &= (x_0, e, x_1, (A(x_0, x_1))^{-1}), \\ (x_0, x_1)^h &= [(x_0, e, x_1, (A(x_0, x_1))^{-1})]_G. \end{aligned}$$

By the properties of the discrete horizontal lift, this extends to $\pi^{-1}(x_0, x_1) \subset Q \times Q$,

$$\begin{aligned} (x_0, x_1)^h_{(x_0,g)} &= (x_0, x_1)^h_{g(x_0,e)} \\ &= g \cdot (x_0, x_1)^h_{(x_0,e)} \\ &= g(x_0, e, x_1, (A(x_0, x_1))^{-1}) \\ &= (x_0, g, x_1, g(A(x_0, x_1))^{-1}). \end{aligned}$$

To prove the second claim, we have in the local trivialization of $Q \times Q$, $(q_0, q_1) = (x_0, g_0, x_1, g_1)$. Then, by the result above,

$$(\pi(q_0, q_1))^h_{q_0} = (\pi(q_0, q_1))^h_{(x_0,g_0)} = (x_0, g_0, x_1, g_0(A(x_0, x_1))^{-1}).$$

Also, by the local representation of the discrete connection,

$$\mathcal{A}_d(q_0, q_1) = g_1 A(x_0, x_1) g_0^{-1}.$$

Therefore,

$$\begin{aligned} i_{q_0}(\mathcal{A}_d(q_0, q_1) \cdot (\pi(q_0, q_1))^h_{q_0} &= (e, \mathcal{A}_d(q_0, q_1)) \cdot (\pi(q_0, q_1))^h_{q_0} \\ &= (e, g_1 A(x_0, x_1) g_0^{-1}) \cdot (x_0, g_0, x_1, g_0(A(x_0, x_1))^{-1}) \\ &= (x_0, g_0, x_1, (g_1 A(x_0, x_1) g_0^{-1})(g_0(A(x_0, x_1))^{-1})) \\ &= (x_0, g_0, x_1, g_1) \\ &= (q_0, q_1), \end{aligned}$$

as claimed. $\square$

Discrete Connection 1-Forms from Discrete Horizontal Lifts. Given a horizontal lift $(\cdot,\cdot)_q^h : S \times S \to Q \times Q$, we wish to construct a discrete connection 1-form, $\mathcal{A}_d : Q \times Q \to G$.

Lemma 4.11. *Given a discrete horizontal lift, $(\cdot,\cdot)_q^h : S \times S \to Q \times Q$, the **discrete connection 1-form**, $\mathcal{A}_d : Q \times Q \to G$, is uniquely defined by the following identity,*

$$i_{q_0}(\mathcal{A}_d(q_0, q_1)) \cdot (\pi(q_0, q_1))_{q_0}^h = (q_0, q_1).$$

Proof. To show that this construction is well-defined, we note that $\pi_1(q_0, q_1) = \pi_1(\pi(q_0, q_1))_{q_0}^h$, by the construction of $(\cdot,\cdot)_{q_0}^h$ from $(\cdot,\cdot)^h : S \times S \to (Q \times Q)/G$. Furthermore, $\pi_2(q_0, q_1)$ and $\pi_2(\pi(q_0, q_1))_{q_0}^h$ are in the same fiber of the principal bundle $\pi : Q \to Q/G$ and are therefore related by a unique element $g \in G$. Since this element is unique, $\mathcal{A}_d(q_0, q_1)$ is uniquely defined by the identity. $\square$

4.4.6 Splitting of the Discrete Atiyah Sequence (Connection 1-Form)

Consider the discrete Atiyah sequence,

$$0 \longrightarrow \tilde{G} \underset{(\pi_1, \mathcal{A}_d)}{\overset{(q, gq)}{\rightleftarrows}} (Q \times Q)/G \underset{(\cdot,\cdot)^h}{\overset{(\pi,\pi)}{\rightleftarrows}} S \times S \longrightarrow 0 \ .$$

As we see from Theorem A.2, given a short exact sequence

$$0 \longrightarrow A_1 \underset{k}{\overset{f}{\rightleftarrows}} B \underset{h}{\overset{g}{\rightleftarrows}} A_2 \longrightarrow 0 \ ,$$

there are three equivalent conditions under which the exact sequence is split. They are as follows,

1. There is a homomorphism $h : A_2 \to B$ with $g \circ h = 1_{A_2}$;
2. There is a homomorphism $k : B \to A_1$ with $k \circ f = 1_{A_1}$;
3. The given sequence is isomorphic (with identity maps on A_1 and A_2) to the direct sum short exact sequence,

   $$0 \longrightarrow A_1 \xrightarrow{i_1} A_1 \oplus A_2 \xrightarrow{\pi_2} A_2 \longrightarrow 0 \ ,$$

   and in particular, $B \cong A_1 \oplus A_2$.

We will address all three conditions in this and the next two subsections.

Splittings from Discrete Connection 1-Forms. A discrete connection 1-form, $\mathcal{A}_d : Q\times Q \to G$, induces a splitting of the discrete Atiyah sequence, in the sense that

$$(\pi_1, \mathcal{A}_d) \circ i = 1_{\tilde{G}}\,.$$

Lemma 4.12. *Given a discrete connection* 1*-form,* $\mathcal{A}_d : Q \times Q \to G$*, we obtain a splitting of the discrete Atiyah sequence,* $\varphi : (Q \times Q)/G \to \tilde{G}$*, which is given by*

$$\varphi([q_0, q_1]_G) = [q_0, \mathcal{A}_d(q_0, q_1)]_G.$$

We denote this map by $(\pi_1, \mathcal{A}_d)$*.*

Proof. This expression is well-defined, as the following computation shows,

$$\begin{aligned}\varphi([gq_0, gq_1]_G) &= [gq_0, \mathcal{A}_d(gq_0, gq_1)]_G\\ &= [gq_0, g\mathcal{A}_d(q_0, q_1)g^{-1}]_G\\ &= \varphi([q_0, q_1]_G).\end{aligned}$$

Furthermore, since

$$\begin{aligned}(\pi_1, \mathcal{A}_d) \circ i([q, g]_G) &= (\pi_1, \mathcal{A}_d)([q, gq]_G)\\ &= [\pi_1(q, gq), \mathcal{A}_d(q, gq)]_G\\ &= [q, g]_G,\end{aligned}$$

it follows that we obtain a splitting of the discrete Atiyah sequence. □

Discrete Connection 1-Forms from Splittings. Given a splitting of the discrete Atiyah sequence, we can obtain a discrete connection 1-form using the following construction.

Given $[q_0, q_1]_G \in (Q \times Q)/G$, we obtain from the splitting of the discrete Atiyah sequence an element, $[q, g]_G \in \tilde{G}$. Viewing $[q, g]_G$ as a subset of $Q \times G$, consider the unique $\tilde{g}$ such that $(q_0, \tilde{g}) \in [q, g]_G \subset Q \times G$. Then, we define

$$\mathcal{A}_d(x_0, e, x_1, g_0^{-1}g_1) = \tilde{g}.$$

We extend this definition to the whole of $Q \times Q$ by equivariance,

$$\mathcal{A}_d(x_0, g_0, x_1, g_1) = g_0\tilde{g}g_0^{-1}.$$

Lemma 4.13. *Given a splitting of the discrete Atiyah sequence, the construction above yields a discrete connection* 1*-form with the requisite properties.*

Proof. To show that the $\mathcal{A}_d$ satisfies the properties of a discrete connection 1-form, we first note that equivariance follows from the construction.

Since we have a splitting, it follows that $\varphi([q, gq]_G) = [q, g]_G$, as φ composed with the map from $\tilde{G}$ to $(Q \times Q)/G$ is the identity on $\tilde{G}$. Using a local trivialization, we have,

$$\begin{aligned} [q_0, g]_G &= \varphi([q_0, gq_0]_G) \\ &= \varphi([(x_0, e), (x_0, g_0^{-1} g g_0)]_G) \\ &= [(x_0, e), \tilde{g}]_G \\ &= [(x_0, g_0), g_0 \tilde{g} g_0^{-1}]_G. \end{aligned}$$

Then, by definition,

$$\mathcal{A}_d((x_0, e), (x_0, g_0^{-1} g g_0)) = \tilde{g},$$

and furthermore, $g = g_0 \tilde{g} g_0^{-1}$. From this, we conclude that

$$\begin{aligned} \mathcal{A}_d(q_0, gq_0) &= \mathcal{A}_d((x_0, g_0), (x_0, gg_0)) \\ &= g_0 \mathcal{A}_d((x_0, e), (x_0, g_0^{-1} g g_0)) g_0^{-1} \\ &= g_0 \tilde{g} g_0^{-1} \\ &= g. \end{aligned}$$

Therefore, we have that $\mathcal{A}_d(q_0, gq_0) = g$, which together with equivariance implies that $\mathcal{A}_d$ is a discrete connection 1-form. □

4.4.7 Splitting of the Discrete Atiyah Sequence (Horizontal Lift)

As was the case with the discrete connection 1-form, the discrete horizontal lift is in one-to-one correspondence with splittings of the discrete Atiyah sequence, and they are related by taking the quotient, or extending by G-equivariance, as appropriate.

Splittings from Discrete Horizontal Lifts. Given a discrete horizontal lift, we obtain a splitting by taking its quotient.

Lemma 4.14. *Given a discrete horizontal lift,* $(\cdot, \cdot)_q^h : S \times S \to Q \times Q$*, the map* $(\cdot, \cdot)^h : S \times S \to (Q \times Q)/G$*, which is given by*

$$(x_0, x_1)^h = [(x_0, x_1)^h_{(x_0, e)}]_G\,,$$

induces a splitting of the discrete Atiyah sequence.

Proof. We compute,

$$\begin{aligned}(\pi,\pi)\circ(x_0,x_1)^h &= (\pi,\pi)([(x_0,x_1)^h_{(x_0,e)}]_G)\\ &= (x_0,x_1)\,,\end{aligned}$$

where we used the G-equivariance of the discrete horizontal lift, and the property that $(\pi,\pi)\cdot(x_0,x_1)^h_q = (x_0,x_1)$ for any $q\in Q$. This implies that $(\pi,\pi)\circ(\cdot,\cdot)^h = 1_{S\times S}$, as desired. □

Discrete Horizontal Lifts from Splittings. Given a splitting, $(\cdot,\cdot)^h : S\times S\to(Q\times Q)/G$, we obtain a discrete horizontal lift, $(\cdot,\cdot)^h_q : S\times S\to Q\times Q$, using the following construction.

We denote by $(x_0,x_1)^h_{q_0}$ the unique element in $(x_0,x_1)^h$, thought of as a subset of $Q\times Q$, such that the first component is q_0. This is the discrete horizontal lift of the point $(x_0,x_1)\in S\times S$ where the base point is specified.

Lemma 4.15. *Given a splitting of the discrete Atiyah sequence, the construction above yields a discrete horizontal lift with the requisite properties.*

Proof. Since the quotient space $(Q\times Q)/G$ is obtained by the diagonal action of G on $Q\times Q$, it follows that if $(x_0,x_1)^h_{q_0}\in(x_0,x_1)^h\subset Q\times Q$, then $g\cdot(x_0,x_1)^h_{q_0}\in(x_0,x_1)^h\subset Q\times Q$. Since the first component of $G\cdot(x_0,x_1)^h_{q_0}$ is gq_0, and $g\cdot(x_0,x_1)^h_{q_0}\in(x_0,x_1)^h\subset Q\times Q$, we have that

$$(x_0,x_1)^h_{gq_0} = g\cdot(x_0,x_1)^h_{q_0}\,,$$

which is to say that the discrete horizontal lift constructed above is G-equivariant.

Since $(\cdot,\cdot)^h$ is a splitting of the discrete Atiyah sequence, we have that $(\pi,\pi)\circ(\cdot,\cdot)^h = 1_{S\times S}$, and this implies that any element in $(x_0,x_1)^h$, viewed as a subset of $Q\times Q$, projects to (x_0,x_1). Therefore, the discrete horizontal lift we constructed above has the requisite properties. □

4.4.8 Isomorphism between $(Q\times Q)/G$ and $(S\times S)\oplus\tilde{G}$

The notion of a discrete connection is motivated by the desire to construct a global diffeomorphism between $(Q\times Q)/G\to S$ and $(S\times S)\oplus\tilde{G}\to S$. This is the discrete analogue of the identification between $TQ/G\to Q/G$ and $T(Q/G)\oplus\tilde{\mathfrak{g}}\to Q/G$ which is the context for Lagrangian Reduction in Cendra et al. [2001]. Since a choice of discrete connection corresponds to a choice of splitting of the discrete Atiyah sequence, we have the following commutative diagram, where each row is a short exact sequence.

$$\begin{array}{ccccccccc}
0 & \longrightarrow & \tilde{G} & \underset{(\pi_1,\mathcal{A}_d)}{\overset{(q,gq)}{\rightleftarrows}} & (Q\times Q)/G & \underset{(\cdot,\cdot)^h}{\overset{(\pi,\pi)}{\rightleftarrows}} & S\times S & \longrightarrow & 0 \\
 & & \Big\| 1_{\tilde{G}} & & \Big\downarrow \alpha_{\mathcal{A}_d} & & \Big\| 1_{S\times S} & & \\
0 & \longrightarrow & \tilde{G} & \underset{\pi_1}{\overset{i_1}{\rightleftarrows}} & \tilde{G}\oplus(S\times S) & \underset{i_2}{\overset{\pi_2}{\rightleftarrows}} & S\times S & \longrightarrow & 0
\end{array}$$

Here, we see how the identification between $(Q\times Q)/G$ and $(S\times S)\oplus\tilde{G}$ are naturally related to the discrete connection and the discrete horizontal lift.

Recall that the discrete adjoint bundle $\tilde{G}$ is the associated bundle one obtains when $M = G$, and ρ_g acts by conjugation. Furthermore, the action of G on $Q\times Q$ is by the diagonal action, and the action of $G\times G$ on $Q\times Q$ is component-wise.

Proposition 4.16. *The map $\alpha_{\mathcal{A}_d} : (Q\times Q)/G \to (S\times S)\oplus\tilde{G}$ defined by*

$$\alpha_{\mathcal{A}_d}([q_0,q_1]_G) = (\pi q_0, \pi q_1)\oplus[q_0, \mathcal{A}_d(q_0,q_1)]_G,$$

is a well-defined bundle isomorphism. The inverse of α_{A_d} is given by

$$\alpha^{-1}_{\mathcal{A}_d}((x_0,x_1)\oplus[q,g]_G) = [(e,g)\cdot(x_0,x_1)^h_q]_G,$$

for any $q\in Q$ such that $\pi q = x_0$.

Proof. To show that $\alpha_{\mathcal{A}_d}$ is well-defined, note that for any $g\in G$, we have that

$$(\pi g q_0, \pi g q_1) = (\pi q_0, \pi q_1),$$

and also,

$$\begin{aligned}
[gq_0, \mathcal{A}_d(gq_0, gq_1)]_G &= [gq_0, g\mathcal{A}_d(q_0,q_1)g^{-1}]_G \\
&= [q_0, \mathcal{A}_d(q_0,q_1)]_G.
\end{aligned}$$

Then, we see that

$$\alpha_{\mathcal{A}_d}([gq_0, gq_1]_G) = \alpha_{\mathcal{A}_d}([q_0,q_1]_G).$$

To show that $\alpha^{-1}_{\mathcal{A}_d}$ is well-defined, note that for any $k\in G$,

$$(x_0,x_1)^h_{kq} = k\cdot(x_0,x_1)^h_q,$$

and that

$$
\begin{aligned}
\alpha_{\mathcal{A}_d}^{-1}((x_0,x_1)\oplus[kq,kgk^{-1}]_G) &= [(e,kgk^{-1})\cdot(x_0,x_1)^h_{kq}]_G \\
&= [(e,kgk^{-1})\cdot k\cdot(x_0,x_1)^h_q]_G \\
&= [(ek,kgk^{-1}k)\cdot(x_0,x_1)^h_q]_G \\
&= [(ke,kg)\cdot(x_0,x_1)^h_q]_G \\
&= [k\cdot(e,g)\cdot(x_0,x_1)^h_q]_G \\
&= [(e,g)\cdot(x_0,x_1)^h_q]_G \\
&= \alpha_{\mathcal{A}_d}^{-1}((x_0,x_1)\oplus[q,g]_G).
\end{aligned}
$$

□

Example 4.2. *It is illustrative to consider the notion of a discrete connection, and the isomorphism, in the degenerate case when $Q=G$, which is the context of discrete Euler–Poincaré reduction. Here, the isomorphism is between $(G\times G)/G$ and $\tilde{G}$, and the connection $\mathcal{A}_d : G\times G\to G$ is given by*

$$\mathcal{A}_d(g_0,g_1)=g_1\cdot g_0^{-1}.$$

Then, we have that

$$
\begin{aligned}
\alpha_{\mathcal{A}_d}([g_0,g_1]_G) &= (\pi g_0,\pi g_1)\oplus[g_0,\mathcal{A}_d(q_0,q_1)]_G \\
&= (e,e)\oplus[g_0,g_1g_0^{-1}]_G\,.
\end{aligned}
$$

Taking the inverse, we have,

$$
\begin{aligned}
\alpha_{\mathcal{A}_d}^{-1}([g_0,g_1g_0^{-1}]_G) &= [(e,g_1g_0^{-1}]\cdot(e,e)^h_{g_0}]_G \\
&= [(e,g_1g_0^{-1}]\cdot(g_0,g_0)]_G \\
&= [eg_0,g_1g_0^{-1}g_0]_G \\
&= [g_0,g_1]_G\,,
\end{aligned}
$$

as expected.

4.4.9 Discrete Horizontal and Vertical Subspaces Revisited

Having now fully introduces all the equivalent representations of a discrete connection, we can revisit the notion of discrete horizontal and vertical subspaces in light of the new structures we have introduced.

Consider the following split exact sequence,

$$0 \longrightarrow A_1 \underset{k}{\overset{f}{\rightleftarrows}} B \underset{h}{\overset{g}{\rightleftarrows}} A_2 \longrightarrow 0 \ .$$

We can decompose any element in B into a A_1 and A_2 term by considering the following isomorphism,

$$B \cong f \circ k(B) \oplus h \circ g(B).$$

Similarly, in the discrete Atiyah sequence, we can decompose an element of $(Q \times Q)/G$ into a horizontal and vertical piece by performing the analogous construction on the split exact sequence

$$0 \longrightarrow \tilde{G} \underset{(\pi_1, \mathcal{A}_d)}{\overset{(q,gq)}{\rightleftarrows}} (Q \times Q)/G \underset{(\cdot,\cdot)^h}{\overset{(\pi,\pi)}{\rightleftarrows}} S \times S \longrightarrow 0 \ .$$

This allows us to define horizontal and vertical spaces associated with the pair groupoid $Q \times Q$, in terms of all the structures we have introduced.

Definition 4.12. *The **horizontal space** is given by*

$$\begin{aligned} \mathrm{Hor}_q &= \{(q, q') \in Q \times Q \mid \mathcal{A}_d(q, q') = e\} \\ &= \{(\pi q, x_1)_q^h \in Q \times Q \mid x_1 \in S\}. \end{aligned}$$

This is the discrete analogue of the statement $\mathrm{Hor}_q = \{v_q \in TQ \mid \mathcal{A}(v_q) = 0\} = \{(v_{\pi q})_q^h \in TQ \mid v_{\pi q} \in TS\}$.

Definition 4.13. *The **vertical space** is given by*

$$\begin{aligned} \mathrm{Ver}_q &= \{(q, q') \in Q \times Q \mid (\pi, \pi)(q, q') = e_{S\times S}\} \\ &= \{i_q(g) \mid g \in G\}. \end{aligned}$$

This is the discrete analogue of the statement $\mathrm{Ver}_q = \{v_q \in TQ \mid \pi_*(v_q) = 0\} = \{\xi_Q \mid \xi \in \mathfrak{g}\}$.

In particular, we can decompose an element of $Q \times Q$ into a horizontal and vertical component.

Definition 4.14. *The **horizontal component** of* $(q_0, q_1) \in Q \times Q$ *is given by*

$$\mathrm{hor}(q_0, q_1) = ((\cdot, \cdot)^h \circ (\pi, \pi))(q_0, q_1) = (\pi q_0, \pi q_1)_{q_0}^h.$$

Definition 4.15. *The **vertical component** of* $(q_0, q_1) \in Q \times Q$ *is given by*

$$\mathrm{ver}(q_0, q_1) = (i \circ (\pi_1, \mathcal{A}_d))(q_0, q_1) = (q_0, \mathcal{A}_d(q_0, q_1)q_0) = i_{q_0}(\mathcal{A}_d(q_0, q_1)).$$

Lemma 4.17. *The horizontal component can be expressed as*

$$\mathrm{hor}(q_0, q_1) = i_{q_0}((\mathcal{A}_d(q_0, q_1))^{-1}) \cdot (q_0, q_1).$$

Proof.

$$\begin{aligned} i_{q_0}(\mathcal{A}_d(q_0, q_1)^{-1}) \cdot (q_0, q_1) &= (q_0, (\mathcal{A}_d(q_0, q_1))^{-1} q_0) \cdot (q_0, q_1) \\ &= (e, (\mathcal{A}_d(q_0, q_1))^{-1})(q_0, q_1) \\ &= (q_0, (\mathcal{A}_d(q_0, q_1))^{-1} q_1). \end{aligned}$$

Clearly, $(\pi, \pi)(q_0, (\mathcal{A}_d(q_0, q_1))^{-1} q_1) = (\pi, \pi)(q_0, q_1)$. Furthermore,

$$\mathcal{A}_d(q_0, (\mathcal{A}_d(q_0, q_1))^{-1} q_1) = (\mathcal{A}_d(q_0, q_1))^{-1} \mathcal{A}_d(q_0, q_1) = e.$$

Therefore, by definition, $(q_0, (\mathcal{A}_d(q_0, q_1))^{-1} q_1) = \mathrm{hor}(q_0, q_1)$. □

Lemma 4.18. *The horizontal and vertical operators satisfy the following identity,*

$$\mathrm{ver}(q_0, q_1) \cdot \mathrm{hor}(q_0, q_1) = (q_0, q_1).$$

Proof.

$$\begin{aligned} \mathrm{ver}(q_0, q_1) \cdot \mathrm{hor}(q_0, q_1) &= i_{q_0}(\mathcal{A}_d(q_0, q_1)) \cdot (i_{q_0}((\mathcal{A}_d(q_0, q_1))^{-1}) \cdot (q_0, q_1)) \\ &= (e, \mathcal{A}_d(q_0, q_1))(e, (\mathcal{A}_d(q_0, q_1))^{-1})(q_0, q_1) \\ &= (e, \mathcal{A}_d(q_0, q_1))(q_0, (\mathcal{A}_d(q_0, q_1))^{-1} q_1) \\ &= (q_0, \mathcal{A}_d(q_0, q_1)(\mathcal{A}_d(q_0, q_1))^{-1} q_1) \\ &= (q_0, q_1), \end{aligned}$$

as desired. □

4.5 Geometric Structures Derived from the Discrete Connection

In this section, we will introduce some of the additional geometric structures that can be derived from a choice of discrete connection. These structures include an extension of the pair groupoid composition to take into account the principal bundle structure, continuous connections that are a limit of a discrete connection, and higher-order connection-like structures.

4.5.1 Extending the Pair Groupoid Composition

Recall that the composition of a vertical element (q_0, gq_0) with an element (q_0, q_1) is given by

$$(q_0, gq_0) \cdot (q_0, q_1) = (q_0, gq_1).$$

The choice of a discrete connection allows us to further extend the composition, in a manner that is relevant in describing the curvature of a discrete connection. The decomposition of an element of $Q \times Q$ into a horizontal and vertical piece naturally suggests a generalization of the composition operation on $Q \times Q$ (viewed as a pair groupoid), by using the discrete connection, and the principal bundle structure of Q.

We wish to define a composition on $Q\times Q$ such that the composition of $(q_0, q_1)\cdot(\tilde{q}_0, \tilde{q}_1)$ is defined whenever $\pi q_1 = \pi\tilde{q}_0$. Furthermore, we require that the extended composition be consistent with the vertical composition we introduced previously, as well as the pair groupoid composition, whenever their domains of definition coincide.

The extended composition is obtained by left translating $(\tilde{q}_0, \tilde{q}_1)$ by a group element h, such that $q_1 = h\tilde{q}_0$, and then using the pair groupoid composition on (q_0, q_1) and the left translated term $h(\tilde{q}_0, \tilde{g}_1)$. This yields the following intrinsic definition of the extended composition.

Definition 4.16. *The* ***extended pair groupoid composition*** *of* $(q_0, q_1), (\tilde{q}_0, \tilde{q}_1) \in Q\times Q$ *is defined whenever* $\pi q_1 = \pi\tilde{q}_0$*, and it is given by*

$$(q_0, q_1) \cdot (\tilde{q}_0, \tilde{q}_1) = (q_0, \mathcal{A}_d(\tilde{q}_0, q_1)\tilde{q}_1).$$

As the following lemmas show, this extended composition is consistent with the vertical composition and the pair groupoid composition.

Lemma 4.19. *The extended pair groupoid composition is consistent with the composition of a vertical element with an arbitrary element.*

Proof. Consider the composition of a vertical element with an arbitrary element,

$$(q_0, gq_0) \cdot (q_0, q_1) = (q_0, gq_1).$$

This is consistent with the result using the extended composition,

$$
\begin{aligned}
(q_0, gq_0) \cdot (q_0, q_1) &= (q_0, \mathcal{A}_d(q_0, gq_0)q_1) \\
&= (q_0, gq_1)\,,
\end{aligned}
$$

where we used that the discrete connection yields a splitting of the Atiyah sequence. □

Lemma 4.20. *The extended pair groupoid composition is consistent with the pair groupoid composition.*

Proof. The pair groupoid composition is given by

$$
(q_0, q_1) \cdot (q_1, q_2) = (q_0, q_2)\,.
$$

This is consistent with the extended composition,

$$
\begin{aligned}
(q_0, q_1) \cdot (q_1, q_2) &= (q_0, \mathcal{A}_d(q_1, q_1)q_2) \\
&= (q_0, eq_2) \\
&= (q_0, q_2)\,.
\end{aligned}
$$

□

The extended composition is G-equivariant, and is well-defined on the quotient space, as the following lemma shows.

Lemma 4.21. *The composition* $\cdot : (Q \times Q) \times (Q \times Q) \to (Q \times Q)$ *is* G*-equivariant, that is,*

$$
(gq_0, gq_1) \cdot (g\tilde{q}_0, g\tilde{q}_1) = g \cdot ((q_0, q_1) \cdot (\tilde{q}_0, \tilde{q}_1)).
$$

Furthermore, the composition induces a well-defined quotient composition $\cdot : ((Q\times Q)\times(Q\times Q))/G \to (Q \times Q)/G$.

Proof. Given $g \in G$, we consider,

$$
\begin{aligned}
(gq_0, gq_1) \cdot (g\tilde{q}_0, g\tilde{q}_1) &= (gq_0, \mathcal{A}_d(g\tilde{q}_0, gq_1)g\tilde{q}_1) \\
&= (gq_0, g\mathcal{A}_d(\tilde{q}_0, q_1)g^{-1}g\tilde{q}_1) \\
&= (gq_0, g\mathcal{A}_d(\tilde{q}_0, q_1)\tilde{q}_1) \\
&= g \cdot (q_0, \mathcal{A}_d(\tilde{q}_0, q_1)\tilde{q}_1) \\
&= g \cdot ((q_0, q_1) \cdot (\tilde{q}_0, \tilde{q}_1))\,,
\end{aligned}
$$

where we used the equivariance of the discrete connection. It follows that the composition is equivariant. Furthermore,

$$[(g\tilde{q}_0, g\tilde{q}_1) \cdot (gq_0, gq_1)]_G = [(\tilde{q}_0, \tilde{q}_1) \cdot (q_0, q_1)]_G,$$

which means that $\cdot : ((Q \times Q) \times (Q \times Q))/G \to (Q \times Q)/G$ is well-defined. □

Corollary 4.22. *The composition of n-terms is G-equivariant. That is to say,*

$$\begin{aligned}(gq_0^1, gq_1^1) \cdot (gq_0^2, gq_1^2) \cdot \ldots \cdot (gq_0^{n-1}, gq_1^{n-1}) \cdot (gq_0^n, gq_1^n)& \\ = g \cdot ((q_0^1, q_1^1) \cdot (q_0^2, q_1^2) \cdot \ldots \cdot (q_0^{n-1}, q_1^{n-1}) \cdot (q_0^n, q_1^n)).&\end{aligned}$$

Proof. The result follows by induction on the previous lemma. □

We find that the extended composition we have constructed on the pair groupoid is associative. However, as we shall see in §4.7.3, composing pair groupoid elements about a loop in the shape space will not in general yield the identity element $e_{Q\times Q}$, and the defect represents the holonomy about the loop, which is related to curvature. This may yield the discrete analogue of the expression giving the geometric phase in terms of a loop integral (in shape space) of the curvature of the connection.

Lemma 4.23. *The composition $\cdot : (Q \times Q) \times (Q \times Q) \to (Q \times Q)$ is associative. That is,*

$$((q_0^0, q_1^0) \cdot (q_0^1, q_1^1)) \cdot (q_0^2, q_1^2) = (q_0^0, q_1^0) \cdot ((q_0^1, q_1^1) \cdot (q_0^2, q_1^2)).$$

Proof. Evaluating the left-hand side, we obtain

$$\begin{aligned}((q_0^0, q_1^0) \cdot (q_0^1, q_1^1)) \cdot (q_0^2, q_1^2) &= (q_0^0, \mathcal{A}_d(q_0^1, q_1^0)q_1^1) \cdot (q_0^2, q_1^2) \\ &= (q_0^0, \mathcal{A}_d(q_0^2, \mathcal{A}_d(q_0^1, q_1^0)q_1^1)q_1^2) \\ &= (q_0^0, \mathcal{A}_d(q_0^1, q_1^0)\mathcal{A}_d(q_0^2, q_1^1)q_1^2),\end{aligned}$$

and the right-hand side is given by

$$\begin{aligned}(q_0^0, q_1^0) \cdot ((q_0^1, q_1^1) \cdot (q_0^2, q_1^2)) &= (q_0^0, q_1^0) \cdot (q_0^1, \mathcal{A}_d(q_0^2, q_1^1)q_1^2) \\ &= (q_0^0, \mathcal{A}_d(q_0^1, q_1^0)\mathcal{A}_d(q_0^2, q_1^1)q_1^2).\end{aligned}$$

Therefore,

$$((q_0^0, q_1^0) \cdot (q_0^1, q_1^1)) \cdot (q_0^2, q_1^2) = (q_0^0, q_1^0) \cdot ((q_0^1, q_1^1) \cdot (q_0^2, q_1^2)),$$

and the extended groupoid composition is associative. □

4.5.2 Continuous Connections from Discrete Connections

Given a discrete G-valued connection 1-form, $\mathcal{A}_d : Q \times Q \to G$, we associate to it a continuous $\mathfrak{g}$-valued connection 1-form, $\mathcal{A} : TQ \to \mathfrak{g}$, by the following construction,

$$\mathcal{A}([q(\cdot)]) = [\mathcal{A}_d(q(0), q(\cdot))],$$

where $[\cdot]$ denotes the equivalence class of curves associated with a tangent vector.

This uses the intrinsic representation of the tangent bundle, which is obtained by identifying a tangent vector at a point on the manifold with the equivalence class of curves on the manifold going through the point, such that the tangent to the curve at the point is given by the tangent vector, which was illustrated earlier in Figure 4.9 on page 151.

More explicitly, given $v_q \in TQ$, we consider an associated curve $q : [0,1] \to Q$, and construct the curve $g : [0,1] \to G$, given by

$$g(t) = \mathcal{A}_d(q(0), q(t)).$$

Then,

$$\mathcal{A}(v_q) = \left.\frac{d}{dt}\right|_{t=0} g(t).$$

When computing the equations in discrete reduction theory, it is often necessary to consider horizontal and vertical variations, which we introduce below.

Definition 4.17. *We introduce the* ***vertical variation*** *of a point* $(q_0, q_1) \in Q \times Q$*. Given a curve* $q_1^\epsilon : [0,1] \to Q$*, such that* $q_1^\epsilon(0) = q_1$*, the vertical variation is given by*

$$\operatorname{ver} \delta q = \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \operatorname{ver}(q_0, q_1^\epsilon) = \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} i_{q_0}(\mathcal{A}_d(q_0, q_1^\epsilon)) \,.$$

Definition 4.18. *We introduce the* ***horizontal variation*** *of a point* $(q_0, q_1) \in Q \times Q$*. Given a curve* $q_1^\epsilon : [0,1] \to Q$*, such that* $q_1^\epsilon(0) = q_1$*, the horizontal variation is given by*

$$\operatorname{hor} \delta q = \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \operatorname{hor}(q_0, q_1^\epsilon) = \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} (\pi(q_0, q_1^\epsilon))_{q_0}^h \,.$$

4.5.3 Connection-Like Structures on Higher-Order Tangent Bundles

Given a continuous connection, we can construct connection-like structures on higher-order tangent bundles. This construction is described in detail in Lemma 3.2.1 of Cendra et al. [2001]. In particular, given a connection 1-form, $\mathcal{A} : TQ \to \mathfrak{g}$, we obtain a well-defined map, $\mathcal{A}^k : T^{(k)}Q \to k\mathfrak{g}$.

As we will see later, these connection-like structures on higher-order tangent bundles will provide an intrinsic method of characterizing the order of approximation of a continuous connection by a discrete connection.

We will describe the discrete analogue of this construction. To begin, the discrete analogue of the k-th order tangent bundle, $T^{(k)}Q$, is $k+1$ copies of Q, namely Q^{k+1}. Intermediate spaces between $T^{(k)}Q$ and Q^{k+1} arise in the general theory of multi-spaces, which is introduced in Olver [2001].

The discrete analogue of tangent lifts, and their higher-order analogues, are obtained by componentwise application of the map, since a tangent lift of a map is computed by applying the map to a representative curve, and taking its equivalence class. Therefore, given a map $f : M \to N$, we have the naturally induced map,

$$T^{(k)}f : M^{k+1} \to N^{k+1} \quad \text{given by} \quad T^{(k)}f(m_0, \dots, m_k) = (f(m_0), \dots, f(m_k)).$$

And in particular, the group action is lifted to the diagonal group action on the product space.

The discrete connection can be extended to Q^{k+1} in the natural way, $\mathcal{A}_d^k : Q^{k+1} \to \oplus_{l=0}^{k-1} G \equiv kG$,

$$\mathcal{A}_d^k(q_0, \dots, q_k) = \oplus_{l=0}^{k-1} \mathcal{A}_d(q_l, q_{l+1}).$$

Similarly, we can define the map from Q^{k+1} to the Whitney sum of k copies of the conjugate bundle $\tilde{G}$ by

$$Q^{k+1} \to k\tilde{G} \quad \text{by} \quad (q_0, \dots, q_k) \mapsto \oplus_{l=0}^{k-1} [q_0, \mathcal{A}_d(q_l, q_{l+1})]_G.$$

In a natural way, we have the following proposition.

Proposition 4.24. *The map*

$$\alpha_{\mathcal{A}_d^k} : Q^{k+1} \to (Q/G)^{k+1} \times_{Q/G} k\tilde{G}$$

defined by

$$\alpha_{\mathcal{A}_d^k}(q_0, \dots, q_k) = (\pi q_0, \dots, \pi q_k) \times_{Q/G} \oplus_{l=0}^{k-1} [q_0, \mathcal{A}_d(q_l, q_{l+1})]_G,$$

is a well-defined bundle isomorphism. The inverse of $\alpha_{\mathcal{A}_d^k}$ *is given by*

$$\begin{aligned} &\alpha_{\mathcal{A}_d^k}^{-1} \left((x_0, \dots, x_k) \times_{Q/G} \oplus_{l=0}^{k-1} [q_l, g_l]_G \right) \\ &\qquad = [(e, g_0, g_1 g_0, \dots, g_{k-1} \dots g_0)) \cdot (x_0, \dots, x_k)_{q_0}^h]_G, \end{aligned}$$

where $(x_0, \ldots, x_k)^h_{q_0} = (\bar{q}_0, \ldots, \bar{q}_k)$ *is defined by the conditions:*

$$\begin{aligned} \bar{q}_0 &= q_0, \\ \pi \bar{q}_l &= x_l, \\ \mathcal{A}_d(\bar{q}_l, \bar{q}_{l+1}) &= e. \end{aligned}$$

Remark 4.2. *In a local trivialization, where* $q_0 = (h_0, x_0)$*, we have,*

$$\bar{q}_{l+1} = \left((A(x_l, x_{l+1}) \cdots A(x_0, x_1))^{-1} h_0, x_{l+1} \right).$$

4.6 Computational Aspects

While we saw in the previous section that a discrete connection induces a continuous connection in the limit, we are often concerned with constructing discrete connections that approximate a continuous connection to a given order of approximation. This section will address the question of what it means for a discrete connection to approximate a continuous connection to a given order, as well as introduce methods for constructing such discrete connections.

4.6.1 Exact Discrete Connection

It is interesting from the point of view of computation to construct an ***exact discrete connection*** associated with a prescribed continuous connection, so that we can make sense of the statement that a given discrete connection is a k-th order approximation of a continuous connection.

Additional Structure. To construct the exact discrete connection, we require that the configuration manifold Q be endowed with a bi-invariant Riemannian metric, with the property that the associated exponential map,

$$\exp : TQ \to Q,$$

is consistent with the group action, in the sense that

$$\exp(\xi_Q(q)) = \exp(\xi) \cdot q.$$

We extend the exponential to $Q \times Q$ as follows,

$$\begin{aligned} \overline{\exp} : TQ &\to Q \times Q, \\ v_q &\mapsto (q, \exp(v_q)), \end{aligned}$$

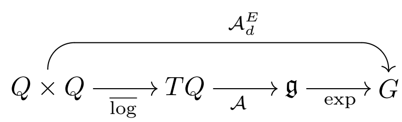
and denote the inverse by $\overline{\log} : Q \times Q \to TQ$, which is defined in a neighborhood of the diagonal of $Q \times Q$.

Construction. Having introduced the appropriate structure on the configuration manifold, we define the exact discrete connection as follows.

Definition 4.19. *The* ***Exact Discrete Connection*** $\mathcal{A}_d^E$ *associated with a prescribed continuous connection* $\mathcal{A} : TQ \to \mathfrak{g}$ *and a Riemannian metric is given by*

$$\mathcal{A}_d^E(q_0, q_1) = \exp(\mathcal{A}(\overline{\log}(q_0, q_1))).$$

This construction is more clearly illustrated in the following diagram,



Properties. The exact discrete connection satisfies the properties of the discrete connection 1-form, in that it is G-equivariant, and it induces a splitting of the discrete Atiyah sequence. The equivariance of the exact discrete connection arises from the fact that each of the composed maps is equivariant, and the splitting condition,

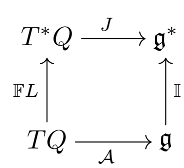
$$\mathcal{A}_d^E(i_q(g)) = g,$$

is a consequence of the compatibility condition,

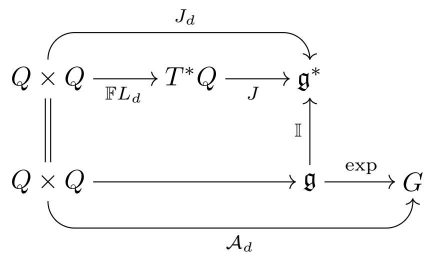
$$\exp(\xi_Q(q)) = \exp(\xi) \cdot q.$$

Since the logarithm map is only defined on a neighborhood of the diagonal of $Q \times Q$, it follows that the exact discrete connection will have the same restriction on its domain of definition.

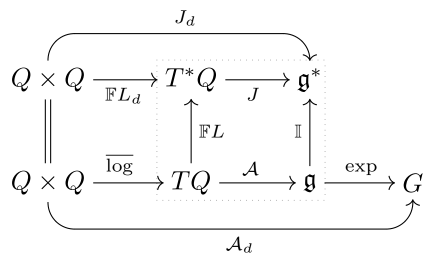
Example 4.3 (Discrete Mechanical Connection). *The continuous mechanical connection is defined by the following diagram,*



Correspondingly, the discrete mechanical connection is defined by the following diagram,



This is consistent with our notion of an exact discrete mechanical connection as the following diagram illustrates,



where the portion in the dotted box recovers the continuous mechanical connection. In checking G-equivariance, we use the equivariance of $\exp : \mathfrak{g} \to G$, $J_d : Q \times Q \to \mathfrak{g}^*$, *and the equivariance of* $\mathbb{I}$ *in the sense of a map* $\mathbb{I} : Q \to L(\mathfrak{g}, \mathfrak{g}^*)$, *namely,* $\mathbb{I}(gq) \cdot \mathrm{Ad}_g \xi = \mathrm{Ad}^*_{g^{-1}} \mathbb{I}(q) \cdot \xi$.

4.6.2 Order of Approximation of a Connection

We have the necessary constructions to consider the order to which a discrete connection approximates a continuous connection. There are two equivalent ways of defining the order of approximation of a continuous connection by a discrete connection, the first is more analytical, and is given by the order of convergence in an appropriate norm on the group.

Definition 4.20 (Order of Connection, Analytic). *A discrete connection* $\mathcal{A}_d$ *is a* k*-th order discrete connection if,* k *is the maximum integer for which*

$$\exists 0 < c < \infty,$$

$$\exists h_0 > 0,$$

such that

$$\sup_{\substack{v_q \in TQ, \\ |v_q| = 1}} \| \mathcal{A}_d^E(q, \exp(hv_q))(\mathcal{A}_d(q, \exp(hv_q)))^{-1} \| \leq c h^{k+1}, \quad \forall h < h_0.$$

The second definition is more intrinsic, and is related to considering the infinitesimal limit of a discrete connection to connection-like structures on higher-order tangent bundles, without the need for the introduction of the exact discrete connection.

Recall from §4.5.2 that we can construct a continuous connection from a discrete connection by the following construction,

$$\mathcal{A}([q(\cdot)]) = [\mathcal{A}_d(q(0), q(\cdot))].$$

Given $\mathcal{A}_d^k : Q^{k+1} \to kG$, we can obtain the continuous limit $\mathcal{A}^k : T^{(k)}Q \to k\mathfrak{g}$ in a similar fashion.

Definition 4.21 (Order of Connection, Intrinsic). *A discrete connection $\mathcal{A}_d$ is a k-th order approximation to $\mathcal{A}$ if, k is the maximum integer for which the diagram holds,*

$$\begin{array}{ccc}
\mathcal{A}_d : Q \times Q \to G & & \mathcal{A} : TQ \to \mathfrak{g} \\
\Big\Downarrow & & \Big\Downarrow \\
\mathcal{A}_d^k : Q^{k+1} \to kG & \dashrightarrow & \mathcal{A}^k : T^{(k)}Q \to k\mathfrak{g}
\end{array}$$

Here, the double arrows represent the higher-order structures induced by the connections, and the dotted arrow represents convergence in the limit.

4.6.3 Discrete Connections from Exponentiated Continuous Connections

To apply the exponential and logarithm approach to construct a discrete connection from a prescribed connection, in the sense of the diagram,

$$Q \times Q \xrightarrow[\log]{} TQ \xrightarrow[\mathcal{A}]{} \mathfrak{g} \xrightarrow[\exp]{} G \,, \qquad \mathcal{A}_d : Q \times Q \to G$$

we can rely on explicit expressions for the exponential and logarithm, such as those given in Appendix B for the special Euclidean group, or we can rely on approximations to the exponential and logarithm.

The explicit formulas for the special Euclidean group are particularly useful for applying the theory of discrete connections to the geometric control of problems such as robotic manipulators, and clusters of satellites. In dealing with other configuration manifolds, approximants to the exponential and logarithm may be required due to the absence of explicit formulas.

Even when explicit formulas are available, it may be desirable to rely on a more computationally efficient approximation, such as the Cayley transformation, methods based on Padé approximants (see, for example, Cardoso and Silva Leite [2001]; Higham [2001]), or Lie group techniques (see, for example, Celledoni and Iserles [2000, 2001]; Zanna and Munthe-Kaas [2001/02]). Clearly, these will yield a discrete connection that has an order of approximation equal to the lower of the two orders of approximation of the numerical schemes used for the exponential and the logarithm.

When used in the context of geometric control, high-order approximations to the continuous connection may not be necessary, since the optimal trajectory is often recomputed at each step, and in such instances, a low-order approximation suffices.

4.6.4 Discrete Mechanical Connections and Discrete Lagrangians

We will introduce a discrete mechanical connection that is consistent with the structure of discrete variational mechanics, and will yield a discrete connection that has an order of approximation that is equation to that obtained from the discrete mechanics.

Consider a G-invariant k-th order discrete Lagrangian, $L_d : Q \times Q \to \mathbb{R}$, which is to say that

$$L_d(gq_0, gq_1) = L_d(q_0, q_1),$$

and

$$L_d = L_d^{\text{exact}} + \mathcal{O}(h^{k+1}),$$

where the exact discrete Lagrangian, $L_d^{\text{exact}} : Q \times Q \to \mathbb{R}$, is given by

$$L_d^{\text{exact}}(q_0, q_1) = \int_0^h L(q_{01}(t), \dot{q}_{01}(t))dt.$$

Here, $q_{01} : [0, h] \to Q$ is the solution of the Euler–Lagrange equations with $q_{01}(0) = q_0$, and $q_{01}(h) = q_1$. The exact discrete Lagrangian is a generator of the symplectic flow, coming from the Jacobi solution of the Hamilton–Jacobi equation.

This k-th order discrete Lagrangian yields a k-th order accurate numerical update scheme, through the discrete Euler–Lagrange equations,

$$D_2 L_d(q_0, q_1) + D_1 L_d(q_1, q_2) = 0,$$

which implicitly defines a discrete flow $\Phi : (q_0, q_1) \mapsto (q_1, q_2)$. By pushing this numerical scheme forward to T^*Q using the discrete fiber derivative $\mathbb{F}L_d : Q \times Q \to T^*Q$, which maps $(q_0, q_1) \mapsto (q_0, -D_1 L_d(q_0, q_1))$, we can obtain a Symplectic Partitioned Runge–Kutta scheme of the same order.

We also introduce the discrete momentum map, $J_d : Q \times Q \to \mathfrak{g}^*$, given by

$$\langle J_d(q_0, q_1), \xi \rangle = -D_1 L_d(q_0, q_1) \cdot \xi_Q(q_0).$$

The discrete Lagrangian is G-invariant, which implies that for any $\xi \in \mathfrak{g}$, we have,

$$\begin{aligned} L_d(q_0, q_1) &= L_d(\exp(\xi t) \cdot q_0, \exp(\xi t) \cdot q_1), \\ 0 &= \left.\frac{d}{dt}\right|_{t=0} L_d(\exp(\xi t) \cdot q_0, \exp(\xi t) \cdot q_1) \\ &= D_1 L_d(q_0, q_1) \cdot \xi_Q(q_0) + D_2 L_d(q_0, q_1) \cdot \xi_Q(q_1). \end{aligned}$$

If we restrict to the flow of the discrete Euler–Lagrange equations, we have that

$$(D_1 L_d(q_0, q_1) + D_2 L_d q(q_1, q_2)) \cdot \xi_Q(q_1) = 0,$$

which upon substitution into the previous equation, yields

$$\begin{aligned} D_1 L_d(q_0, q_1) \cdot \xi_Q(q_0) - D_1 L_d(q_1, q_2) \cdot \xi_Q(q_1) &= 0, \\ -D_1 L_d(q_1, q_2) \cdot \xi_Q(q_1) &= -D_1 L_d(q_0, q_1) \cdot \xi_Q(q_0), \\ \langle J_d(q_1, q_2), \xi_Q(q_1) \rangle &= \langle J_d(q_0, q_1), \xi_Q(q_0) \rangle, \\ \Phi^* J_d &= J_d. \end{aligned}$$

which is the statement of the discrete Noether theorem, that the discrete momentum map is preserved by the discrete Euler–Lagrange flow.

We note that the mechanical connection corresponds to a choice of horizontal space corresponding to the zero momentum surface. That is to say that the horizontal distribution corresponding to the continuous mechanical connection is

$$\mathrm{Hor}_q = \{ v_q \in TQ \mid J(v_q) = 0 \},$$

and the discrete horizontal subspace corresponding to the discrete mechanical connection is

$$\mathrm{Hor}_q^d = \{ (q, q') \in Q \times Q \mid J_d(q, q') = 0 \}$$

Remark 4.3. *For the discrete horizontal subspace we defined above to have the correct dimensionality, the discrete Lagrangian needs to satisfy certain non-degeneracy conditions, which dictates the size of the neighborhood of the diagonal that the discrete connection is defined on.*

Since the continuous momentum map is preserved by the continuous Euler–Lagrange flow, and the discrete momentum map is preserved by the discrete Euler–Lagrange flow, it follows that the order of approximation of the continuous mechanical connection by the discrete mechanical connection is equal to the order of approximation of the continuous Euler–Lagrange flow by the discrete Euler–Lagrange flow. To construct a discrete mechanical connection of a prescribed order, we use the following procedure.

1. Consider a k-th order G-invariant discrete Lagrangian, $L_d : Q \times Q \to \mathbb{R}$,

$$L_d = L_d^{\text{exact}} + \mathcal{O}(h^{k+1}).$$

2. Construct the corresponding discrete momentum map, $J_d(q_0, q_1) \to \mathfrak{g}^*$,

$$\langle J_d(q_0, q_1), \xi \rangle = -D_1 L_d(q_0, q_1) \cdot \xi_Q(q_0).$$

3. Then, the k-th order discrete mechanical connection is given implicitly by considering the condition for the discrete horizontal space,

$$\mathcal{A}_d(q_0, q_1) = e \qquad \text{iff} \qquad J_d(q_0, q_1) = 0,$$

   and then extending the construction to the domain of definition by G-equivariance.

4. More explicitly, given $(q_0, q_1) \in Q \times Q$, we consider a local trivialization, in which $(q_0, q_1) = (x_0, g_0, x_1, g_1)$, and we find the unique $g \in G$ such that

$$J_d(x_0, g_0, x_1, g) = 0.$$

   Then, we have that

$$\mathcal{A}_d(x_0, g_0, x_1, g) = e,$$

   from which we conclude that

$$\begin{aligned}\mathcal{A}_d(x_0, g_0, x_1, g_1) &= \mathcal{A}_d(x_0, g_0, x_1, g_1 g^{-1} g) \\ &= g_1 g^{-1} \cdot \mathcal{A}_d(x_0, g_0, x_1, g) \\ &= g_1 g^{-1}.\end{aligned}$$

4.7 Applications

This section will sketch some of the applications of the mathematical machinery of discrete connections and discrete exterior calculus to problems in computational geometric mechanics, geometric control theory, and discrete Riemannian geometry.

4.7.1 Discrete Lagrangian Reduction

Lagrangian reduction, which is the Lagrangian analogue of Poisson reduction on the Hamiltonian side, is associated with the reduction of Hamilton's variational principle for systems with symmetry.

The variation of the action integral associated with a variation in the curve can be expressed in terms of the Euler–Lagrange operator, $\mathcal{EL} : T^{(2)}Q \to T^*Q$. When the Lagrangian is G-invariant, the associated Euler–Lagrange operator is G-equivariant, and this induces a reduced Euler–Lagrange operator, $[\mathcal{EL}]_G : T^{(2)}Q/G \to T^*Q/G$. The choice of a connection allows us to construct intrinsic coordinates on $T^{(2)}/G$ and T^*Q/G, and the representation of the reduced Euler–Lagrange operator in these coordinates correspond to the Lagrange–Poincaré operator, $\mathcal{LP} : T^{(2)}(Q/G) \times_{Q/G} 2\tilde{\mathfrak{g}} \to T^*(Q/G) \oplus \tilde{\mathfrak{g}}^*$.

The reduced equations obtained by reduction tend to have non-canonical symplectic structures. As such, naïvely applying standard symplectic algorithms to reduced equations can have undesirable consequences for the longtime behavior of the simulation, since it preserves the canonical symplectic form on the reduced space, as opposed to the reduced (non-canonical) symplectic form that is invariant under the reduced dynamics.

This sends a cautionary message, that it is important to understand the reduction of discrete variational mechanics, since applying standard numerical algorithms to the reduced equations obtained from continuous reduction theory may yield undesirable results, inasmuch as long-term stability is concerned.

Discrete connections on principal bundles provide the appropriate geometric structure to construct a discrete analogue of Lagrangian reduction. We first introduce the discrete Euler–Lagrange operator, which is constructed as follows.

Discrete Euler–Lagrange Operator. The discrete Euler–Lagrange operator, $\mathcal{EL}_d : Q^3 \to T^*Q$ satisfies the following property,

$$\mathbf{d}\mathfrak{S}_d(L_d) \cdot \delta\mathbf{q} = \sum \mathcal{EL}_d(L_d)(q_{k-1}, q_k, q_{k+1}) \cdot \delta q_k.$$

In coordinates, the discrete Euler–Lagrange operator has the form

$$[D_2 L_d(q_{k-1}, q_k) + D_1 L_d(q_k, q_{k+1})]\, dq_k.$$

Discrete Lagrange–Poincaré Operator. The map $\mathcal{EL}_d(L_d) : Q^3 \to T^*Q$, being G-equivariant, induces a quotient map

$$[\mathcal{EL}_d(L_d)]_G : Q^3/G \to T^*Q/G,$$

which depends only on the reduced discrete Lagrangian $l_d : (Q \times Q)/G \to \mathbb{R}$. We can therefore identify $[\mathcal{EL}_d(L_d)]_G$ with an operator $\mathcal{EL}_d(l_d)$ which we call the ***reduced discrete Euler–Lagrange operator***.

If in addition to the principal bundle structure, we have a discrete principal connection as described in the previous section, we can identify

$$Q^3/G \quad \text{with} \quad (Q/G)^3 \times_{Q/G} (\tilde{G} \oplus \tilde{G}).$$

The isomorphism between these two spaces is a consequence of Proposition 4.24, which is higher-order generalization of Proposition 4.16. The discrete mechanical connection which was introduced in §4.6.4 is a particularly natural choice of discrete connection, since it does not require any *ad hoc* choices, as it is constructed directly from the discrete Lagrangian.

Furthermore, each discrete G-valued connection 1-form, $\mathcal{A}_d : Q \times Q \to G$, induces in the infinitesimal limit a continuous $\mathfrak{g}$-valued connection 1-form, $\mathcal{A} : TQ \to \mathfrak{g}$, as shown in §4.5.2. This continuous principal connection allows us to identify

$$T^*Q/G \quad \text{with} \quad T^*(Q/G) \oplus \tilde{\mathfrak{g}}^*.$$

The discrete Lagrange–Poincaré operator, $\mathcal{LP}_d(l_d) : (Q/G)^3 \times_{Q/G} (\tilde{G} \oplus \tilde{G}) \to T^*(Q/G) \oplus \tilde{\mathfrak{g}}^*$, is obtained from the reduced discrete Euler–Lagrange operator by making the identifications obtained from the discrete connection structure.

The splitting of the range space of $\mathcal{LP}_d(l_d)$ as a direct product (as in §3.3 of Cendra et al. [2001]) naturally induces a decomposition of the discrete Lagrange–Poincaré operator,

$$\mathcal{LP}_d(l_d) = \text{Hor}(\mathcal{LP}_d(l_d)) \oplus \text{Ver}(\mathcal{LP}_d(l_d)),$$

and this allows the discrete reduced equations to be decomposed in horizontal and vertical equations.

4.7.2 Geometric Control Theory and Formations

There are well-established control algorithms for actuating a control system to achieve a desired reference configuration. In many problems of practical interest, the actuation of the mechanical system decomposes into shape and group variables in a natural fashion.

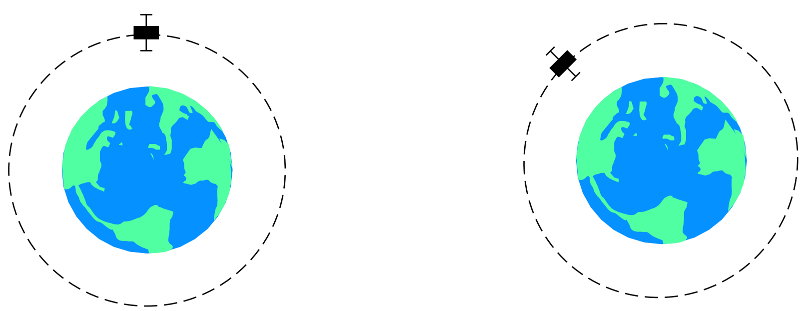
A canonical example of this is a satellite in motion about the Earth, where the orientation of the satellite is controlled by internal rotors through the use of holonomy and geometric phases, and the position is controlled by chemical propulsion.

In this example, the configuration space is SE(3), the group is SO(3), and the shape space is

$\mathbb{R}^3$. The group variable corresponds to the orientation, and the shape variable corresponds to the position. When given an initial and desired configuration, it is desirable, while computing the control inputs, to decompose the relative motion into a shape component and a group component, so that they can be individually actuated.

Since the discrete connection is used here to provide an efficient choice of local coordinates for optimal control, the discrete connection is most naturally obtained by exponentiating the continuous connection, in the manner described in §4.6.3, in conjunction with the explicit formulas for the exponential and logarithm for SE(3) that are given in Appendix B. The natural choice of the continuous connection is one in which the horizontal space is given by the momentum surface corresponding to the current value of the momentum.

To illustrate why it may not be desirable from a control-theoretic point of view to decompose the space using a trivial connection, consider a satellite that is in a tidally locked orbit about the Earth, with the initial and desired configuration as illustrated in Figure 4.10.



Initial configuration

Desired configuration

Figure 4.10: Application of discrete connections to control.

Here, if we choose a trivial connection, then the relative group element would be a rotation by $\pi/4$, but this choice is undesirable, since the motion is tidally locked, and moving the center of mass to the new location would result in a shift in the orientation by precisely the desired amount. In this case, the optimal control input should therefore only actuate in the shape variables, and the relative group element assigned to this pair of configurations should be the identity element.

As such, the extension of mechanically relevant connections to pairs of points in the configuration space with finite separation, through the use of a discrete connection, can be of immense value in geometric control theory.

Similarly, in the case of formations, discrete connections allow for the orientation coordination problem to be handled in a more efficient manner, by taking into account the dynamic coupling of the shape and group motions automatically through the use of the discrete mechanical connection.

4.7.3 Discrete Levi-Civita Connection

Vector bundle connections can be cast in the language of connections on principal bundles by considering the frame bundle consisting of oriented orthonormal frames over the manifold M, which is a principal SO(n) bundle, as originally proposed by Cartan [1983, 2001]. For related work on discrete connections on triangulated manifolds with applications to algebraic topology and the computation of Chern classes, please see Novikov [2003].

To construct our model of a discrete Riemannian manifold, we first trivialize the frame bundle to yield SO$(n) \times M$. Then, $Q = \mathrm{SO}(n) \times M$, and $G = \mathrm{SO}(n)$.

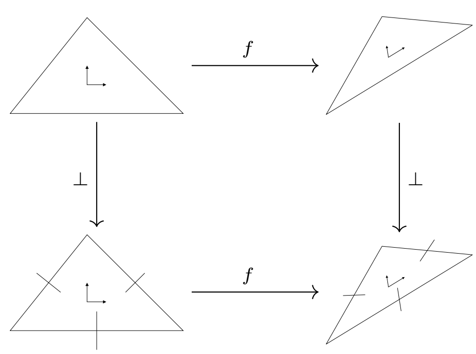
Here, we introduce the notion of a semidiscretized principal bundle, where the shape space, $S = Q/G$, is discretized as a simplicial complex K, and the structure group G remains continuous. In this context, the semidiscretization of the trivialization of the frame bundle is given by $Q = \mathrm{SO}(n) \times K$.

A discrete connection is a map $\mathcal{A}_d : Q \times Q \to G$, and we can construct a candidate for the Levi-Civita connection on a simplicial complex K, using the discrete analogue of the frame bundle described above. However, we will first introduce the notion of a discrete Riemannian manifold.

Definition 4.22. *A **discrete dual Riemannian manifold** is a simplicial complex where each n-simplex σ^n is endowed with a constant Riemannian metric tensor g, such that the restriction of the metric tensor to a common face with an adjacent n-simplex is consistent.*

This is referred to as a discrete dual Riemannian manifold as we can equivalently think of associating a Riemannian metric tensor to each dual vertex, and as we shall see, by adopting Cartan's method of orthogonal frames (see, for example, Cartan [1983, 2001]), the connection is a SO(n)-valued discrete dual 1-form, and the curvature is a SO(n)-valued discrete dual 2-form.

For each n-simplex σ^n, consider an invertible transformation f of $\mathbb{R}^n$ such that $f^*g = I$. In the orthonormal space, we have a normal operator that maps a $(n-1)$-dimensional subspace to a generator of the orthogonal complement, denoted by $\perp$. Then, we obtain a normal operator on the faces of σ^n by making the following diagram commute.



The coordinate axes in the diagram represent the normalized eigenvectors of the metric, scaled by their respective eigenvalues.

The local representation of the discrete connection is given by

$$\mathcal{A}_d((\sigma_0^n, R_0), (\sigma_1^n, R_1)) = R_1 A(\sigma_0^n, \sigma_1^n) R_0^{-1},$$

and so the discrete connection is uniquely defined if we specify $A(\sigma_0^n, \sigma_1^n)$, where σ_0^n and σ_1^n are adjacent n-simplices. Since they are adjacent, they share a $(n-1)$-simplex, denoted σ^{n-1}. In particular, this can then be thought of as a SO(n)-valued discrete dual 1-form, since to each dual 1-cell, $\star\sigma^{n-1}$, we associate an element of SO(n).

This element of SO(n) is computed as follows.

1. In each of the n-simplices, we have a normal direction associated with σ^{n-1}, denoted by

$$\perp(\sigma^{n-1}, \sigma_i^n) \in \mathbb{R}^n.$$

2. If these two normal directions are parallel, we set

$$\langle A, \star\sigma^{n-1}\rangle = I,$$

otherwise, we continue.

3. Construct the $(n-2)$-dimensional hyperplane P^{n-2}, given by the orthogonal complement to the span of the two normal directions.

$$P^{n-2} = \perp(\text{span}(\perp(\sigma^{n-1}, \sigma_0^n), \perp(\sigma^{n-1}, \sigma_1^n))).$$

4. If $\star\sigma^{n-1}$ is oriented from σ_0^n to σ_1^n, we set

$$\langle A, \star\sigma^{n-1}\rangle = \{R \in \text{SO}(n) \mid R|_{P^{n-2}} = I_{P^{n-2}}, R(\perp(\sigma^{n-1}, \sigma_0^n)) = \perp(\sigma^{n-1}, \sigma_1^n)\}.$$

The curvature of this discrete Levi-Civita connection is then a SO(n)-valued discrete dual 2-form. There is however the curious property that the boundary operator for a dual cell complex may not necessarily agree with the standard notion of boundary, since that may not be expressible in terms of a chain in the dual cell complex. This is primarily an issue on the boundary of the simplicial complex, and if we are in the interior, this is not a problem.

Since curvature is a dual 2-form, it is associated with the dual of a codimension-two simplex, given by $\star\sigma^{n-2}$. Consider the example illustrated in Figure 4.11.

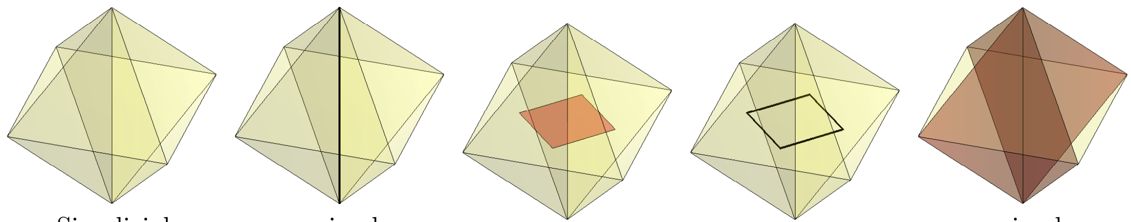


Figure 4.11: Discrete curvature as a discrete dual 2-form.

The curvature $\mathcal{B}$ of the discrete Levi-Civita connection is given by

$$\langle\mathcal{B},\star\sigma^{n-2}\rangle = \langle\mathbf{d}A,\star\sigma^{n-2}\rangle = \langle A,\partial\star\sigma^{n-2}\rangle.$$

As can be seen from the geometric region $\star\partial\star\sigma^{n-2}$, the curvature associated with $\star\sigma^{n-2}$ is given by the ordered product of the connection associated with the dual cells, $\star\sigma^{n-1}$, where $\sigma^{n-1}\succ\sigma^{n-2}$. This also suggests that we can also think of the discrete connection as a primal $(n-1)$-form, and the curvature as a primal $(n-2)$-form, where the curvature is obtained from the connection using the codifferential.

When the group G is nonabelian, we see that the curvature is only defined up to conjugation, since we need to specify a dual vertex on the dual one-chain $\partial\star\sigma^{n-2}$ from which to start composing group elements. To make this well-defined, we can adopt the approach used in defining the simplicial cup product, and assume that there is a partial ordering on dual vertices, which would make the curvature unambiguous.

As a quality measure for simplicial triangulations of a Riemannian manifold, having the curvature defined up to conjugation may be sufficient if we have a norm on $\mathrm{SO}(n)$ which is invariant under conjugation. As an example, taking the logarithm to get an element of the Lie algebra $\mathfrak{so}(n)$, and then using a norm on this vector space yields a conjugation-invariant norm on $\mathrm{SO}(n)$. This allows us to detect regions of the mesh with high curvature, and selectively subdivide the triangulation in such regions.

Similarly, we can define a discrete primal Riemannian manifold, where the Riemannian metric tensor is associated with primal vertices, and the connection is a G-valued primal 1-form, and the curvature is a G-valued primal 2-form.

Abstract Simplicial Complex with a Local Metric. Recall that in the §3.4, we introduced the notion of an abstract simplicial complex with a local metric defined on pairs of vertices that are adjacent.

In this situation, we can compute the curvature around a loop in the mesh using local embeddings. We start with an initial n-simplex, which we endow with an orthonormal frame. By locally embedding adjacent n-simplices into Euclidean space, and parallel transporting the orthonormal frame, we will eventually transport the frame back to the initial simplex.

The relative orientation between the original frame and the transported frame yields the integral of the curvature of the surface which is bounded by the traversed curve. This results from a simple application of the Generalized Stokes' theorem, and the fact that the curvature is given by the exterior derivative of the connection 1-form.

4.8 Conclusions and Future Work

We have introduced a complete characterization of discrete connections, in terms of horizontal and vertical spaces, discrete connection 1-forms, horizontal lifts, and splittings of the discrete Atiyah sequence. Geometric structures that can be derived from a given discrete connection have been discussed, including continuous connections, an extended pair groupoid composition, and higher-order analogues of the discrete connection. In addition, we have explored computational issues, such as order of accuracy, and the construction of discrete connections from continuous connections.

Applications to discrete reduction theory, geometric control theory, and discrete geometry, have also been discussed, and it would be desirable to systematically apply the machinery of discrete connections to these problems.

In addition, connections play a crucial role in representing the nonholonomic constraint distribution in nonholonomic mechanics, particularly when considering nonholonomic mechanical systems with symmetry, wherein the nonholonomic connection enters (see, for example, Bloch [2003]). There has been recent progress on constructing nonholonomic integrators in the work of Cortés [2002] and McLachlan and Perlmutter [2003], but an intrinsically discrete notion of a connection remains absent from their work, and they do not consider the role of symmetry reduction in discrete nonholonomic mechanics.

It would be very interesting to apply the general theory of discrete connections on principal bundles to nonholonomic mechanical systems with symmetry, and to cast the notion of a discrete nonholonomic constraint distribution and the nonholonomic connection in the language of discrete connections, and thereby develop a discrete theory of nonholonomic mechanics with symmetry. This would be particularly important for the numerical implementation of geometric control algorithms.

The role of discrete connections in the study of discrete geometric phases would also be an area worth pursuing. A discrete analogue of the rigid-body phase formula, that involves the discrete mechanical connection, that is exact for rigid-body simulations that use discrete variational mechanics, would yield significant insights into the geometric structure-preservation properties of variational integrators. In particular, it would provide much needed insight into how discretization interacts with geometric phases, and yield an understanding how much of the phase drift observed in a numerical simulation is due to the underlying geometry of the mechanical system, and how much is due to the process of discretizing the system.

Chapter 5

Generalized Variational Integrators

Abstract

In this chapter, we introduce generalized Galerkin variational integrators, which are a natural generalization of discrete variational mechanics, whereby the discrete action, as opposed to the discrete Lagrangian, is the fundamental object. This is achieved by approximating the action integral with appropriate choices of a finite-dimensional function space that approximate sections of the configuration bundle and numerical quadrature to approximate the integral. We discuss how this general framework allows us to recover higher-order Galerkin variational integrators, asynchronous variational integrators, and symplectic-energy-momentum integrators. In addition, we will consider function spaces that are not parameterized by field values evaluated at nodal points, which allows the construction of Lie group, multiscale, and pseudospectral variational integrators. The construction of pseudospectral variational integrators is illustrated by applying it to the (linear) Schrödinger equation. G-invariant discrete Lagrangians are constructed in the context of Lie group methods through the use of natural charts and interpolation at the level of the Lie algebra. The reduction of these G-invariant Lagrangians yield a higher-order analogue of discrete Euler–Poincaré reduction. By considering nonlinear approximation spaces, spatio-temporally adaptive variational integrators can be introduced as well.

5.1 Introduction

We will review some of the previous work on discrete mechanics and their multisymplectic generalizations (see, for example, Marsden et al. [1998, 2001]), before introducing a general formulation of discrete mechanics that recovers higher-order variational integrators (see, for example, Marsden and West [2001]), asynchronous variational integrators (see, for example, Lew et al. [2003]), as well symplectic-energy-momentum integrators (see, for example, Kane et al. [1999]).

While discrete variational integrators exhibit desirable properties such as symplecticity, momentum preservation, and good energy behavior, it does not address other important issues in numerical analysis, such as adaptivity and approximability. Generalized variational integrators are introduced with a view towards addressing such issues in the context of discrete variational mechanics.

By formulating the construction of a generalized variational integrator in terms of the choice of a finite-dimensional function space and a numerical quadrature scheme, we are able to draw upon the extensive literature on approximation theory and numerical quadrature to construct variational schemes that are appropriate for a larger class of problems. Within this framework, we will introduce multiscale, spatio-temporally adaptive, Lie group, and pseudospectral variational integrators.

5.1.1 Standard Formulation of Discrete Mechanics

The standard formulation of discrete variational mechanics (see, for example, Marsden and West [2001]) is to consider the ***discrete Hamilton's principle***,

$$\delta \mathbb{S}_d = 0,$$

where the ***discrete action sum***, $\mathbb{S}_d : Q^{n+1} \to \mathbb{R}$, is given by

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

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***,

$$L_d^{\text{exact}}(q_0, q_1) = \int_0^h L(q_{01}(t), \dot{q}_{01}(t)) dt,$$

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

$$D_2 L_d(q_0, q_1) + D_1 L_d(q_1, q_2) = 0,$$

which yields an implicit update map $(q_0, q_1) \mapsto (q_1, q_2)$ that is valid for initial conditions (q_0, q_1) that as sufficiently close to the diagonal of $Q \times Q$.

5.1.2 Multisymplectic Geometry

The generalization of the variational principle to the setting of partial differential equations involves a multisymplectic formulation (see, for example, Marsden et al. [1998, 2001]). Here, the ***base space*** $\mathcal{X}$ consists of the independent variables, which are denoted by $(x^0, \ldots, x^n)$, where x^0 is time, and $x^1, \ldots, x^n$ are space variables.

The independent or field variables, denoted $(q^1, \ldots, q^m)$, form a fiber over each space-time basepoint. The set of independent variables, together with the field variables over them, form a fiber bundle, $\pi : Y \to \mathcal{X}$, referred to as the ***configuration bundle***. The configuration of the system is specified by giving the field values at each space-time point. More precisely, this can be represented as a section of Y over $\mathcal{X}$, which is a continuous map $q : \mathcal{X} \to Y$, such that $\pi \circ q = 1_{\mathcal{X}}$. This means that for every $x \in \mathcal{X}$, $q(x)$ is in the fiber over x, which is $\pi^{-1}(x)$.

In the case of ordinary differential equations, the Lagrangian is dependent on the position variable, and its time derivative, and the action integral is obtained by integrating the Lagrangian in time. In the multisymplectic case, the Lagrangian density is dependent on the field variables, and the derivatives of the field variables with respect to the space-time variables, and the action integral is obtained by integrating the Lagrangian density over a region of space-time.

The analogue of the tangent bundle TQ in the multisymplectic setting is referred to as the ***first jet bundle*** J^1Y, which consists of the configuration bundle Y, together with the first derivatives of the field variables with respect to independent variables. We denote these as,

$$v^i{}_j = q^i{}_{,j} = \frac{\partial q^i}{\partial x^j},$$

for $i = 1, \ldots, m$, and $j = 0, \ldots, n$.

We can think of J^1Y as a fiber bundle over $\mathcal{X}$. Given a section $q : \mathcal{X} \to Y$, we obtain its ***first jet extension***, $j^1q : \mathcal{X} \to J^1Y$, that is given by

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

which is a section of the fiber bundle J^1Y over $\mathcal{X}$.

The Lagrangian density is a map $L : J^1Y \to \Omega^{n+1}(\mathcal{X})$, and the action integral is given by

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

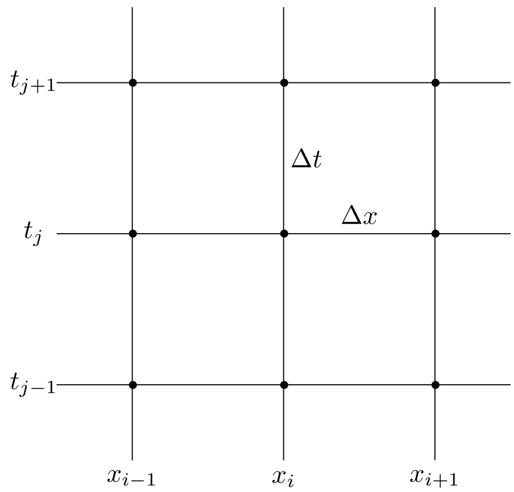
and then Hamilton's principle states that

$$\delta\mathcal{S} = 0.$$

We will see in the next subsection how this allows us to construct multisymplectic variational integrators.

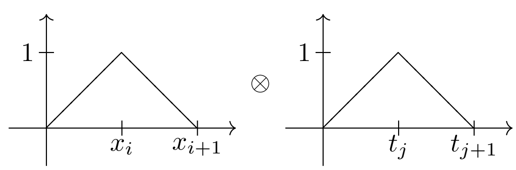
5.1.3 Multisymplectic Variational Integrator

We introduce a multisymplectic variational integrator through the use of a simple but illustrative example. We consider a tensor product discretization of $(1+1)$-space-time, given by



and tensor product shape functions given by

$\varphi_{i,j}(x,t) =$



We construct the discrete Lagrangian as follows,

$$L_d(q_{i,j}, q_{i+1,j}, q_{i,j+1}, q_{i+1,j+1}) = \int_{[x_i, x_{i+1}]} \int_{[t_j, t_{j+1}]} L\Big(j^1\Big(\sum_{a=i}^{i+1} \sum_{b=j}^{j+1} q_{a,b}\varphi_{a,b}\Big)\Big),$$

where $q_{i,j} \simeq q(i\Delta x, j\Delta t)$.

Consider a variation that varies the value of $q_{i,j}$, and leaves the other degrees of freedom fixed, then we obtain the following discrete Euler–Lagrange equation,

$$\begin{aligned} D_1 L_d(q_{i,j}, q_{i+1,j}, q_{i,j+1}, q_{i+1,j+1}) + & D_2 L_d(q_{i-1,j}, q_{i,j}, q_{i-1,j+1}, q_{i,j+1}) \\ & + D_3 L_d(q_{i,j-1}, q_{i+1,j-1}, q_{i,j}, q_{i+1,j}) \\ & + D_4 L_d(q_{i-1,j-1}, q_{i,j-1}, q_{i-1,j}, q_{i,j}) = 0\,, \end{aligned}$$

In general, when we take variations in a degree of freedom, we will have a discrete Euler–Lagrange equation that involves all terms in the discrete action sum that are associated with regions in space-time that overlap with the support of the shape function associated with that degree of freedom.

5.2 Generalized Galerkin Variational Integrators

There are a few essential observations that go into constructing a general framework that encompasses the prior work on variational integrators, asynchronous variational integrators, and symplectic-energy-momentum integrators, while yielding generalizations that allow the construction of multiscale, spatio-temporally adaptive, Lie group, and pseudospectral variational integrators.

The first is that a generalized Galerkin variational integrator involves the choice of a finite-dimensional function space that discretizes a section of the configuration bundle, and the second is that we approximate the action integral though a numerical quadrature scheme to yield a discrete action sum. The discrete variational equations we obtain from this discrete variational principle are simply the Karush–Kuhn–Tucker (KKT) conditions (see, for example, Nocedal and Wright [1999]) with respect to the degrees of freedom that generate the finite-dimensional function space.

To recap, the choices which are made in discretizing a variational problem are:

1. A finite-dimensional function space to represent sections of the configuration bundle.

2. A numerical quadrature scheme to evaluate the action integral.

Given these two choices, we obtain an expression for the discrete action in terms of the degrees of freedom, and the KKT conditions for the discrete action to be stationary with respect to variations in the degrees of freedom yield the generalized discrete Euler–Lagrange equations.

Current variational integrators are based on piecewise polynomial interpolation, with function spaces that are parameterized by the value of the field variables at nodal points, and a set of internal points. By relaxing the condition that the interpolation is piecewise, we will be able to consider pseudospectral discretizations, and by relaxing the condition that the parameterization is in terms of field values, we will be able to consider Lie group variational integrators. By considering shape functions motivated by multiscale finite elements (see, for example, Hou and Wu [1999]; Efendiev et al. [2000]; Chen and Hou [2003]), we will obtain multiscale variational integrators. And by generalizing the approach used in symplectic-energy-momentum integrators, and considering nonlinear approximation spaces (see, for example, DeVore [1998]), we will be able to introduce spatio-temporally adaptive variational integrators.

As we will see, there is nothing canonical about the form of the discrete Euler–Lagrange equations, or the notion that the discrete Lagrangian is a map $L_d : Q \times Q \to \mathbb{R}$. These expressions arise because of the finite-dimensional function space which has been chosen.

5.2.1 Special Cases of Generalized Galerkin Variational Integrators

In this subsection, we will show how higher-order Galerkin variational integrators, multisymplectic variational integrators, and symplectic-energy-momentum integrators are all special cases of generalized Galerkin variational integrators.

Higher-Order Galerkin Variational Integrators. In the case of higher-order Galerkin variational integrators, we have chosen a piecewise interpolation for each time interval $[0,h]$, that is parameterized by control points $q_0^1, \dots q_0^s$, corresponding to the value of the curve at a set of control times $0 = d_0 < d_1 < \dots < d_{s-1} < d_s = 1$. The interpolation within each interval $[0,h]$ is given by the unique degree s polynomial $q_d(t; q_0^\nu, h)$, such that $q_d(d_\nu h) = g_0^\nu$, for $\nu = 0, \dots, s$.

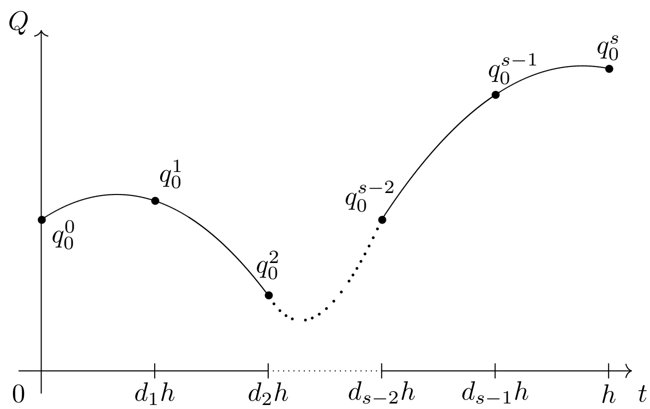


Figure 5.1: Polynomial interpolation used in higher-order Galerkin variational integrators.

By an appropriate choice of quadrature scheme, we can break up the action integral into pieces, which we denote by

$$\mathbb{S}_d^i(q_i^\nu) \approx \int_0^h L(q_d(t; q_i^\nu, h), \dot{q}_d(t; q_i^\nu, h))dt.$$

If we further require that the piecewise defined curve is continuous at the node points, we obtain the following augmented discrete action,

$$\mathbb{S}_d\left(\{q_i^\nu\}_{\substack{i=0,\dots,N-1\\ \nu=0,\dots,s}}\right) = \sum_{i=0}^{N-1} \mathbb{S}_d^i\left(\{q_i^\nu\}_{\nu=0}^s\right) - \sum_{i=0}^{N-2} \lambda_i(q_i^s - q_{i+1}^0).$$

The discrete action is stationary when

$$\frac{\partial \mathbb{S}_d^i}{\partial q_i^s}(q_i^\nu) = \lambda_i,$$

$$\frac{\partial \mathbb{S}_d^i}{\partial q_{i+1}^0}(q_{i+1}^\nu) = -\lambda_i,$$
$$\frac{\partial \mathbb{S}_d^i}{\partial q_i^j}(q_i^\nu) = 0.$$

We can identify the pieces of the discrete action with the discrete Lagrangian, $L_d : Q \times Q \to \mathbb{R}$, by setting

$$L_d(q_i, q_{i+1}) = \mathbb{S}_d^i(q_i^\nu), \tag{5.2.1}$$

where, $q_i^0 = q_i$, $q_i^s = q_{i+1}$, and the other q_i^j's are defined implicitly by the system of equations

$$\frac{\partial \mathbb{S}_d^i}{\partial q_i^j}(q_i^\nu) = 0, \tag{5.2.2}$$

for $\nu = 1, \ldots, s-1$. Once we have made this identification, we have that

$$\begin{aligned} -D_1 L_d(q_{i+1}, q_{i+2}) &= -\frac{\mathbb{S}_d^{i+1}}{\partial q_{i+1}^0}(q_{i+1}^\nu) \\ &= \lambda_i \\ &= \frac{\partial \mathbb{S}_d^i}{\partial q_i^s}(q_i^\nu) \\ &= D_2 L_d(q_i, q_{i+1}), \end{aligned}$$

from which we recover the discrete Euler–Lagrange equation,

$$D_1 L_d(q_{i+1}, q_{i+2}) + D_2 L_d(q_i, q_{i+1}) = 0.$$

The DEL equations, together with the definition of the discrete Lagrangian, given in Equations 5.2.1 and 5.2.2, yield a higher-order Galerkin variational integrator. As we have shown, it is only because the interpolation was piecewise that we were able to decompose the equations into a DEL equation, and a set of equations that define the discrete Lagrangian in terms of conditions on the internal control points.

Multisymplectic Variational Integrators. Recall the example of a multisymplectic variational integrator we introduced in §5.1.3, where we used tensor product linear shape functions with localized supports to discretize the configuration bundle. The discrete action is then given by

$$\mathbb{S}_d\left(\{q_{a,b}\}_{\substack{a=0,\ldots,M-1\\ b=0,\ldots,N-1}}\right) = \int_{[x_0,x_M]} \int_{[t_0,t_N]} L\Big(j^1\Big(\sum_{a=0}^{N}\sum_{b=0}^{N} q_{a,b}\varphi_{a,b}\Big)\Big)$$

$$= \sum_{i=0}^{M-1} \sum_{j=0}^{N-1} \int_{[x_i, x_{i+1}]} \int_{[t_j, t_{j+1}]} L\Big(j^1\Big(\sum_{a=0}^{N} \sum_{b=0}^{N} q_{a,b}\varphi_{a,b}\Big)\Big)$$

$$= \sum_{i=0}^{M-1} \sum_{j=0}^{N-1} \int_{[x_i, x_{i+1}]} \int_{[t_j, t_{j+1}]} L\Big(j^1\Big(\sum_{a=i}^{i+1} \sum_{b=j}^{j+1} q_{a,b}\varphi_{a,b}\Big)\Big),$$

where we first decomposed the integral into pieces, and then used the local support of the shape functions to simplify the inner sums over $q_{a,b}\varphi_{a,b}$. As before, it is due to the local support of the shape functions that we can express the discrete action as

$$\mathbb{S}_d = \sum_{i=0}^{M-1} \sum_{j=0}^{N-1} L_d(q_{i,j}, q_{i+1,j}, q_{i,j+1}, q_{i+1,j+1}),$$

where

$$L_d(q_{i,j}, q_{i+1,j}, q_{i,j+1}, q_{i+1,j+1}) = \int_{[x_i, x_{i+1}]} \int_{[t_j, t_{j+1}]} L\Big(j^1\Big(\sum\nolimits_{a=i}^{i+1} \sum\nolimits_{b=j}^{j+1} q_{a,b}\varphi_{a,b}\Big)\Big),$$

This localized support is also the reason why the discrete Euler–Lagrange equation in this case consists of four terms, since to each degree of freedom, there are four other degrees of freedom that have shape functions with overlapping support. In the case of ordinary differential equations, this was two. In general, for tensor product meshes of $(n+1)$-space-times, with tent function shape functions, the number of terms in the discrete Euler–Lagrange equation will be 2^{n+1}. In contrast, for pseudospectral variational integrators with m spatial degrees of freedom per time level, and k degrees of freedom per piecewise polynomial in time, each of the $m(k-1)$ discrete Euler–Lagrange equations will involve $m(k-1)$ terms.

This is simply a reflection of the fact that shape functions with compact support yield schemes with banded matrix structure, whereas pseudospectral and spectral methods tend to yield fuller matrices. The payoff in using pseudospectral and spectral methods for problems with smooth or analytic solutions is due to the approximation theoretic property that these solutions are approximated at an exponential rate of accuracy by spectral expansions.

Symplectic-Energy-Momentum Integrators. In the case of symplectic-energy-momentum integrators, the degrees of freedom involve both the base variables and the field variables. We will first derive a second-order symplectic-energy momentum integrator, and in the next section, we will derive a higher-order generalization. We choose a piecewise linear interpolation for our configuration bundle. Each piece is parameterized by the endpoint values of the field variable q_i^0, q_i^1, and the endpoint times h_i^0, h_i^1, and we approximate the action integral using the midpoint rule. To ensure continuity, we require that, $q_i^1 = q_{i+1}^0$, and $h_i^1 = h_{i+1}^0$.

Remark 5.1. *The approach of allowing each piecewise defined curve to float around freely, and imposing the continuity conditions using Lagrange multipliers was used in Lall and West [2003] to unify the formulation of discrete variational mechanics and optimal control. Through the use of a primal-dual formalism, discrete analogues of Hamiltonian mechanics and the Hamilton–Jacobi equation were also introduced.*

This yields the following discrete action,

$$\mathbb{S}_d = \sum_{i=0}^{N-1} (h_i^1 - h_i^0) L\left(\frac{q_i^0 + q_i^1}{2}, \frac{q_i^1 - q_i^0}{h_i^1 - h_1^0}\right) - \sum_{i=0}^{N-2} \lambda_i (q_i^1 - q_{i+1}^0) - \sum_{i=0}^{N-2} \omega_i (h_i^1 - h_{i+1}^0).$$

To simplify the expressions, we define

$$\begin{aligned} h_i &\equiv h_i^1 - h_i^0, \\ q_{i+\frac{1}{2}} &\equiv \frac{q_i^0 + q_i^1}{2}, \\ \dot{q}_{i+\frac{1}{2}} &\equiv \frac{q_i^1 - q_i^0}{h_i}. \end{aligned}$$

Then, the variational equations are given by

$$\begin{aligned}
0 &= L\left(q_{i+\frac{1}{2}}, \dot{q}_{i+\frac{1}{2}}\right) - h_i \frac{\partial L}{\partial \dot{q}}\left(q_{i+\frac{1}{2}}, \dot{q}_{i+\frac{1}{2}}\right) \frac{1}{h_i} \dot{q}_{i+\frac{1}{2}} - \omega_i, && \text{for } i = 0, \ldots, N-2, \\
0 &= -L\left(q_{i+\frac{1}{2}}, \dot{q}_{i+\frac{1}{2}}\right) + h_i \frac{\partial L}{\partial \dot{q}}\left(q_{i+\frac{1}{2}}, \dot{q}_{i+\frac{1}{2}}\right) \frac{1}{h_i} \dot{q}_{i+\frac{1}{2}} + \omega_{i-1}, && \text{for } i = 1, \ldots, N-1, \\
0 &= h_i \left[\frac{\partial L}{\partial q}\left(q_{i+\frac{1}{2}}, \dot{q}_{i+\frac{1}{2}}\right) \frac{1}{2} + \frac{\partial L}{\partial \dot{q}}\left(q_{i+\frac{1}{2}}, \dot{q}_{i+\frac{1}{2}}\right) \frac{1}{h_i}\right] - \lambda_i, && \text{for } i = 0, \ldots, N-2, \\
0 &= h_i \left[\frac{\partial L}{\partial q}\left(q_{i+\frac{1}{2}}, \dot{q}_{i+\frac{1}{2}}\right) \frac{1}{2} - \frac{\partial L}{\partial \dot{q}}\left(q_{i+\frac{1}{2}}, \dot{q}_{i+\frac{1}{2}}\right) \frac{1}{h_i}\right] + \lambda_{i-1}, && \text{for } i = 1, \ldots, N-1, \\
q_i^1 &= q_{i+1}^0, && \text{for } i = 0, \ldots, N-2, \\
h_i^1 &= h_{i+1}^0, && \text{for } i = 0, \ldots, N-2.
\end{aligned}$$

If we define the discrete Lagrangian to be

$$L_d(q_i, q_{i+1}, h_i) \equiv h_i L\left(\frac{q_i + q_{i+1}}{2}, \frac{q_{i+1} - q_i}{h_i}\right),$$

and the discrete energy to be

$$\begin{aligned} E_d(q_i, q_{i+1}, h_i) &\equiv -D_3 L_d(q_i, q_{i+1}, h_i) \\ &= -L\left(\frac{q_i + q_{i+1}}{2}, \frac{q_{i+1} - q_i}{h_i}\right) + h_i \frac{\partial L}{\partial \dot{q}}\left(\frac{q_i + q_{i+1}}{2}, \frac{q_{i+1} - q_i}{h_i}\right) \frac{1}{h_i} \frac{q_{i+1} - q_i}{h_i}, \end{aligned}$$

and identify points as follows,

$$q_i = q_{i-1}^1 = q_i^0,$$
$$h_i = h_{i-1}^1 = h_i^0,$$

we obtain

$$\begin{aligned}
0 =& E_d(q_i, q_{i+1}, h_i) - \omega_i, && \text{for } i = 0, \ldots, N-2,\\
0 =& -E_d(q_i, q_{i+1}, h_i) + \omega_{i-1}, && \text{for } i = 1, \ldots, N-1,\\
0 =& D_2 L_d(q_i, q_{i+1}, h_i) - \lambda_i, && \text{for } i = 0, \ldots, N-2,\\
0 =& D_1 L_d(q_i, q_{i+1}, h_i) + \lambda_{i-1}, && \text{for } i = 1, \ldots, N-1.
\end{aligned}$$

After eliminating the Lagrange multipliers, we obtain the conservation of discrete energy equation,

$$E_d(q_i, q_{i+1}, h_i) = E_d(q_{i+1}, q_{i+2}, h_{i+1}),$$

and the discrete Euler–Lagrange equation,

$$D_2 L_d(q_i, q_{i+1}, h_i) + D_1 L_d(q_{i+1}, q_{i+2}, h_{i+1}) = 0.$$

This recovers the results obtained in Kane et al. [1999], but the derivation is new. In §5.5, we will see how this derivation can be generalized to yield a higher-order scheme.

Discrete Action as the Fundamental Object. The message of this section is that the discrete action is the fundamental object in discrete mechanics, as opposed to the discrete Lagrangian. In instances whereby the shape function associated with individual degrees of freedom have localized supports, it is possible to decompose the discrete action into terms that can be identified with discrete Lagrangians. While this approach might seem artificial at first, we will find that in discussing pseudospectral variational integrators, it does not make sense to break up the discrete action into individual pieces.

5.3 Lie Group Variational Integrators

In this section, we will introduce higher-order Lie group variational integrators. The basic idea behind all Lie group techniques is to express the update map of the numerical scheme in terms of the exponential map,

$$g_1 = g_0 \exp(\xi_{01}) ,$$

and thereby reduce the problem to finding an appropriate Lie algebra element $\xi_{01} \in \mathfrak{g}$, such that the update scheme has the desired order of accuracy. This is a desirable reduction, as the Lie algebra is a vector space, and as such the interpolation of elements can be easily defined. In our construction, the interpolatory method we use on the Lie group relies on interpolation at the level of the Lie algebra.

For a more in depth review of Lie group methods, please refer to Iserles et al. [2000]. In the case of variational Lie group methods, we will express the variational problem in terms of finding Lie algebra elements, such that the discrete action is stationary.

As we will consider the reduction of these higher-order Lie group integrators in the next section, we will chose a construction that yields a G-invariant discrete Lagrangian whenever the continuous Lagrangian is G-invariant. This is achieved through the use of G-equivariant interpolatory functions, and in particular, natural charts on G.

5.3.1 Galerkin Variational Integrators

We first recall the construction of higher-order Galerkin variational integrators, as originally described in Marsden and West [2001]. Given a Lie group G, the associated ***state space*** is given by the tangent bundle TG. In addition, the dynamics on G is described by a ***Lagrangian***, $L : TG \to \mathbb{R}$. Given a time interval $[0, h]$, the ***path space*** is defined to be

$$\mathcal{C}(G) = \mathcal{C}([0, h], G) = \{g : [0, h] \to G \mid g \text{ is a } C^2 \text{ curve}\},$$

and the ***action map***, $\mathfrak{S} : \mathcal{C}(G) \to \mathbb{R}$, is given by

$$\mathfrak{S}(g) \equiv \int_0^h L(g(t), \dot{g}(t))dt.$$

We approximate the action map, by numerical quadrature, to yield $\mathfrak{S}^s : \mathcal{C}([0, h], G) \to \mathbb{R}$,

$$\mathfrak{S}^s(g) \equiv h \sum_{i=1}^{s} b_i L(g(c_i h), \dot{g}(c_i h)),$$

where $c_i \in [0, 1]$, $i = 1, \ldots, s$ are the quadrature points, and b_i are the quadrature weights.

Recall that the discrete Lagrangian should be an approximation of the form

$$L_d(g_0, g_1, h) \approx \operatorname*{ext}_{g \in \mathcal{C}([0,h],G), g(0)=g_0, g(h)=g_1} \mathfrak{S}(g) .$$

If we restrict the extremization procedure to the subspace spanned by the interpolatory function that is parameterized by $s+1$ internal points, $\varphi : G^{s+1} \to \mathcal{C}([0,h],G)$, we obtain the following discrete Lagrangian,

$$\begin{aligned} L_d(g_0,g_1) &= \operatorname*{ext}_{g^\nu \in G; g^0=g_0; g^s=g_1} \mathfrak{S}(T\varphi(g^\nu;\cdot)) \\ &= \operatorname*{ext}_{g^\nu \in G; g^0=g_0; g^s=g_1} h\sum_{i=1}^{s} b_i L(T\varphi(g^\nu;c_i h)). \end{aligned}$$

The interpolatory function is G-equivariant if

$$\varphi(gg^\nu;t) = g\varphi(g^\nu;t).$$

Lemma 5.1. *If the interpolatory function $\varphi(g^\nu;t)$ is G-equivariant, and the Lagrangian, $L : TG \to \mathbb{R}$, is G-invariant, then the discrete Lagrangian, $L_d : G\times G \to \mathbb{R}$, given by*

$$L_d(g_0,g_1) = \operatorname*{ext}_{g^\nu \in G; g^0=g_0; g^s=g_1} h\sum_{i=1}^{s} b_i L(T\varphi(g^\nu;c_i h)),$$

is G-invariant.

Proof.

$$\begin{aligned} L_d(gg_0,gg_1) &= \operatorname*{ext}_{\tilde{g}^\nu \in G; \tilde{g}^0=gg_0; \tilde{g}^s=gg_1} h\sum_{i=1}^{s} b_i L(T\varphi(\tilde{g}^\nu;c_i h)), \\ &= \operatorname*{ext}_{g^\nu \in g^{-1}G; g^0=g_0; g^s=g_1} h\sum_{i=1}^{s} b_i L(T\varphi(gg^\nu;c_i h)), \\ &= \operatorname*{ext}_{g^\nu \in G; g^0=g_0; g^s=g_1} h\sum_{i=1}^{s} b_i L(TL_g\cdot T\varphi(g^\nu;c_i h)), \\ &= \operatorname*{ext}_{g^\nu \in G; g^0=g_0; g^s=g_1} h\sum_{i=1}^{s} b_i L(T\varphi(g^\nu;c_i h)), \\ &= L_d(g_0,g_1), \end{aligned}$$

where we used the G-equivariance of the interpolatory function in the third equality, and the G-invariance of the Lagrangian in the forth equality. □

Remark 5.2. *While G-equivariant interpolatory functions provide a computationally efficient method of constructing G-invariant discrete Lagrangians, we can construct a G-invariant discrete Lagrangian (when G is compact) by averaging an arbitrary discrete Lagrangian. In particular, given a discrete*

Lagrangian $L_d : Q \times Q \to \mathbb{R}$, the averaged discrete Lagrangian, given by

$$\bar{L}_d(q_0, q_1) = \frac{1}{|G|} \int_{g \in G} L_d(gq_0, gq_1) dg$$

is G-equivariant. Therefore, in the case of compact symmetry groups, a G-invariant discrete Lagrangian always exists.

5.3.2 Natural Charts

Following the construction in Marsden et al. [1999], we use the group exponential map at the identity, $\exp_e : \mathfrak{g} \to G$, to construct a G-equivariant interpolatory function, and a higher-order discrete Lagrangian. As shown in Lemma 5.1, this construction yields a G-invariant discrete Lagrangian if the Lagrangian itself is G-invariant.

In a finite-dimensional Lie group G, $\exp_e$ is a local diffeomorphism, and thus there is an open neighborhood $U \subset G$ of e such that $\exp_e^{-1} : U \to \mathfrak{u} \subset \mathfrak{g}$. When the group acts on the left, we obtain a chart $\psi_g : L_g U \to \mathfrak{u}$ at $g \in G$ by

$$\psi_g = \exp_e^{-1} \circ L_{g^{-1}}.$$

Lemma 5.2. *The interpolatory function given by*

$$\varphi(g^\nu; \tau h) = \psi_{g^0}^{-1} \left(\sum\nolimits_{\nu=0}^{s} \psi_{g^0}(g^\nu) \tilde{l}_{\nu,s}(\tau) \right),$$

is G-equivariant.

Proof.

$$\begin{aligned}
\varphi(gg^\nu; \tau h) &= \psi_{(gg^0)}^{-1} \left(\sum\nolimits_{\nu=0}^{s} \psi_{gg^0}(gg^\nu) \tilde{l}_{\nu,s}(\tau) \right) \\
&= L_{gg^0} \exp_e \left(\sum\nolimits_{\nu=0}^{s} \exp_e^{-1}((gg^0)^{-1}(gg^\nu)) \tilde{l}_{\nu,s}(\tau) \right) \\
&= L_g L_{g^0} \exp_e \left(\sum\nolimits_{\nu=0}^{s} \exp_e^{-1}((g^0)^{-1} g^{-1} g g^\nu) \tilde{l}_{\nu,s}(\tau) \right) \\
&= L_g \psi_{g^0}^{-1} \left(\sum\nolimits_{\nu=0}^{s} \exp_e^{-1} \circ L_{(g^0)^{-1}}(g^\nu) \tilde{l}_{\nu,s}(\tau) \right) \\
&= L_g \psi_{g^0}^{-1} \left(\sum\nolimits_{\nu=0}^{s} \psi_{g^0}(g^\nu) \tilde{l}_{\nu,s}(\tau) \right) \\
&= L_g \varphi(g^\nu; \tau h).
\end{aligned}$$

□

Remark 5.3. *In the proof that φ is G-equivariant, it was important that the base point for the chart should transform in the same way as the internal points g^ν. As such, the interpolatory function will be G-equivariant for a chart that it based at any one of the internal points g^ν that parameterize the function, but will not be G-equivariant if the chart is based at a fixed $g \in G$. Without loss of* *generality, we will consider the case when the chart is based at the first point g_0.*

We will now consider a discrete Lagrangian based on the use of interpolation in a natural chart, which is given by

$$L_d(g_0, g_1) = \underset{g^\nu \in G; g^0 = g_0; g^s = g_0^{-1} g_1}{\text{ext}} h \sum_{i=1}^{s} b_i L(T\varphi(\{g^\nu\}_{\nu=0}^{s}; c_i h)\,.$$

To further simplify the expression, we will express the extremal in terms of the Lie algebra elements ξ^ν associated with the ν-th control point. This relation is given by

$$\xi^\nu = \psi_{g_0}(g^\nu)\,,$$

and the interpolated curve in the algebra is given by

$$\xi(\xi^\nu; \tau h) = \sum_{\kappa=0}^{s} \xi^\kappa \tilde{l}_{\kappa,s}(\tau),$$

which is related to the curve in the group,

$$g(g^\nu; \tau h) = g_0 \exp(\xi(\psi_{g_0}(g^\nu); \tau h)).$$

The velocity $\dot{\xi} = g^{-1}\dot{g}$ is given by

$$\dot{\xi}(\tau h) = g^{-1}\dot{g}(\tau h) = \frac{1}{h} \sum_{\kappa=0}^{s} \xi^\kappa \dot{\tilde{l}}_{\kappa,s}(\tau).$$

Using the standard formula for the derivative of the exponential,

$$T_\xi \exp = T_e L_{\exp(\xi)} \cdot \mathrm{dexp}_{\mathrm{ad}_\xi}\,,$$

where

$$\mathrm{dexp}_w = \sum_{n=0}^{\infty} \frac{w^n}{(n+1)!}\,,$$

we obtain the following expression for discrete Lagrangian,

$$L_d(g_0, g_1) = \underset{\xi^\nu \in \mathfrak{g}; \xi^0 = 0; \xi^s = \psi_{g_0}(g_1)}{\text{ext}} h \sum_{i=1}^{s} b_i L\Big(L_{g_0} \exp(\xi(c_i h)),$$
$$T_{\exp(\xi(c_i h))} L_{g_0} \cdot T_e L_{\exp(\xi(c_i h))} \cdot \mathrm{dexp}_{\mathrm{ad}_{\xi(c_i h)}}(\dot{\xi}(c_i h))\Big)\,.$$

More explicitly, we can compute the conditions on the Lie algebra elements for the expression above to be extremal. This implies that

$$L_d(g_0, g_1) = h\sum_{i=1}^{s} b_i L\Big(L_{g_0}\exp(\xi(c_ih)), T_{\exp(\xi(c_ih))}L_{g_0}\cdot T_eL_{\exp(\xi(c_ih))}\cdot \operatorname{dexp}_{\operatorname{ad}_{\xi(c_ih)}}(\dot{\xi}(c_ih))\Big)$$

with $\xi^0 = 0$, $\xi^s = \psi_{g_0}(g_1)$, and the other Lie algebra elements implicitly defined by

$$\begin{aligned} 0 = h\sum_{i=1}^{s} b_i \Bigg[&\frac{\partial L}{\partial g}(c_ih)T_{\exp(\xi(c_ih))}L_{g_0}\cdot T_eL_{\exp(\xi(c_ih))}\cdot \operatorname{dexp}_{\operatorname{ad}_{\xi(c_ih)}}\tilde{l}_{\nu,s}(c_i) \\ &+ \frac{1}{h}\frac{\partial L}{\partial \dot{g}}(c_ih)T^2_{\exp(\xi(c_ih))}L_{\exp(\xi(c_ih))}\cdot T^2_eL_{\exp(\xi(c_ih))}\cdot \operatorname{ddexp}_{\operatorname{ad}_{\xi(c_ih)}}\dot{\tilde{l}}_{\nu,s}(c_i)\Bigg]\,, \end{aligned}$$

for $\nu = 1, \ldots, s-1$, and where

$$\operatorname{ddexp}_w = \sum_{n=0}^{\infty}\frac{w^n}{(n+2)!}\,.$$

This expression for the higher-order discrete Lagrangian, together with the discrete Euler–Lagrange equation,

$$D_2L_d(g_0, g_1) + D_1L_d(g_1, g_2) = 0\,,$$

yields a ***higher-order Lie group variational integrator***.

5.4 Higher-Order Discrete Euler–Poincaré Equations

In this section, we will apply discrete Euler–Poincaré reduction (see, for example, Marsden et al. [1999]) to the Lie group variational integrator we derived previously, to construct a higher-order generalization of discrete Euler–Poincaré reduction.

5.4.1 Reduced Discrete Lagrangian

We first proceed by computing an expression for the reduced discrete Lagrangian in the case when the Lagrangian is G-invariant. Recall that our discrete Lagrangian uses G-equivariant interpolation, which, when combined with the G-invariance of the Lagrangian, implies that the discrete Lagrangian is G-invariant as well. We compute the reduced discrete Lagrangian,

$$\begin{aligned} l_d(g_0^{-1}g_1) &\equiv L_d(g_0, g_1) \\ &= L_d(e, g_0^{-1}g_1) \\ &= \operatorname*{ext}_{\xi^\nu\in\mathfrak{g};\xi^0=0;\xi^s=\log(g_0^{-1}g_1)} h\sum_{i=1}^{s} b_i L\Big(L_e\exp(\xi(c_ih)), \\ &\qquad\qquad T_{\exp(\xi(c_ih))}L_e\cdot T_eL_{\exp(\xi(c_ih))}\cdot \operatorname{dexp}_{\operatorname{ad}_{\xi(c_ih)}}(\dot{\xi}(c_ih))\Big) \end{aligned}$$

$$= \operatorname*{ext}_{\xi^\nu\in\mathfrak{g};\xi^0=0;\xi^s=\log(g_0^{-1}g_1)} h\sum_{i=1}^s b_i L\Big(\exp(\xi(c_ih)), T_eL_{\exp(\xi(c_ih))}\cdot \operatorname{dexp}_{\operatorname{ad}_{\xi(c_ih)}}(\dot{\xi}(c_ih))\Big)\,.$$

Setting $\xi^0 = 0$, and $\xi^s = \log(g_0^{-1}g_1)$, we can solve the stationarity conditions for the other Lie algebra elements $\{\xi^\nu\}_{\nu=1}^{s-1}$ using the following implicit system of equations,

$$\begin{aligned} 0 = h\sum_{i=1}^s b_i \bigg[&\frac{\partial L}{\partial g}(c_ih)T_eL_{\exp(\xi(c_ih))}\cdot \operatorname{dexp}_{\operatorname{ad}_{\xi(c_ih)}} \tilde{l}_{\nu,s}(c_i)\\ &+\frac{1}{h}\frac{\partial L}{\partial \dot{g}}(c_ih)T_e^2L_{\exp(\xi(c_ih))}\cdot \operatorname{ddexp}_{\operatorname{ad}_{\xi(c_ih)}} \dot{\tilde{l}}_{\nu,s}(c_i)\bigg]\end{aligned}$$

where $\nu = 1, \dots, s-1$.

This expression for the reduced discrete Lagrangian is not fully satisfactory however, since it involves the Lagrangian, as opposed to the reduced Lagrangian. If we revisit the expression for the reduced discrete Lagrangian,

$$l_d(g_0^{-1}g_1) = \operatorname*{ext}_{\xi^\nu\in\mathfrak{g};\xi^0=0;\xi^s=\log(g_0^{-1}g_1)} h\sum_{i=1}^s b_i L\Big(\exp(\xi(c_ih)), T_eL_{\exp(\xi(c_ih))}\cdot \operatorname{dexp}_{\operatorname{ad}_{\xi(c_ih)}}(\dot{\xi}(c_ih))\Big)\,,$$

we find that by G-invariance of the Lagrangian, each of the terms in the summation,

$$L\Big(\exp(\xi(c_ih)), T_eL_{\exp(\xi(c_ih))}\cdot \operatorname{dexp}_{\operatorname{ad}_{\xi(c_ih)}}(\dot{\xi}(c_ih))\Big)\,,$$

can be replaced by

$$l\Big(\operatorname{dexp}_{\operatorname{ad}_{\xi(c_ih)}}(\dot{\xi}(c_ih))\Big)\,,$$

where $l : \mathfrak{g} \to \mathbb{R}$ is the ***reduced Lagrangian*** given by

$$l(\eta) = L(L_{g^{-1}}g, TL_{g^{-1}}\dot{g}) = L(e,\eta),$$

where $\eta = TL_{g^{-1}}\dot{g} \in \mathfrak{g}$.

From this observation, we have an expression for the reduced discrete Lagrangian in terms of the reduced Lagrangian,

$$l_d(g_0^{-1}g_1) = \operatorname*{ext}_{\xi^\nu\in\mathfrak{g};\xi^0=0;\xi^s=\log(g_0^{-1}g_1)} h\sum_{i=1}^s b_i l\Big(\operatorname{dexp}_{\operatorname{ad}_{\xi(c_ih)}}(\dot{\xi}(c_ih))\Big)\,.$$

As before, we set $\xi^0 = 0$, and $\xi^s = \log(g_0^{-1}g_1)$, and solve the stationarity conditions for the other

Lie algebra elements $\{\xi^\nu\}_{\nu=1}^{s-1}$ using the following implicit system of equations,

$$0 = h \sum_{i=1}^{s} b_i \left[\frac{\partial l}{\partial \eta}(c_i h) \, \mathrm{ddexp}_{\mathrm{ad}_{\xi(c_i h)}} \dot{\tilde{l}}_{\nu,s}(c_i) \right] ,$$

where $\nu = 1, \ldots, s-1$.

5.4.2 Discrete Euler–Poincaré Equations

As shown above, we have constructed a higher-order reduced discrete Lagrangian that depends on

$$f_{kk+1} \equiv g_k g_{k+1}^{-1} .$$

We will now recall the derivation of the discrete Euler–Poincaré equations, introduced in Marsden et al. [1999]. The variations in f_{kk+1} induced by variations in g_k, g_{k+1} are computed as follows,

$$\begin{aligned} \delta f_{kk+1} &= -g_k^{-1} \delta g_k g_k - 1 g_{k+1} + g_k^{-1} \delta g_{k+1} \\ &= TR_{f_{kk+1}} (-g_k^{-1} \delta g_k + \mathrm{Ad}_{f_{kk+1}} g_{k+1} \delta g_{k+1}) \, . \end{aligned}$$

Then, the variation in the discrete action sum is given by

$$\begin{aligned} \delta \mathbb{S} &= \sum_{k=0}^{N-1} l_d'(f_{kk+1}) \delta f_{kk+1} \\ &= \sum_{k=0}^{N-1} l_d'(f_{kk+1}) TR_{f_{kk+1}} (-g_k^{-1} \delta g_k + \mathrm{Ad}_{f_{kk+1}} g_{k+1} \delta g_{k+1}) \\ &= \sum_{k=1}^{N-1} \left[l_d'(f_{k-1k}) TR_{f_{k-1k}} \mathrm{Ad}_{f_{k-1k}} - l_d'(f_{kk+1}) TR_{f_{kk+1}} \right] \vartheta_k \, , \end{aligned}$$

with variations of the form $\vartheta_k = g_k^{-1} \delta g_k$. In computing the variation of the discrete action sum, we have collected terms involving the same variations, and used the fact that $\vartheta_0 = \vartheta_N = 0$. This yields the ***discrete Euler–Poincaré equation***,

$$l_d'(f_{k-1k}) TR_{f_{k-1k}} \mathrm{Ad}_{f_{k-1k}} - l_d'(f_{kk+1}) TR_{f_{kk+1}} = 0, \qquad k = 1, \ldots, N-1.$$

For ease of reference, we will recall the expressions from the previous subsection that define the ***higher-order reduced discrete Lagrangian***,

$$l_d(f_{kk+1}) = h \sum_{i=1}^{s} b_i l \Big(\mathrm{dexp}_{\mathrm{ad}_{\xi(c_i h)}} (\dot{\xi}(c_i h)) \Big) ,$$

where

$$\xi(\xi^\nu;\tau h) = \sum_{\kappa=0}^{s} \xi^\kappa \tilde{l}_{\kappa,s}(\tau)\,,$$

and

$$\begin{aligned} \xi^0 &= 0\,, \\ \xi^s &= \log(f_{kk+1})\,, \end{aligned}$$

and the remaining Lie algebra elements $\{\xi^\nu\}_{\nu=1}^{s-1}$, are defined implicitly by

$$0 = h\sum_{i=1}^{s} b_i \left[\frac{\partial l}{\partial \eta}(c_i h)\, \mathrm{ddexp}_{\mathrm{ad}_{\xi(c_i h)}}\, \dot{\tilde{l}}_{\nu,s}(c_i) \right],$$

for $\nu = 1,\ldots,s-1$, and where

$$\mathrm{ddexp}_w = \sum_{n=0}^{\infty} \frac{w^n}{(n+2)!}\,.$$

When the discrete Euler–Poincaré equation is used in conjunction with the higher-order reduced discrete Lagrangian, we obtain the ***higher-order Euler–Poincaré equations***.

5.5 Higher-Order Symplectic-Energy-Momentum Variational Integrators

In this section, we will generalize our new derivation of the symplectic-energy-momentum preserving variational integrators (see, Kane et al. [1999]) to yield integrators with higher-order accuracy.

As before, we consider a piecewise interpolation, with both the control points in the field variables, q_i^ν, and the endpoints of the interval, h_i^0, h_i^1, as degrees of freedom. The continuity conditions for this function space are $q_i^s = q_{i+1}^0$, and $h_i^1 = h_{i+1}^0$. Then, we have that the discrete action is given by

$$\begin{aligned} \mathbb{S}_d = \sum_{i=0}^{N-1} (h_i^1 - h_i^0) \sum_{j=1}^{s} b_j L(q_i(c_j(h_i^1 - h_i^0); q_i^\nu), \dot{q}_i(c_j(h_i^1 - h_i^0); q_i^\nu)) \\ - \sum_{i=0}^{N-2} \lambda_i (q_i^s - q_{i+1}^0) - \sum_{i=0}^{N-2} \omega_i (h_i^1 - h_{i+1}^0), \end{aligned}$$

where

$$q_i(\tau(h_i^1 - h_i^0); q_i^\nu) = \sum_{\kappa=0}^{s} q_i^\kappa \tilde{l}_{\kappa,s}(\tau),$$

$$\dot{q}_i(\tau(h_i^1 - h_i^0); q_i^\nu) = \frac{1}{h_i^1 - h_i^0} \sum_{\kappa=0}^{s} q_i^\kappa \dot{\tilde{l}}_{\kappa,s}(\tau).$$

To simplify the expressions, we define $h_i \equiv h_i^1 - h_i^0$. Then, the variational equations are given by

$$\begin{aligned}
0 =& \sum_{j=1}^{s} b_j L(q_i(c_j h_i), \dot{q}_i(c_j h_i)) - h_i \sum_{j=1}^{s} b_j \frac{\partial L}{\partial \dot{q}}(c_j h_i) \frac{1}{h_i} \dot{q}_i(c_j h_i) - \omega_i, && \text{for } i = 0, \dots, N-2,\\
0 =& -\sum_{j=1}^{s} b_j L(q_i(c_j h_i), \dot{q}_i(c_j h_i)) + h_i \sum_{j=1}^{s} b_j \frac{\partial L}{\partial \dot{q}}(c_j h_i) \frac{1}{h_i} \dot{q}_i(c_j h_i) + \omega_{i-1}, && \text{for } i = 1, \dots, N-1,\\
0 =& h_i \sum_{j=1}^{s} b_j \left[\frac{\partial L}{\partial q}(c_j h_i) \tilde{l}_{s,s}(c_j) + \frac{1}{h_i} \frac{\partial L}{\partial \dot{q}}(c_j h_i) \dot{\tilde{l}}_{s,s}(c_j) \right] - \lambda_i, && \text{for } i = 0, \dots, N-2,\\
0 =& h_i \sum_{j=1}^{s} b_j \left[\frac{\partial L}{\partial q}(c_j h_i) \tilde{l}_{0,s}(c_j) + \frac{1}{h_i} \frac{\partial L}{\partial \dot{q}}(c_j h_i) \dot{\tilde{l}}_{0,s}(c_j) \right] + \lambda_{i-1}, && \text{for } i = 1, \dots, N-1,\\
0 =& h_i \sum_{j=1}^{s} b_j \left[\frac{\partial L}{\partial q}(c_j h_i) \tilde{l}_{\nu,s}(c_j) + \frac{1}{h_i} \frac{\partial L}{\partial \dot{q}}(c_j h_i) \dot{\tilde{l}}_{\nu,s}(c_j) \right], && \begin{array}{r}\text{for } i = 0, \dots, N-1,\\ \nu = 1, \dots, s-1,\end{array}\\
q_i^s =& q_{i+1}^0, && \text{for } i = 0, \dots, N-2,\\
h_i^1 =& h_{i+1}^0, && \text{for } i = 0, \dots, N-2.
\end{aligned}$$

We can eliminate the Lagrange multipliers, to yield

$$\begin{aligned}
0 =& \sum_{j=1}^{s} b_j L(q_i(c_j h_i), \dot{q}_i(c_j h_i)) - \sum_{j=1}^{s} b_j \frac{\partial L}{\partial \dot{q}}(c_j h_i) \dot{q}_i(c_j h_i)\\
&+ \sum_{j=1}^{s} b_j L(q_{i-1}(c_j h_{i-1}), \dot{q}_{i-1}(c_j h_{i-1}))\\
&- \sum_{j=1}^{s} b_j \frac{\partial L}{\partial \dot{q}}(c_j h_{i-1}) \dot{q}_{i-1}(c_j h_{i-1}), && \text{for } i = 1, \dots, N-1,\\
0 =& h_i \sum_{j=1}^{s} b_j \left[\frac{\partial L}{\partial q}(c_j h_i) \tilde{l}_{s,s}(c_j) + \frac{1}{h_i} \frac{\partial L}{\partial \dot{q}}(c_j h_i) \dot{\tilde{l}}_{s,s}(c_j) \right]\\
&+ h_{i-1} \sum_{j=1}^{s} b_j \left[\frac{\partial L}{\partial q}(c_j h_{i-1}) \tilde{l}_{0,s}(c_j) + \frac{1}{h_{i-1}} \frac{\partial L}{\partial \dot{q}}(c_j h_{i-1}) \dot{\tilde{l}}_{0,s}(c_j) \right], && \text{for } i = 1, \dots, N-1,\\
0 =& h_i \sum_{j=1}^{s} b_j \left[\frac{\partial L}{\partial q}(c_j h_i) \tilde{l}_{\nu,s}(c_j) + \frac{1}{h_i} \frac{\partial L}{\partial \dot{q}}(c_j h_i) \dot{\tilde{l}}_{\nu,s}(c_j) \right], && \begin{array}{r}\text{for } i = 0, \dots, N-1,\\ \nu = 1, \dots, s-1,\end{array}\\
q_i^s =& q_{i+1}^0, && \text{for } i = 0, \dots, N-2,\\
h_i^1 =& h_{i+1}^0, && \text{for } i = 0, \dots, N-2.
\end{aligned}$$

If we define the discrete Lagrangian as follows,

$$L_d(q_i, q_{i+1}, h_i) \equiv h_i \sum_{j=1}^{s} b_j L(q_i(c_j h_i), \dot{q}_i(c_j h_i)),$$

where

$$q_i(\tau h_i; q_i^\nu) = \sum_{\kappa=0}^{s} q_i^\kappa \tilde{l}_{\kappa,s}(\tau),$$
$$\dot{q}_i(\tau h_i; q_i^\nu) = \frac{1}{h_i} \sum_{\kappa=0}^{s} q_i^\kappa \dot{\tilde{l}}_{\kappa,s}(\tau),$$

and $q_i^0 = q_i$, $q_i^s = q_1$, and the remaining terms were defined implicitly by

$$0 = h_i \sum_{j=1}^{s} b_j \left[\frac{\partial L}{\partial q}(c_j h_i) \tilde{l}_{\nu,s}(c_j) + \frac{1}{h_i} \frac{\partial L}{\partial \dot{q}}(c_j h_i) \dot{\tilde{l}}_{\nu,s}(c_j) \right],$$

then the equations reduce to the following,

$$E_d(q_i, q_{i+1}, h_i) = -\frac{\partial}{\partial h_i}[L_d(q_i, q_{i+1}, h_i)],$$
$$E_d(q_i, q_{i+1}, h_i) = E_d(q_{i+1}, q_{i+2}, h_{i+1}),$$
$$0 = D_2 L_d(q_i, q_{i+1}, h_i) + D_1 L_d(q_{i+1}, q_{i+2}, h_{i+1}).$$

which is a ***higher-order symplectic-energy-momentum variational integrator***.

Solvability of the Energy Equation. It should be noted that the discrete energy conservation equation is not necessarily solvable, in general, particularly near stationary points. This issue is discussed in Kane et al. [1999]; Lew et al. [2004], and can be addressed by reformulating the discrete energy conservation equation as an optimization problem that chooses the time step by minimizing the discrete energy error squared. Clearly, reformulating the discrete energy conservation equation yields the desired behavior whenever the discrete energy conservation equation can be solved, while allowing the computation to proceed when discrete energy conservation cannot be achieved, albeit with a slight energy error in that case. This does not degrade performance significantly, since instances in which discrete energy conservation cannot be achieved are rare.

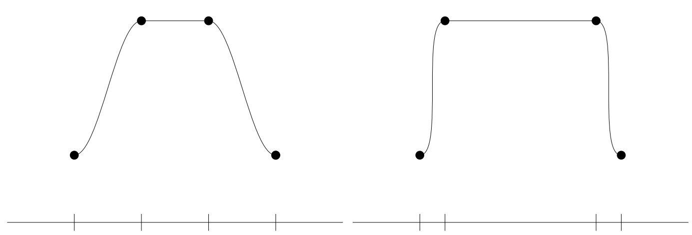
5.6 Spatio-Temporally Adaptive Variational Integrators

As is the case with all inner approximation techniques in numerical analysis, the quality of the numerical solution we obtain is dependent on the rate at which the sequence of finite-dimensional function spaces approximates the actual solution as the number of degrees of freedom is increased.

For problems that exhibit shocks, nonlinear approximation spaces (see, for example, DeVore [1998]), as opposed to linear approximation spaces, are clearly preferable. Adaptive techniques have been developed in the context of finite elements under the name of r-adaptivity and moving finite elements (see, for example, Baines [1995]), and has been developed in a variational context for elasticity in Thoutireddy and Ortiz [2003]. The standard motivation in discrete mechanics to introduce function spaces that have degrees of freedom associated with the base space is to achieve energy or momentum conservation, as discussed in §5.5, or Kane et al. [1999]; Oliver et al. [2004]. However, if the solution to be approximated exhibits shocks, nonlinear approximation techniques achieve better results for a given number of degrees of freedom.

In this section, we will sketch the use of regularizing transformations of the base space, to achieve a computational representation of sections of the configuration bundle that will yield more accurate numerical results.

Consider the situation when we are representing a characteristic function using piecewise spline interpolation. We show in Figure 5.2, the difference between linear and nonlinear approximation of the characteristic function.



(a) Using equispaced nodes (b) Using adaptive nodes

Figure 5.2: Linear and nonlinear approximation of a characteristic function.

When the derivatives of the solution vary substantially in a spatially distributed manner, we obtain additional accuracy, for a fixed representation cost, if we allow nodal points to cluster near regions of high curvature. It is therefore desirable to consider variational integrators based on function spaces that are parameterized by both the position of the nodal points on the base space, as well as the field values over the nodes.

This is represented by having a regular grid for the computational domain $\mathcal{R}$, which is then mapped to the physical base space $\mathcal{X}$, as shown in Figure 5.3.

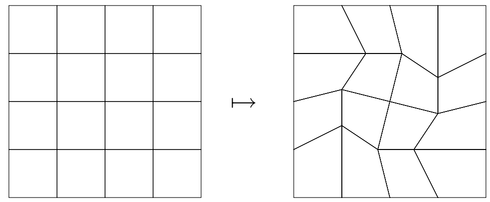
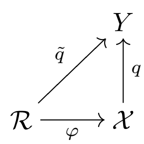


Figure 5.3: Mapping of the base space from the computational to the physical domain.

The sections of the configuration bundle factor as follows,



The mapping $\varphi : \mathcal{R} \to \mathcal{X}$ results in a regularized computational representation $\tilde{q} : \mathcal{R} \to Y$ of the original section $q : \mathcal{X} \to Y$. The relationship between the discrete section of the configuration bundle and its computational representation is illustrated in Figure 5.4.

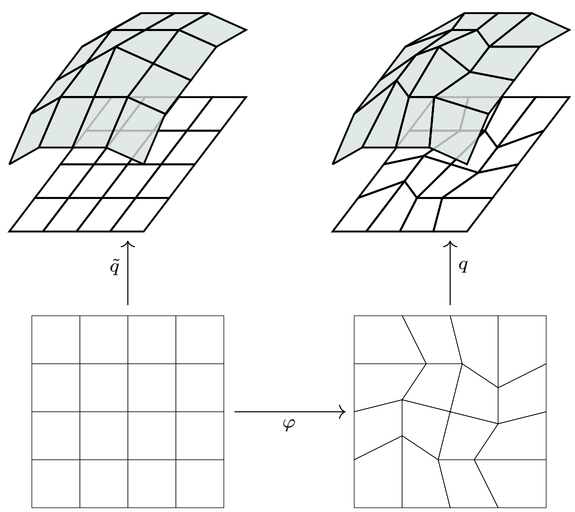


Figure 5.4: Factoring the discrete section.

The action integral is then given by

$$\mathcal{S}(q) = \int_{\mathcal{X}} L(j^1 q) = \int_{\mathcal{R}} L(j^1 \tilde{q}) |\mathbf{D}\varphi|.$$

Thus, even though $q : \mathcal{X} \to Y$ may exhibit shocks, the computational representation we work with, $\tilde{q} : \mathcal{R} \to Y$, is substantially more regular, and consequently, a numerical quadrature scheme in $\mathcal{R}$

applied to

$$\int_{\mathcal{R}} L(j^1\tilde{q})|\mathbf{D}\varphi|$$

is significantly more accurate than the corresponding numerical quadrature scheme in $\mathcal{X}$ applied to

$$\int_{\mathcal{X}} L(j^1 q).$$

As such, spatio-temporally adaptive variational integrators achieve increased accuracy by allowing the accurate representation of shock solutions using an adapted free knot representation, while using a smooth computational representation to compute the action integral.

5.7 Multiscale Variational Integrators

In the work on multiscale finite elements (MsFEM), introduced and developed in Hou and Wu [1999]; Efendiev et al. [2000]; Chen and Hou [2003], shape functions that are solutions of the fast dynamics in the absence of slow forces are constructed to yield finite element schemes that achieve convergence rates that are independent of the ratio of fast to slow scales.

In constructing a multiscale variational integrator, we need to choose finite-dimensional function spaces that do a good job of approximating the fast dynamics of the problem, when the slow variables are frozen. In addition, we require an appropriate choice of numerical quadrature scheme to be able to evaluate the action, which involves integrating a highly-oscillatory Lagrangian. In this section, we will discuss how to go about making such choices of function spaces and quadrature methods.

We will start with a discussion of the multiscale finite element method, to illustrate the importance of a good choice of shape functions in computing solutions to problems with multiple scales. After that, we will walk through the construction of a multiscale variational integrator for the case of a planar pendulum with a stiff spring. Finally, we will discuss how we might proceed if we do not possess knowledge of which variables, or forces, are fast or slow.

5.7.1 Multiscale Shape Functions

We will illustrate the idea of constructing shape functions that are solutions of the fast dynamics by introducing a model multiscale second-order elliptic partial differential equation given by

$$\nabla \cdot a(x/\epsilon)\nabla u^\epsilon(x) = f(x),$$

with homogeneous boundary conditions. In the one-dimensional case, we can solve for the solution analytically, and it has the form

$$u^\epsilon(x) = \int_0^x \frac{F(y)}{a(y/\epsilon)}dy - \frac{\int_0^1 \frac{F(y)}{a(y/\epsilon)}dy}{\int_0^1 \frac{dy}{a(y/\epsilon)}} \int_0^x \frac{dy}{a(y/\epsilon)},$$

where $F(x) = \int_0^x f(y)dy$. If we have nodal points at $\{x_i\}_{i=0}^N$, then the appropriate multiscale shape functions to adopt in this example is to use shape functions that are solutions of the homogeneous problem at the element level. These shape functions φ_i^ϵ satisfy

$$\begin{cases} \frac{\partial}{\partial x}\left(a(x/\epsilon)\frac{\partial}{\partial x}\varphi_i^\epsilon\right) = 0, & \text{for } x_{i-1} < x < x_{i+1}; \\ \varphi_i^\epsilon(x_{i-1}) = 0; \quad \varphi_i^\epsilon(x_{i+1}) = 0; \quad \varphi_i^\epsilon(x_i) = 1. \end{cases}$$

And they have the explicit form given by

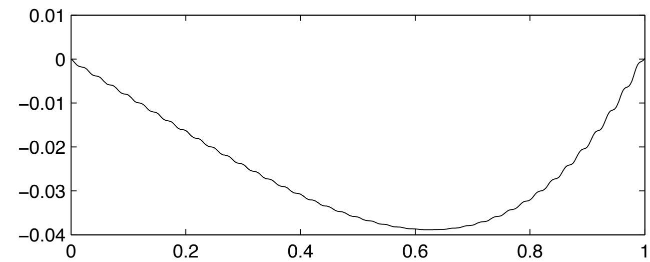
$$\varphi_i^\epsilon(x) = \begin{cases} \left[\int_{x_{i-1}}^{x_i} \frac{ds}{a(s/\epsilon)}\right]^{-1} \left[\int_{x_{i-1}}^{x} \frac{ds}{a(s/\epsilon)}\right], & x \in [x_{i-1}, x_i]\,; \\ \left[\int_{x_i}^{x_{i+1}} \frac{ds}{a(s/\epsilon)}\right]^{-1} \left[\int_{x}^{x_{i+1}} \frac{ds}{a(s/\epsilon)}\right], & x \in (x_i, x_{i+1}]\,; \\ 0, & \text{otherwise}\,. \end{cases}$$

It can be shown that this will yield a numerical scheme that solves exactly for the solution at the nodal points. This analysis is carried out in Appendix C.

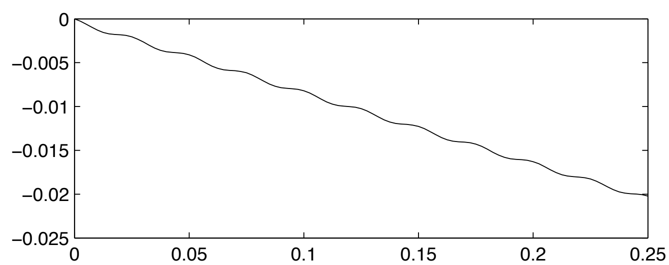
As an example, we will compute the analytical solution for $a(x) = \frac{10}{1+0.95\sin(2\pi x)}$, $f(x) = x^2$, and $\epsilon = 0.025$. This is illustrated in Figure 5.5(a). What is particularly interesting is to compare the zoomed plot of the exact solution and the multiscale shape function over the same interval, shown in Figures 5.5(b) and 5.5(c), respectively. The multiscale finite element method is able to achieve excellent results because the multiscale shape functions are able to capture the fast dynamics well. In the next subsection, we will discuss how this insight is relevant in the construction of multiscale variational integrators.

5.7.2 Multiscale Variational Integrator for the Planar Pendulum with a Stiff Spring

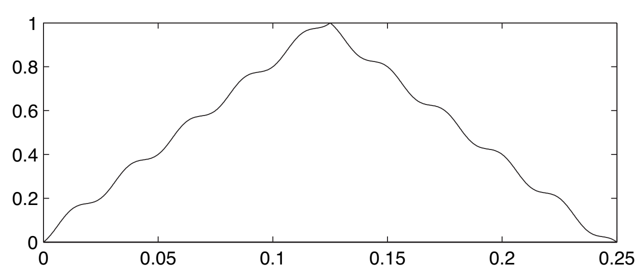
As was shown previously, a shape function that captures the fast dynamics of a multiscale problem is able to achieve superior accuracy when used for computation. While this idea has primarily been used for problems with multiple spatial scales, it is natural to consider its application to a problem with multiple temporal scales, such as the problem of the planar pendulum with a stiff spring, as illustrated in Figure 5.6.



(a) Exact solution



(b) Exact solution (zoomed)



(c) Multiscale shape function

Figure 5.5: Comparison of the multiscale shape function and the exact solution for the elliptic problem.

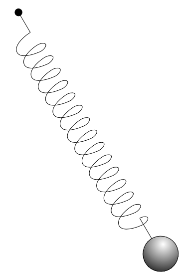


Figure 5.6: Planar pendulum with a stiff spring

We will use this example to illustrate the issues that arise in constructing a multiscale variational integrator. The variables are $q = (a, \theta)$, where a is the spring extension, and θ is the angle from the vertical. The Lagrangian is given by

$$L(a, \theta, \dot{a}, \dot{\theta}) = \frac{m}{2}(\dot{x}^2 + \dot{y}^2) - mgy - \frac{k}{2}a^2,$$

where

$$\begin{aligned}
x &= (l + a)\sin\theta, \\
y &= -(l + a)\cos\theta, \\
\dot{x} &= \dot{a}\sin\theta + \dot{\theta}(l + a)\cos\theta, \\
\dot{y} &= -\dot{a}\cos\theta + \dot{\theta}(l + a)\sin\theta.
\end{aligned}$$

The Hamilton's equations for the planar pendulum with a stiff spring are

$$\begin{aligned}
\dot{a} &= \frac{p_a}{m}, \\
\dot{\theta} &= \frac{p_\theta}{m(l + a)^2}, \\
\dot{p}_a &= -ka + gm\cos\theta + m(l + a)\dot{\theta}^2, \\
\dot{p}_\theta &= -gm(l + a)\sin\theta.
\end{aligned}$$

The timescale arising from the mass-spring system is $2\pi\sqrt{m/k}$. The timescale arising from the planar pendulum system is $2\pi\sqrt{l/g}$. The ratio of timescales is given by $\epsilon = \sqrt{mg/kl}$.

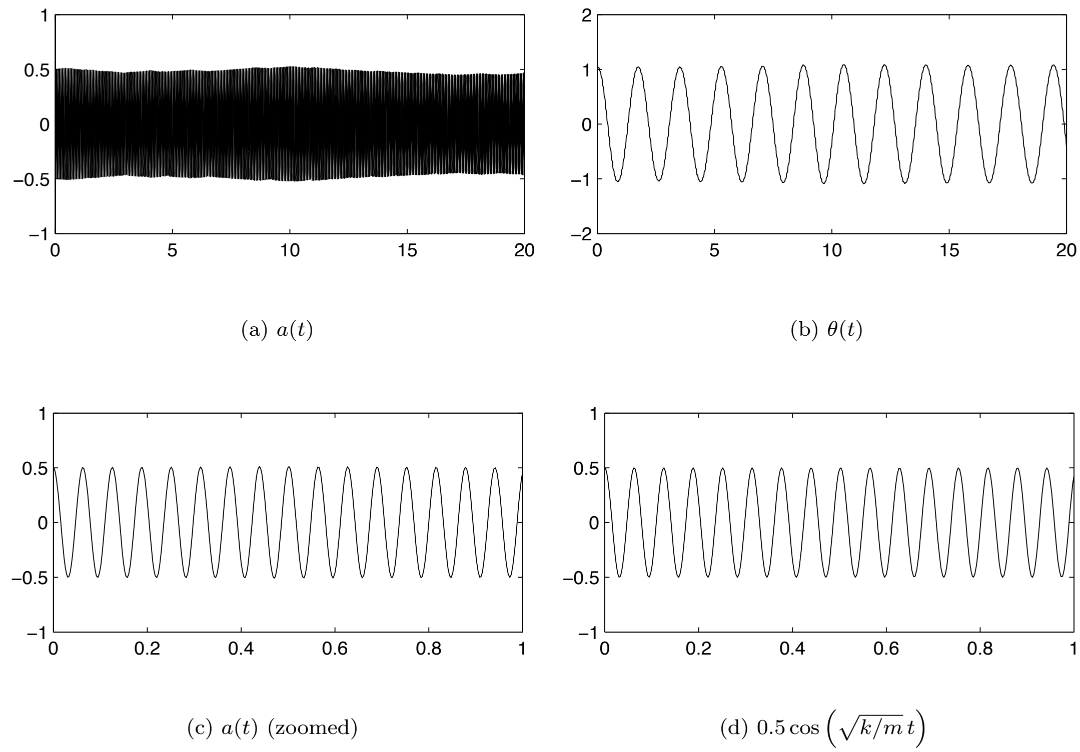
Multiscale Shape Function. In this problem, the fast scale is associated with the stiff spring, and if we set the slow variable $\theta = 0$, we obtain the equation

$$\ddot{a} = \frac{\dot{p}_a}{m} = -\frac{k}{m}a,$$

which has solutions of the form

$$a(t) = a_0 \sin\left(\sqrt{k/m}\, t\right) + a_1 \cos\left(\sqrt{k/m}\, t\right).$$

We will now consider a well-resolved simulation of this system using the `ode15s` stiff solver from MATLAB, with parameters $m = 1$, $g = 9.81$, $k = 10000$, $l = 1$, giving a scale separation of $\epsilon = 0.0313$. The simulation results are show in Figure 5.7.



(a) $a(t)$

(b) $\theta(t)$

(c) $a(t)$ (zoomed)

(d) $0.5\cos\left(\sqrt{k/m}\, t\right)$

Figure 5.7: Comparison of the multiscale shape function and the exact solution for the planar pendulum with a stiff spring.

Clearly, if we wish to choose time steps that do not resolve the fast oscillations in a, but do resolve the slow oscillations in θ, it would be desirable to include $\sin\left(\sqrt{k/m}\, t\right)$, and $\cos\left(\sqrt{k/m}\, t\right)$ in the finite-dimensional function space used to interpolate $a(t)$.

Evaluating the Discrete Lagrangian. Since we have chosen time steps that do not resolve the fast oscillations, it follows that over the interval $[0,h]$, the Lagrangian will oscillate rapidly as well. In computing the discrete Lagrangian, it is therefore necessary to ensure that this highly-oscillatory integral is well-approximated.

It is conventional wisdom, in numerical analysis, that the numerical quadrature of highly-oscillatory integrals is a challenging problem requiring the use of many function evaluations. Recently, there has been a series of papers, Iserles [2003a,b, 2004]; Iserles and Nørsett [2004], that provides an analysis of Filon-type quadrature schemes that provide an efficient and accurate method of evaluating such integrals. The method is applicable to weighted integrals as well, but we will summarize the results from §3 of Iserles [2003a] restricted to unweighted integrals, and refer the reader to the original reference for an in-depth discussion and analysis.

The Filon-type method aims to evaluate an integral of the form

$$I_h[f] = \int_0^h f(x)e^{i\omega x}dx = h\int_0^h f(hx)e^{i\omega x}dx.$$

Given a set of distinct quadrature points, $c_1 < c_2 < \cdots < c_\nu$ in $[0,1]$, the Filon-type quadrature method is given by

$$Q_h^F[f] = h\sum_{i=1}^{\nu} b_i(ih\omega)f(c_i h),$$

where

$$b_i(ih\omega) = \int_0^1 l_i(x)e^{ih\omega x}dx,$$

and l_i are the Legendre polynomials. Here, we draw attention to the fact that the quadrature weights are dependent on $h\omega$.

If the quadrature points correspond to Gauss-Christoffel quadrature of order p, then the error for the Filon-type method is given as follows.

$$\begin{aligned}
\mathcal{O}(h^{p+1}), &\quad \text{if} \quad h\omega \ll 1 \\
\mathcal{O}(h^{\nu}), &\quad \text{if} \quad h\omega = \mathcal{O}(1) \\
\mathcal{O}(h^{\nu+1}/(h\omega)), &\quad \text{if} \quad h\omega \gg 1 \\
\mathcal{O}(h^{\nu+1}/(h\omega)^2), &\quad \text{if} \quad h\omega \gg 1, c_1 = 0, c_\nu = 1.
\end{aligned}$$

Clearly, for highly-oscillatory functions, the last case, which corresponds to the Lobatto quadrature points, is most desirable. Thus, it is appropriate to use the Filon-Lobatto method to evaluate the discrete Lagrangian in our case.

Discrete Variational Equations. As we discussed previously, instead of looking for stationary solutions to the discrete Hamilton's principle in polynomial spaces, we will consider solutions that are piecewise of the form

$$q(t;\{p_j\},\omega,a_0,a_1)=\left(\sum\nolimits_{j=0}^{n} p_j t^j\right)(1+a_0\sin(\omega t)+a_1\cos(\omega t))\,.$$

This function space approximates the highly-oscillatory nature of the solution well, in contrast to a polynomial function space, thereby avoiding approximation-theoretic errors. The degrees of freedom in this function space are $\{p_j\}$, ω, a_0, and a_1. Since there are no distinguished degrees of freedom that are responsible for the endpoint values of the curve, we need to impose continuity at the nodes using a Lagrange multiplier. The augmented discrete action is given by

$$\begin{aligned}\mathbb{S}_d=&\sum_{i=0}^{N-1}\int_0^h L(j^1 q_i(t;\{p_j^i\},\omega^i,a_0^i,a_1^i))dt\\&\quad+\sum_{i=0}^{N-2}\lambda_i(q_i(h;\{p_j^i\},\omega^i,a_0^i,a_1^i)-q_{i+1}(0;\{p_j^{i+1}\},\omega^{i+1},a_0^{i+1},a_1^{i+1}))\,,\end{aligned}$$

where each of the integrals are evaluated using the Filon-Lobatto method. Taking variations with respect to the degrees of freedom yields an update map,

$$\left(\{p_j^i\},\omega^i,a_0^i,a_1^i\right)\mapsto\left(\{p_j^{i+1}\},\omega^{i+1},a_0^{i+1},a_1^{i+1}\right),$$

which gives the ***multiscale variational integrator*** for the planar pendulum with a stiff spring.

5.7.3 Computational Aspects

Multiscale variational integrators have the advantage of directly accounting for the contribution of the fast dynamics, thereby allowing the scheme to use significantly larger time-steps, while maintaining accuracy and stability. It is possible to take advantage of knowledge about which of the variables, or forces, are fast or slow, by using a low degree polynomial and oscillatory functions for the fast variables, and a higher-order polynomial for the slow variables. In the absence of such information, it is appropriate to use a function space with both polynomials and oscillatory functions, and apply it to all the variables.

Recall that the Filon-type method has quadrature coefficients that depend on the frequency. As such, the initial fast frequency has to be estimated numerically using a fully resolved computation for a short period of time. Since both the function space and the quadrature weights depend on the fast frequency ω, the resulting scheme is implicit and fairly nonlinear, and as such, it may be expensive for large systems.

5.8 Pseudospectral Variational Integrators

The use of spectral expansions of the solution in space are particularly appropriate for highly accurate simulations of the evolution of smooth solutions, such as those arising from quantum mechanics. We will introduce pseudospectral variational integrators, and consider the Schrödinger equation as an example.

In particular we will adopt the tensor product of a spectral expansion in space, and a polynomial expansion in time. For example, we could have an interpolatory function of the form

$$\psi(x,(\tau+l)\Delta t) = \frac{1}{2\pi}\sideset{}{'}\sum_{k=-N/2}^{N/2} e^{ikx}\left((1-\tau)\hat{v}_k^l + \tau\hat{v}_k^{l+1}\right),$$

which is the tensor product of a discrete Fourier expansion in space, and linear interpolation in time. Here, the $\sum'$ notation denotes a weighted sum where the terms with indices $\pm N/2$ are weighted by $1/2$, and the other terms are weighted by 1. See page 19 of Trefethen [2000] for a discussion of why this is necessary to fix an issue with derivatives of the interpolant.

The degrees of freedom are given by $\hat{v}_k^l$, which are the discrete Fourier coefficients. We will later see how such an interpolation can be applied to the Schrödinger equation. The action integral can be exactly evaluated for this class of shape functions, as we will see below.

It is straightforward to generalize the pseudospectral approach we present in this section to a spectral variational integrator, with discrete Fourier expansions in space for periodic domains, or Chebyshev expansions in space for non-periodic domains, and Chebyshev expansions in time. This will however result in all the degrees of freedom on the space-time mesh being coupled, and is therefore substantially more expensive computationally than the pseudospectral method. The payoff for adopting the spectral approach is spectral accuracy, which is accuracy beyond all orders.

5.8.1 Variational Derivation of the Schrödinger Equation

Let $\mathcal{H}$ be a complex Hilbert space, for example, the space of complex-valued functions ψ on $\mathbb{R}^3$ with the Hermitian inner product,

$$\langle\psi_1,\psi_2\rangle = \int \psi_1(x)\overline{\psi}_2(x)d^3x\,,$$

where the overbar denotes complex conjugation. We will present a Lagrangian derivation of the Schrödinger equation, following worked example 9.1 on pages 568–569 of José and Saletan [1998].

Consider the Lagrangian density $\mathcal{L}$ given by

$$\mathcal{L}(j^1\psi) = \frac{i\hbar}{2}\{\dot{\psi}\overline{\psi} - \psi\dot{\overline{\psi}}\} - \hat{H}\psi\overline{\psi},$$

where $\hat{H} : \mathcal{H} \to \mathcal{H}$ is given by

$$\hat{H}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi,$$

which yields

$$\mathcal{L}(j^1\psi) = \frac{i\hbar}{2}\{\dot{\psi}\overline{\psi} - \psi\dot{\overline{\psi}}\} - \frac{\hbar^2}{2m}\nabla\psi \cdot \nabla\overline{\psi} - V\psi\overline{\psi}.$$

We take $\psi, \overline{\psi}$ as independent variables, and compute,

$$\begin{aligned}
\delta \int L dt &= \int \left[\left(\frac{\partial \mathcal{L}}{\partial \overline{\psi}} \delta\overline{\psi} + \frac{\partial \mathcal{L}}{\partial \dot{\overline{\psi}}} \delta\dot{\overline{\psi}} + \frac{\partial \mathcal{L}}{\partial \nabla\overline{\psi}} \delta\nabla\overline{\psi} \right) + \left(\frac{\partial \mathcal{L}}{\partial \psi} \delta\psi + \frac{\partial \mathcal{L}}{\partial \dot{\psi}} \delta\dot{\psi} + \frac{\partial \mathcal{L}}{\partial \nabla\psi} \delta\nabla\psi \right) \right] d^3x dt \\
&= \int \left[\left(\frac{\partial \mathcal{L}}{\partial \overline{\psi}} - \frac{\partial}{\partial t}\frac{\partial \mathcal{L}}{\partial \dot{\overline{\psi}}} - \nabla \cdot \frac{\partial \mathcal{L}}{\partial \nabla\overline{\psi}} \right) \delta\overline{\psi} + \left(\frac{\partial \mathcal{L}}{\partial \psi} - \frac{\partial}{\partial t}\frac{\partial \mathcal{L}}{\partial \dot{\psi}} - \nabla \cdot \frac{\partial \mathcal{L}}{\partial \nabla\psi} \right) \delta\psi \right] d^3x dt \\
&= \int \left[\left(\frac{i\hbar}{2}\dot{\psi} - V\psi + \frac{i\hbar}{2}\dot{\psi} + \frac{\hbar^2}{2m}\nabla^2\psi \right) \delta\overline{\psi} + \left(\frac{i\hbar}{2}\dot{\overline{\psi}} - V\overline{\psi} + \frac{i\hbar}{2}\dot{\overline{\psi}} + \frac{\hbar^2}{2m}\nabla^2\overline{\psi} \right) \delta\psi \right] d^3x dt,
\end{aligned}$$

where we integrated by parts, and neglected boundary terms as the variations vanish at the boundary of the space-time region. Since the variations are arbitrary, we obtain the nonrelativistic (linear) Schrödinger equation as a result,

$$i\hbar\dot{\psi} = \left\{ -\frac{\hbar^2}{2m}\nabla^2 + V \right\} \psi\,.$$

We note that the Lagrangian density is invariant under the internal phase shift given by

$$\psi \mapsto e^{i\epsilon}\psi, \qquad \overline{\psi} \mapsto e^{-i\epsilon}\overline{\psi}.$$

The space part of the multi-momentum map is given by

$$j^k = \frac{\partial \mathcal{L}}{\partial(\partial_k \psi)} i\psi + \frac{\partial \mathcal{L}}{\partial(\partial_k \overline{\psi})}(-i\overline{\psi}) = \frac{i\hbar^2}{2m}(\psi\partial_k\overline{\psi} - \overline{\psi}\partial_k\psi),$$

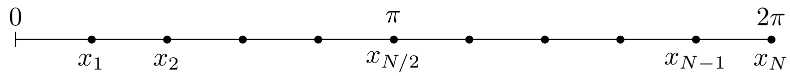
and the time part is given by

$$j^0 = \frac{\partial \mathcal{L}}{\partial \dot{\psi}} i\psi - \frac{\partial \mathcal{L}}{\partial \dot{\overline{\psi}}}(-i\overline{\psi}) = -\frac{\hbar}{2}(\dot{\overline{\psi}}\psi - \dot{\psi}\overline{\psi}).$$

The norm of the wavefunction is automatically preserved by variational integrators, since the norm is a quadratic invariant.

5.8.2 Pseudospectral Variational Integrator for the Schrödinger Equation

Consider a periodic domain $[0, 2\pi]$, discretized with a discrete Fourier series expansion in space, and a linear interpolation in time. Let N be an even integer, then, our computation is done on the following mesh,



This implies that the grid spacing is given by

$$h = \frac{2\pi}{N}\,.$$

The interpolation is given by

$$\psi(x,(\tau+l)\Delta t) = \frac{1}{2\pi}\sideset{}{'}\sum_{k=-N/2}^{N/2} e^{ikx}\left((1-\tau)\hat{v}_k^l + \tau\hat{v}_k^{l+1}\right),$$

$$\dot{\psi}(x,(\tau+l)\Delta t) = \frac{1}{2\pi\Delta t}\sideset{}{'}\sum_{k=-N/2}^{N/2} e^{ikx}\left(\hat{v}_k^{l+1} - \hat{v}_k^l\right),$$

$$\bar{\psi}(x,(\tau+l)\Delta t) = \frac{1}{2\pi}\sideset{}{'}\sum_{k=-N/2}^{N/2} e^{-ikx}\left((1-\tau)\bar{\hat{v}}_k^l + \tau\bar{\hat{v}}_k^{l+1}\right),$$

$$\dot{\bar{\psi}}(x,(\tau+l)\Delta t) = \frac{1}{2\pi\Delta t}\sideset{}{'}\sum_{k=-N/2}^{N/2} e^{-ikx}\left(\bar{\hat{v}}_k^{l+1} - \bar{\hat{v}}_k^l\right),$$

and the discrete Fourier transformation is given by

$$\hat{v}_j = \frac{1}{2\pi}h\sum_{j=1}^{N} e^{-ikx_j}v_j\,,$$

for $k = -N/2+1,\ldots,N/2$, and $\hat{v}_{-N/2} \equiv \hat{v}_{N/2}$. Recall that

$$\mathcal{L}(j^1\psi) = \frac{i\hbar}{2}\{\dot{\psi}\overline{\psi} - \psi\dot{\overline{\psi}}\} - \hat{H}\psi\overline{\psi},$$

where $\hat{H} : \mathcal{H} \to \mathcal{H}$ is given by

$$\hat{H}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi.$$

Furthermore, the potential V is expressed using a discrete Fourier expansion,

$$V(x) = \frac{1}{2\pi}\sideset{}{'}\sum_{k=-N/2}^{N/2} e^{ikx}\hat{V}_k\,.$$

In addition, we will need to introduce a normalization condition, so as to eliminate trivial solutions of the partial differential equation. The normalization condition is

$$1 = \langle \psi_l, \psi_l \rangle = \int_0^{2\pi} \left(\frac{1}{2\pi} \sum_{k=-N/2}^{N/2}{}' e^{ikx} \hat{v}_k^l \right) \left(\frac{1}{2\pi} \sum_{k=-N/2}^{N/2}{}' e^{-ikx} \bar{\hat{v}}_k^l \right) dx = \frac{1}{2\pi} \sum_{k=-N/2}^{N/2}{}'' \hat{v}_k^l \bar{\hat{v}}_k^l,$$

which is enforced using a Lagrange multiplier.

Discrete Action for the Schrödinger Equation. The discrete action in the space-time region $[0, 2\pi] \times [l\Delta t, (l+1)\Delta t]$ is given by

$$\begin{aligned}
\mathbb{S}_d &= \int_{l\Delta t}^{(l+1)\Delta t} \int_0^{2\pi} \mathcal{L}(j^1\psi) dx dt + \lambda_l (1 - \langle \psi_l, \psi_l \rangle) \\
&= \int_{l\Delta t}^{(l+1)\Delta t} \int_0^{2\pi} \left[\frac{i\hbar}{2} \{ \dot{\psi}\bar{\psi} - \psi\dot{\bar{\psi}} \} + \frac{\hbar^2}{2m} \nabla^2 \psi \bar{\psi} - V\psi\bar{\psi} \right] dx dt + \lambda_l \left(1 - \frac{1}{2\pi} \sum_{k=-N/2}^{N/2}{}'' \hat{v}_k^l \bar{\hat{v}}_k^l \right) \\
&= \int_0^1 \int_0^{2\pi} \frac{i\hbar}{2} \left[\left(\frac{1}{2\pi\Delta t} \sum_{k=-N/2}^{N/2}{}' e^{ikx} \left(\hat{v}_k^{l+1} - \hat{v}_k^l \right) \right) \left(\frac{1}{2\pi} \sum_{k=-N/2}^{N/2}{}' e^{-ikx} \left((1-\tau) \bar{\hat{v}}_k^l + \tau \bar{\hat{v}}_k^{l+1} \right) \right) \right. \\
&\qquad \left. - \left(\frac{1}{2\pi} \sum_{k=-N/2}^{N/2}{}' e^{ikx} \left((1-\tau) \hat{v}_k^l + \tau \hat{v}_k^{l+1} \right) \right) \left(\frac{1}{2\pi\Delta t} \sum_{k=-N/2}^{N/2}{}' e^{-ikx} \left(\bar{\hat{v}}_k^{l+1} - \bar{\hat{v}}_k^l \right) \right) \right] \Delta t \, dx d\tau \\
&\quad + \int_0^1 \int_0^{2\pi} \frac{\hbar^2}{2m} \left(\frac{1}{2\pi} \sum_{k=-N/2}^{N/2}{}' (-k^2) e^{ikx} \left((1-\tau) \hat{v}_k^l + \tau \hat{v}_k^{l+1} \right) \right) \\
&\qquad \cdot \left(\frac{1}{2\pi} \sum_{k=-N/2}^{N/2}{}' e^{-ikx} \left((1-\tau) \bar{\hat{v}}_k^l + \tau \bar{\hat{v}}_k^{l+1} \right) \right) \Delta t \, dx d\tau \\
&\quad - \int_0^1 \int_0^{2\pi} \left[\left(\frac{1}{2\pi} \sum_{k=-N/2}^{N/2}{}' e^{ikx} \hat{V}_k \right) \left(\frac{1}{2\pi} \sum_{m=-N/2}^{N/2}{}' e^{imx} \left((1-\tau) \hat{v}_m^l + \tau \hat{v}_m^{l+1} \right) \right) \right. \\
&\qquad \left. \cdot \left(\frac{1}{2\pi} \sum_{n=-N/2}^{N/2}{}' e^{-inx} \left((1-\tau) \bar{\hat{v}}_n^l + \tau \bar{\hat{v}}_n^{l+1} \right) \right) \right] \Delta t \, dx dt \\
&\quad + \lambda_l \left(1 - \frac{1}{2\pi} \sum_{k=-N/2}^{N/2}{}'' \hat{v}_k^l \bar{\hat{v}}_k^l \right)
\end{aligned}$$

$$= \int_0^1 \frac{i\hbar}{2}\left[\frac{1}{2\pi}\sum_{k=-N/2}^{N/2}{}'' \Big((\hat{v}_k^{l+1}-\hat{v}_k^l)((1-\tau)\bar{\hat{v}}_k^l+\tau\bar{\hat{v}}_k^{l+1})-((1-\tau)\hat{v}_k^l+\tau\hat{v}_k^{l+1})(\bar{\hat{v}}_k^{l+1}-\bar{\hat{v}}_k^l)\Big)\right]d\tau$$

$$-\int_0^1\left[\frac{\hbar^2}{2\pi}\frac{k^2}{2\pi}\sum_{k=-N/2}^{N/2}{}''((1-\tau)\hat{v}_k^l+\tau\hat{v}_k^{l+1})((1-\tau)\bar{\hat{v}}_k^l+\tau\bar{\hat{v}}_k^{l+1})\right]\Delta t\,d\tau$$

$$-\int_0^1\left(\frac{1}{2\pi}\right)^2\left[\sum_{n=-N/2}^{-1}{}'\sum_{m=-N/2}^{N/2+n}{}'\Big(\hat{V}_{n-m}((1-\tau)\hat{v}_m^l+\tau\hat{v}_m^{l+1})((1-\tau)\bar{\hat{v}}_n^l+\tau\bar{\hat{v}}_n^{l+1})\Big)\right.$$

$$\left.+\sum_{n=0}^{N/2}{}'\sum_{m=n-N/2}^{N/2}{}'\Big(\hat{V}_{n-m}((1-\tau)\hat{v}_m^l+\tau\hat{v}_m^{l+1})((1-\tau)\bar{\hat{v}}_n^l+\tau\bar{\hat{v}}_n^{l+1})\Big)\right]\Delta t\,d\tau$$

$$+\lambda_l\left(1-\frac{1}{2\pi}\sum_{k=-N/2}^{N/2}{}''\hat{v}_k^l\bar{\hat{v}}_k^l\right)$$

$$=\frac{i\hbar}{4\pi}\sum_{k=-N/2}^{N/2}{}''\left[\hat{v}_k^{l+1}\bar{\hat{v}}_k^l-\hat{v}_k^l\bar{\hat{v}}_k^{l+1}\right]-\frac{\hbar^2k^2\Delta t}{24\pi^2}\sum_{k=-N/2}^{N/2}{}''\left[\hat{v}_k^l(2\bar{\hat{v}}_k^l+\bar{\hat{v}}_k^{l+1})+\hat{v}_k^{l+1}(\bar{\hat{v}}_k^l+2\bar{\hat{v}}_k^{l+1})\right]$$

$$-\frac{\Delta t}{24\pi^2}\left(\sum_{n=-N/2}^{-1}{}'\sum_{m=-N/2}^{N/2+n}{}'+\sum_{n=0}^{N/2}{}'\sum_{m=n-N/2}^{N/2}{}'\right)\hat{V}_{n-m}\left[\hat{v}_m^l(2\bar{\hat{v}}_n^l+\bar{\hat{v}}_n^{l+1})+\hat{v}_m^{l+1}(\bar{\hat{v}}_n^l+2\bar{\hat{v}}_n^{l+1})\right]$$

$$+\lambda_l\left(1-\frac{1}{2\pi}\sum_{k=-N/2}^{N/2}{}''\hat{v}_k^l\bar{\hat{v}}_k^l\right),$$

where we used the fact that

$$\int_0^{2\pi}e^{ikx}dx=2\pi\delta_0^i\,,$$

for $k\in\mathbb{Z}$, and we define $\sum'$ as a weighted sum where the terms with indices $\pm N/2$ are weighted by $1/2$, and $\sum''$ as a weighted sum where the terms with indices $\pm N/2$ are weighted by $1/4$. We should note that using the same approach, it would be possible to exactly evaluate the action integral for the class of tensor product shape functions with a discrete Fourier expansion in space, and a polynomial expansion in time. In particular, a similar approach is valid in exactly evaluating the action integral when we use shape functions that are spectral in both space and time.

Discrete Euler–Lagrange Equations. We are now in a position to compute the discrete Euler–Lagrange equations associated with the Schrödinger equation when using a tensor product of a discrete Fourier expansion in space, and a linear interpolation in time.

The discrete variational equations are given by

$$
\begin{aligned}
0 &= \frac{i\hbar}{4\pi}\left[\bar{\hat{v}}_j^{l-1} - \bar{\hat{v}}_j^{l+1}\right] - \frac{\hbar^2 k^2 \Delta t}{24\pi^2}\left[\bar{\hat{v}}_j^{l-1} + 4\bar{\hat{v}}_j^{l} + \bar{\hat{v}}_j^{l+1}\right] \\
&\quad - \frac{\Delta t}{24\pi^2}\sum_{n=-N/2}^{N/2+j}{}' \hat{V}_{n-j}\left[\bar{\hat{v}}_n^{l-1} + 4\bar{\hat{v}}_n^{l} + \bar{\hat{v}}_n^{l+1}\right] - \frac{\lambda_l}{2\pi}\bar{\hat{v}}_j^{l}, \qquad \text{for } j = -N/2+1,\ldots,-1, \\
0 &= \frac{i\hbar}{4\pi}\left[\hat{v}_j^{l+1} - \hat{v}_j^{l-1}\right] - \frac{\hbar^2 k^2 \Delta t}{24\pi^2}\left[\hat{v}_j^{l-1} + 4\hat{v}_j^{l} + \hat{v}_j^{l+1}\right] \\
&\quad - \frac{\Delta t}{24\pi^2}\sum_{n=-N/2}^{N/2+j}{}' \hat{V}_{j-n}\left[\hat{v}_n^{l-1} + 4\hat{v}_n^{l} + \hat{v}_n^{l+1}\right] - \frac{\lambda_l}{2\pi}\hat{v}_j^{l}, \qquad \text{for } j = -N/2+1,\ldots,-1, \\
0 &= \frac{i\hbar}{4\pi}\left[\bar{\hat{v}}_j^{l-1} - \bar{\hat{v}}_j^{l+1}\right] - \frac{\hbar^2 k^2 \Delta t}{24\pi^2}\left[\bar{\hat{v}}_j^{l-1} + 4\bar{\hat{v}}_j^{l} + \bar{\hat{v}}_j^{l+1}\right] \\
&\quad - \frac{\Delta t}{24\pi^2}\sum_{n=j-N/2}^{N/2}{}' \hat{V}_{n-j}\left[\bar{\hat{v}}_n^{l-1} + 4\bar{\hat{v}}_n^{l} + \bar{\hat{v}}_n^{l+1}\right] - \frac{\lambda_l}{2\pi}\bar{\hat{v}}_j^{l}, \qquad \text{for } j = 0,\ldots,N/2-1, \\
0 &= \frac{i\hbar}{4\pi}\left[\hat{v}_j^{l+1} - \hat{v}_j^{l-1}\right] - \frac{\hbar^2 k^2 \Delta t}{24\pi^2}\left[\hat{v}_j^{l-1} + 4\hat{v}_j^{l} + \hat{v}_j^{l+1}\right] \\
&\quad - \frac{\Delta t}{24\pi^2}\sum_{n=j-N/2}^{N/2}{}' \hat{V}_{j-n}\left[\hat{v}_n^{l-1} + 4\hat{v}_n^{l} + \hat{v}_n^{l+1}\right] - \frac{\lambda_l}{2\pi}\hat{v}_j^{l}, \qquad \text{for } j = 0,\ldots,N/2-1, \\
0 &= \frac{i\hbar}{16\pi}\left[\bar{\hat{v}}_{N/2}^{l-1} - \bar{\hat{v}}_{N/2}^{l+1}\right] - \frac{\hbar^2 k^2 \Delta t}{96\pi^2}\left[\bar{\hat{v}}_{N/2}^{l-1} + 4\bar{\hat{v}}_{N/2}^{l} + \bar{\hat{v}}_{N/2}^{l+1}\right] \\
&\quad - \frac{\Delta t}{48\pi^2}\sum_{n=0}^{N/2}{}' \hat{V}_{n-N/2}\left[\bar{\hat{v}}_n^{l-1} + 4\bar{\hat{v}}_n^{l} + \bar{\hat{v}}_n^{l+1}\right] - \frac{\lambda_l}{2\pi}\bar{\hat{v}}_{N/2}^{l}, \\
0 &= \frac{i\hbar}{16\pi}\left[\hat{v}_{N/2}^{l+1} - \hat{v}_{N/2}^{l-1}\right] - \frac{\hbar^2 k^2 \Delta t}{96\pi^2}\left[\hat{v}_{N/2}^{l-1} + 4\hat{v}_{N/2}^{l} + \hat{v}_{N/2}^{l+1}\right] \\
&\quad - \frac{\Delta t}{48\pi^2}\sum_{n=0}^{N/2}{}' \hat{V}_{N/2-n}\left[\hat{v}_n^{l-1} + 4\hat{v}_n^{l} + \hat{v}_n^{l+1}\right] - \frac{\lambda_l}{2\pi}\hat{v}_{N/2}^{l}, \\
1 &= \frac{1}{2\pi}\sum_{k=-N/2}^{N/2}{}'' \hat{v}_k^{l}\bar{\hat{v}}_k^{l}, \\
0 &= \hat{v}_{-N/2}^{l} - \hat{v}_{N/2}^{l}, \\
0 &= \bar{\hat{v}}_{-N/2}^{l} - \bar{\hat{v}}_{N/2}^{l}.
\end{aligned}
$$

This system of $(2N+3)$-equations, allow us to solve for $\{\hat{v}_k^{l+1}, \bar{\hat{v}}_k^{l+1}\}_{k=-N/2}^{N/2}$ and λ_l from initial data, $\{\hat{v}_k^{l-1}, \bar{\hat{v}}_k^{l-1}\}_{k=-N/2}^{N/2}$ and $\{\hat{v}_k^{l}, \bar{\hat{v}}_k^{l}\}_{k=-N/2}^{N/2}$. As such, this system of equations are an example of a spectral in space, second-order in time, ***pseudospectral variational integrator*** for the time-dependent Schrödinger equation. The expressions for the variational integrator for the time-independent Schrödinger equation, which has spectral accuracy in space, are given by

$$\hbar^2 k^2 \bar{\hat{v}}_j = -\sum_{n=-N/2}^{N/2+j}{}' \hat{V}_{n-j}\bar{\hat{v}}_n - \lambda\bar{\hat{v}}_j\,, \qquad \text{for } j=-N/2+1,\ldots,-1,$$

$$\hbar^2 k^2 \hat{v}_j = -\sum_{n=-N/2}^{N/2+j}{}' \hat{V}_{j-n}\hat{v}_n - \lambda\hat{v}_j\,, \qquad \text{for } j=-N/2+1,\ldots,-1,$$

$$\hbar^2 k^2 \bar{\hat{v}}_j = -\sum_{n=j-N/2}^{N/2}{}' \hat{V}_{n-j}\bar{\hat{v}}_n - \lambda\bar{\hat{v}}_j\,, \qquad \text{for } j=0,\ldots,N/2-1,$$

$$\hbar^2 k^2 \hat{v}_j = -\sum_{n=j-N/2}^{N/2}{}' \hat{V}_{j-n}\hat{v}_n - \lambda\hat{v}_j\,, \qquad \text{for } j=0,\ldots,N/2-1,$$

$$\frac{\hbar^2 k^2}{2}\bar{\hat{v}}_{N/2} = -\sum_{n=0}^{N/2}{}' \hat{V}_{n-N/2}\bar{\hat{v}}_n - \lambda\bar{\hat{v}}_{N/2}\,,$$

$$\frac{\hbar^2 k^2}{2}\hat{v}_{N/2} = -\sum_{n=0}^{N/2}{}' \hat{V}_{N/2-n}\hat{v}_n - \lambda\hat{v}_{N/2},$$

$$1 = \frac{1}{2\pi}\sum_{k=-N/2}^{N/2}{}'' \hat{v}_k\bar{\hat{v}}_k\,,$$

$$\hat{v}^l_{-N/2} = \hat{v}^l_{N/2}\,,$$

$$\bar{\hat{v}}^l_{-N/2} = \bar{\hat{v}}^l_{N/2}\,.$$

As mentioned previously, it is possible generalize this approach to construct a fully spectral variational integrator in space-time, using Chebyshev polynomials to interpolate in time the coefficients of the discrete Fourier expansion used in the spatial interpolation. The computational cost of implementing such a scheme would be significantly higher, since this would require all the spatio-temporal degrees of freedom to be solved for simultaneously.

5.9 Conclusions and Future Work

We have introduced the notion of a generalized Galerkin variational integrator, which is based on the idea of appropriately choosing a finite-dimensional approximation of the section of the configuration bundle, and approximating the action integral by a numerical quadrature scheme.

In contrast to standard variational methods, that are typically formulated in terms of interpolatory schemes parameterized by values of field variables at nodal and internal points, generalized Galerkin methods utilize function spaces that can be generated by arbitrary degrees of freedom. This allows the introduction of Lie group methods, and their symmetry reduction using discrete

Euler–Poincaré reduction, as well as multiscale, and pseudospectral methods. Nonlinear approximation spaces allow the construction of spatio-temporally adaptive methods, which are better able to resolve shocks and other kinds of localized discontinuities in the solution.

It would be interesting to compare the performance of pseudospectral variational integrators with traditional pseudospectral schemes to see if any additional benefits arise from constructing pseudospectral schemes using a variational approach. More interesting still would be the comparison for fully spectral methods, since both variational and non-variational methods would achieve spectral accuracy, and it would make a particularly compelling case for variational integrators if their advantages persist even when compared to numerical methods with spectral accuracy.

Most mesh adaptive methods use the principle of equipartitioning the error of the numerical scheme over the mesh elements to obtain moving mesh equations. These methods rely on *a posteriori* error estimators that are related to the norm in which the accuracy of the numerical method is measured. While adaptive variational integrators exhibit an equipartitioning principle, in the sense that the discrete conjugate momentum associated with the horizontal variations are preserved from element to element in each connected component of the domain, it would be interesting to carefully explore the question of whether this can be understood as arising from error equipartitioning with respect to a geometrically motivated error estimator.

While we have only discussed the application of multiscale variational integrators to the case of ordinary differential equations, it would be natural to consider their generalizations to partial differential equations, whereby the multiscale shape functions are obtained through well-resolved solutions of the cell problem, as in the case with multiscale finite elements (see, for example, Hou and Wu [1999]). In general, short-term simulations at the fine scale can be used to construct appropriate shape functions to obtain generalized Galerkin variational integrators at a coarser level, through the use of principal orthogonal decomposition and balanced truncation, for example. This is consistent with the coarse-fine computational approach proposed in Theodoropoulos et al. [2000], or the framework of heterogeneous multiscale methods as proposed in E and Engquist [2003].

A natural generalization would be to consider wavelet based variational integrators, as well as schemes based on conforming, hierarchical, adaptive refinement methods (CHARMS) introduced in Grinspun et al. [2002] and further developed in Krysl et al. [2003].

Chapter 6

Conclusions

In this thesis, we developed discrete Routh reduction, discrete exterior calculus, discrete connections on principal bundles, and generalized variational integrators, which can be classified into two categories, discrete geometry, and discrete mechanics, which form the basis for computational geometric mechanics.

Computational Geometric Mechanics	
Discrete Geometry	**Discrete Mechanics**
Discrete Exterior Calculus (DEC) Discrete Connections on Principal Bundles (DCPB)	Discrete Routh Reduction (DRR) Generalized Variational Integrators (GVI)

The new machinery that has been developed will aid in the systematic development of computational algorithms that are motivated by the techniques of geometric mechanics. Some of the links between the material in the various chapters are summarized below.

DRR and DEC. The curvature term in the discrete Routh equations can be though of as arising from the discrete exterior derivative applied to the connection 1-form, in the case whereby the spatial discretization goes to the continuum limit.

DRR and DCPB. Discrete connections provide the separation of the space $Q \times Q$ into horizontal (shape) and vertical (group) components, thereby providing the coordinates necessary to realize a discrete theory of reduction.

DRR and GVI. Generalized variational integrators provide a framework for the construction of G-invariant discrete Lagrangians, using G-equivariant natural charts, which are necessary to apply discrete reduction theory.

DEC and DCPB. Discrete connections and discrete exterior calculus provide the necessary tools to make sense of the discrete Levi-Civita connection, and to realize its curvature as a SO(n)-valued discrete dual 2-form, that arises from the exterior derivative of a discrete connection expressed as a discrete dual 1-form.

DEC and GVI. Discrete exterior calculus provides a means of discretizing the action integral, and it can be combined with multiscale or spectral discretizations in time to yield hybrid variational schemes that capture the spatial geometry.

DCPB and GVI. Lie group variational integrators could provide an efficient method of constructing discrete connections that approximate continuous connections to a prescribed degree of accuracy.

Unifying Application. The primary motivation for developing accurate simulations is to provide numerical results that are reliable, and minimizes the use of arbitrary parameters in the simulation in order to obtain a correspondence with reality. In providing a link between physical models across scales, one is in a position to accurately predict large-scale and long-term behavior, and in so doing close the simulation and design cycle.

The next stage of evolution for numerical computation is not simply to predict what happens given a set of initial conditions, but rather to enable simulation driven design through the use of adjoint sensitivity techniques. This can be applied to an optimal design problem in computational electromagnetism, which is to modify the shape of an aircraft wing by homotopy methods so as to minimize its radar cross section. Computational electromagnetism is an application area wherein a large number of the techniques I have been working on converge.

Reduction provides a general framework to remove the gauge symmetries in Maxwell's equations, and discrete exterior calculus discretizes the equations in a geometrically exact fashion. The variational framework of discrete mechanics provides a means of deriving numerical schemes that have good structure-preserving properties, and adaptive mesh movement allow for the resolution of shocks while minimizing computational cost. And incorporating multiscale and numerical homogenization techniques provide the bridge to simulating the effect of complex hybrid materials on the far field scattered wave. More generally, reduction, adaptivity, and multiscale methods increase the efficiency of computations, while discrete exterior calculus and discrete mechanics increase the accuracy. Only by having accurate and efficient numerical methods can one hope to realize the promise of simulation driven design.

Appendix A

Review of Homological Algebra

For the reader's convenience, we will recall some basic definitions and results from homological algebra, which we have reproduced from Hungerford [1974].

Definition A.1. *A pair of homomorphisms,*

$$A \xrightarrow{f} B \xrightarrow{g} C \ ,$$

*is said to be **exact** at B if*

$$\operatorname{Im} f = \operatorname{Ker} g\,.$$

A finite sequence of homomorphisms,

$$A_0 \xrightarrow{f_1} A_1 \xrightarrow{f_2} A_2 \xrightarrow{f_3} \cdots \xrightarrow{f_{n-1}} A_{n-1} \xrightarrow{f_n} A_n \ ,$$

*is **exact** if*

$$\operatorname{Im} f_i = \operatorname{Ker} f_{i+1}, \qquad \textit{for } i = 1, 2, \ldots, n-1.$$

An infinite sequence of homomorphisms,

$$\cdots \xrightarrow{f_{i-1}} A_{i-1} \xrightarrow{f_i} A_i \xrightarrow{f_{i+1}} A_{i+1} \xrightarrow{f_{i+2}} \cdots \ ,$$

*is **exact** if*

$$\operatorname{Im} f_i = \operatorname{Ker} f_{i+1}, \qquad \textit{for all } i \in \mathbb{Z}.$$

Remark A.1. *We record below some of the properties of exact sequences.*

1. *The sequence* $0 \longrightarrow A \xrightarrow{f} B$ *is exact iff f is a monomorphism (one-to-one).*
2. *The sequence* $B \xrightarrow{g} C \longrightarrow 0$ *is exact iff g is a epimorphism (onto).*

3. *If* $A \xrightarrow{f} B \xrightarrow{g} C$ *is exact, then* $gf = 0$.

4. *If* $A \xrightarrow{f} B \xrightarrow{g} C \longrightarrow 0$ *is exact, then*

$$\operatorname{Coker} f = B/\operatorname{Im} f = B/\operatorname{Ker} g = \operatorname{Coim} g \cong C.$$

5. *An exact sequence of the form* $0 \longrightarrow A \xrightarrow{f} B \xrightarrow{g} C \longrightarrow 0$, *is called a* ***short exact sequence****, and in particular,* f *is a monomorphism, and* g *is an epimorphism.*

6. *A short exact sequence is another way of presenting a submodule* ($A \cong \operatorname{Im} f$) *and its quotient module* ($B/\operatorname{Im} f = B/\ker g \cong C$)*.*

We will now consider some results for short exact sequences, such as

$$0 \longrightarrow A_1 \underset{k}{\overset{f}{\rightleftarrows}} B \underset{h}{\overset{g}{\rightleftarrows}} A_2 \longrightarrow 0 ,$$

and their splittings.

Lemma A.1 (The Short Five Lemma). *Consider a commutative diagram,*

$$\begin{array}{ccccccccc} 0 & \longrightarrow & A & \xrightarrow{f} & B & \xrightarrow{g} & C & \longrightarrow & 0 \\ & & \downarrow{\scriptstyle\alpha} & & \downarrow{\scriptstyle\beta} & & \downarrow{\scriptstyle\gamma} & & \\ 0 & \longrightarrow & A' & \xrightarrow{f'} & B' & \xrightarrow{g'} & C' & \longrightarrow & 0 \end{array}$$

such that each row is a short exact sequence. Then,

1. α *and* γ *are monomorphisms, implies* β *is a monomorphism;*

2. α *and* γ *are epimorphisms, implies* β *is an epimorphism;*

3. α *and* γ *are isomorphisms, implies* β *is an isomorphism.*

Proof. The proof involves diagram chasing and the exactness of the rows. See, for example, page 176 of Hungerford [1974]. □

The short five lemma allows the following theorem to be proved. This theorem can be used to relate the various representations of a connection on a principal bundle, in both the continuous and discrete cases.

Theorem A.2. *Given a short exact sequence*

$$0 \longrightarrow A_1 \xrightarrow{f} B \xrightarrow{g} A_2 \longrightarrow 0 ,$$

the following conditions are equivalent.

1. *There is a homomorphism* $h : A_2 \to B$ *with* $g \circ h = 1_{A_2}$*;*

2. *There is a homomorphism* $k : B \to A_1$ *with* $k \circ f = 1_{A_1}$*;*

3. *The given sequence is isomorphic (with identity maps on* A_1 *and* A_2*) to the direct sum short exact sequence,*

$$0 \longrightarrow A_1 \xrightarrow{i_1} A_1 \oplus A_2 \xrightarrow{\pi_2} A_2 \longrightarrow 0\ ,$$

and in particular, $B \cong A_1 \oplus A_2$*.*

A short exact sequence that satisfies the equivalent conditions of Theorem A.2 is said to be ***split*** or a ***split exact*** sequence. The maps in Theorem A.2 are referred to as ***splittings*** of the short exact sequence.

Proof. We present the proof sketched on pages 177–178 of Hungerford [1974].

1 ⇒ 3. Consider the homomorphism $\varphi : A_1 \oplus A_2 \to B$, given by $(a_1, a_2) \mapsto f(a_1) + h(a_2)$, and verify that the diagram

$$\begin{array}{ccccccccc}
0 & \longrightarrow & A & \xrightarrow{i_1} & A_1 \oplus A_2 & \xrightarrow{\pi_2} & A_2 & \longrightarrow & 0 \\
 & & \big\downarrow{\scriptstyle 1_{A_1}} & & \big\downarrow{\scriptstyle \varphi} & & \big\downarrow{\scriptstyle 1_{A_2}} & & \\
0 & \longrightarrow & A_1 & \xrightarrow{f} & B & \underset{h}{\overset{g}{\rightleftarrows}} & A_2 & \longrightarrow & 0
\end{array}$$

is commutative. Use the short five lemma to conclude that φ is an isomorphism.

2 ⇒ 3. Consider the homomorphism $\psi : B \to A_1 \oplus A_2$, given by $b \mapsto (k(b), g(b))$, and verify that the diagram

$$\begin{array}{ccccccccc}
0 & \longrightarrow & A_1 & \underset{k}{\overset{f}{\rightleftarrows}} & B & \xrightarrow{g} & A_2 & \longrightarrow & 0 \\
 & & \big\downarrow{\scriptstyle 1_{A_1}} & & \big\downarrow{\scriptstyle \psi} & & \big\downarrow{\scriptstyle 1_{A_2}} & & \\
0 & \longrightarrow & A & \xrightarrow{i_1} & A_1 \oplus A_2 & \xrightarrow{\pi_2} & A_2 & \longrightarrow & 0
\end{array}$$

is commutative. Use the short five lemma to conclude that ψ is an isomorphism.

3 ⇒ 1, 2. Consider the commutative diagram

$$\begin{array}{ccccccccc}
0 & \longrightarrow & A_1 & \underset{\pi_1}{\overset{i_1}{\rightleftarrows}} & A_1 \oplus A_2 & \underset{i_2}{\overset{\pi_2}{\rightleftarrows}} & A_2 & \longrightarrow & 0 \\
 & & \big\downarrow{\scriptstyle 1_{A_1}} & & \big\downarrow{\scriptstyle \varphi} & & \big\downarrow{\scriptstyle 1_{A_2}} & & \\
0 & \longrightarrow & A_1 & \xrightarrow{f} & B & \xrightarrow{g} & A_2 & \longrightarrow & 0
\end{array}$$

with exact rows, and where φ is an isomorphism. Let $h = \varphi i_2 : A_2 \to B$ and $k = \pi_1 \varphi^{-1} : B \to A_1$, and show using the commutativity of the diagram that $kf = 1_{A_1}$ and $gh = 1_{A_2}$. □

Appendix B

Geometry of the Special Euclidean Group

To allow the reader to apply the construction of the exact discrete connection using exponentials and logarithms to problems arising in geometric control, we review some of the basic geometry of the ***Special Euclidean Group*** in three dimensions, SE(3), which is the Lie group consisting of isometries of $\mathbb{R}^3$. A more detail discussion of the geometry of SE(3), and its applications to robotics can be found in Murray et al. [1994].

Representation of SE(3). The group SE(3) is a semidirect product of SO(3) and $\mathbb{R}^3$. Using homogeneous coordinates, we can represent SE(3) as follows,

$$\mathrm{SE}(3) = \left\{ \begin{pmatrix} R & p \\ 0 & 1 \end{pmatrix} \in \mathrm{GL}(4,\mathbb{R}) \,\middle|\, R \in \mathrm{SO}(3), p \in \mathbb{R}^3 \right\}$$

with the action on $\mathbb{R}^3$ given by the usual matrix-vector product when we identify $\mathbb{R}^3$ with the section $\mathbb{R}^3 \times \{1\} \subset \mathbb{R}^4$. In particular, given

$$g = \begin{pmatrix} R & p \\ 0 & 1 \end{pmatrix} \in \mathrm{SE}(3),$$

and $q \in \mathbb{R}^3$, we have

$$g \cdot q = Rq + p,$$

or as a matrix-vector product,

$$\begin{pmatrix} R & p \\ 0 & 1 \end{pmatrix} \begin{pmatrix} q \\ 1 \end{pmatrix} = \begin{pmatrix} Rq + p \\ 1 \end{pmatrix}.$$

The Lie algebra of SE(3) is given by

$$\mathfrak{se}(3) = \left\{ \begin{pmatrix} \hat{\omega} & v \\ 0 & 0 \end{pmatrix} \in M_4(\mathbb{R}) \,\middle|\, \hat{\omega} \in \mathfrak{so}(3), v \in \mathbb{R}^3 \right\},$$

where $\hat{\cdot} : \mathbb{R}^3 \to \mathfrak{so}(3)$ is given by

$$\hat{\omega} = \begin{pmatrix} 0 & -\omega_z & \omega_y \\ \omega_z & 0 & -\omega_x \\ -\omega_y & \omega_x & 0 \end{pmatrix}.$$

Exponentials and Logarithms. The exponential map, $\exp : \mathfrak{se}(3) \to \mathrm{SE}(3)$, is given by

$$\exp \begin{pmatrix} \hat{\omega} & v \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} \exp(\hat{\omega}) & Av \\ 0 & 1 \end{pmatrix},$$

where

$$A = I + \frac{1 - \cos\|\omega\|}{\|\omega\|^2}\hat{\omega} + \frac{\|\omega\| - \sin\|\omega\|}{\|\omega\|^3}\hat{\omega}^2,$$

and $\exp(\hat{\omega})$ is given by the Rodriguez' formula,

$$\exp(\hat{\omega}) = I + \frac{\sin\|\omega\|}{\|\omega\|}\hat{\omega} + \frac{1 - \cos\|\omega\|}{\|\omega\|^2}\hat{\omega}^2.$$

The logarithm, $\log : \mathrm{SE}(3) \to \mathfrak{se}(3)$, is given by

$$\log \begin{pmatrix} R & p \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} \log(R) & A^{-1}p \\ 0 & 0 \end{pmatrix},$$

where

$$\log(R) = \frac{\phi}{2\sin\phi}(R - R^T) \equiv \hat{\omega},$$

and ϕ satisfies

$$\mathrm{Tr}(R) = 1 - 2\cos\phi, \qquad |\phi| < \pi,$$

and where

$$A^{-1} = I - \frac{1}{2}\hat{\omega} + \frac{2\sin\|\omega\| - \|\omega\|(1 + \cos\|\omega\|)}{2\|\omega\|^2 \sin\|\omega\|}\hat{\omega}^2.$$

Appendix C

Analysis of Multiscale Finite Elements in One Dimension

This appendix will analyze the discrete l_∞ error for multiscale finite elements (MsFEM) in one dimension when applied to a multiscale second-order elliptic equation with homogeneous boundary conditions. This will serve to motivate the use of multiscale shape functions in the construction of variational integrators, for problems with multiple temporal scales, as discussed in §5.7.

Let $a(y)$ be a smooth, periodic function in y, with period 1. Moreover, we assume that $a(y) \geq c_1 > 0$ for some positive constant c_1, and that $f(x)$ is a smooth function. Let $\epsilon > 0$ be a small parameter. Consider the following second-order elliptic PDE,

$$\frac{\partial}{\partial x}\left(a\left(\frac{x}{\epsilon}\right)\frac{\partial}{\partial x}u^\epsilon(x)\right) = f(x), \quad 0 < x < 1\,,$$

with homogeneous boundary conditions, $u^\epsilon(0) = 0 = u^\epsilon(1)$.

Analytical Solution. To obtain convergence estimates, it is relevant to consider the analytical solution of the above PDE. We have

$$\begin{aligned}\frac{\partial}{\partial x}\left(a\left(\frac{x}{\epsilon}\right)\frac{\partial}{\partial x}u^\epsilon(x)\right) &= f(x)\,,\\ a\left(\frac{x}{\epsilon}\right)\frac{\partial}{\partial x}u^\epsilon(x) - a(0)\frac{\partial}{\partial x}u^\epsilon(0) &= \int_0^x f(s)\,ds\,.\end{aligned}$$

Denoting $a(0)\frac{\partial}{\partial x}u^\epsilon(0)$ by c, we obtain

$$\begin{aligned}\frac{\partial}{\partial x}u^\epsilon(x) &= \frac{\int_0^x f(s)\,ds - c}{a\left(\frac{x}{\epsilon}\right)}\,,\\ u^\epsilon(x) &= \int_0^x \frac{\int_0^y f(s)\,ds - c}{a\left(\frac{y}{\epsilon}\right)}dy\,.\end{aligned}$$

We impose the boundary condition $u^\epsilon(1) = 0$, which yields

$$\begin{aligned}
0 &= u^\epsilon(1) \\
&= \int_0^1 \frac{\int_0^y f(s)ds}{a\left(\frac{y}{\epsilon}\right)} dy - c\int_0^1 \frac{dy}{a\left(\frac{y}{\epsilon}\right)}\,, \\
c &= \frac{\int_0^1 \frac{\int_0^y f(s)ds}{a\left(\frac{y}{\epsilon}\right)} dy}{\int_0^1 \frac{dy}{a\left(\frac{y}{\epsilon}\right)}}\,.
\end{aligned}$$

Hence,

$$\begin{aligned}
u^\epsilon(x) &= \int_0^x \frac{\int_0^y f(s)\,ds}{a\left(\frac{y}{\epsilon}\right)} dy - \frac{\int_0^1 \frac{\int_0^y f(s)ds}{a\left(\frac{y}{\epsilon}\right)} dy}{\int_0^1 \frac{dy}{a\left(\frac{y}{\epsilon}\right)}} \int_0^x \frac{dy}{a\left(\frac{y}{\epsilon}\right)} \\
&= \int_0^x \frac{F(y)}{a\left(\frac{y}{\epsilon}\right)} dy - \frac{\int_0^1 \frac{F(y)}{a\left(\frac{y}{\epsilon}\right)} dy}{\int_0^1 \frac{dy}{a\left(\frac{y}{\epsilon}\right)}} \int_0^x \frac{dy}{a\left(\frac{y}{\epsilon}\right)}.
\end{aligned}$$

Analytical Expressions for the MsFEM Shape Functions. The MsFEM shape functions can be obtained analytically as follows,

$$\begin{aligned}
\partial_x a\left(\frac{x}{\epsilon}\right)\partial_x \varphi_i^\epsilon &= 0\,, \\
a\left(\frac{x}{\epsilon}\right)\partial_x \varphi_i^\epsilon &= c_1\,, \\
\partial_x \varphi_i^\epsilon &= \frac{c_1}{a\left(\frac{x}{\epsilon}\right)}\,.
\end{aligned}$$

For $x \in [x_{i-1}, x_i]$, we have

$$\begin{aligned}
\varphi_i^\epsilon(x) &= c_1 \int_{x_{i-1}}^x \frac{ds}{a\left(\frac{s}{\epsilon}\right)}\,, \\
\varphi_i^\epsilon(x_i) &= c_1 \int_{x_{i-1}}^{x_i} \frac{ds}{a\left(\frac{s}{\epsilon}\right)} = 1\,, \\
c_1 &= \frac{1}{\int_{x_{i-1}}^{x_i} \frac{ds}{a\left(\frac{s}{\epsilon}\right)}}\,, \\
\varphi_i^\epsilon(x) &= \frac{\int_{x_{i-1}}^{x} \frac{ds}{a\left(\frac{s}{\epsilon}\right)}}{\int_{x_{i-1}}^{x_i} \frac{ds}{a\left(\frac{s}{\epsilon}\right)}}\,.
\end{aligned}$$

For $x \in [x_i, x_{i+1}]$, we have

$$\varphi_i^\epsilon(x_{i+1}) - \varphi_i^\epsilon(x) = c_1 \int_x^{x_{i+1}} \frac{ds}{a\left(\frac{s}{\epsilon}\right)}\,,$$

$$\begin{aligned}
0-1 &= \varphi_i^{\epsilon}(x_{i+1}) - \varphi_i^{\epsilon}(x_i) \\
&= c_1 \int_{x_i}^{x_{i+1}} \frac{ds}{a\left(\frac{s}{\epsilon}\right)}, \\
c_1 &= -\frac{1}{\int_{x_i}^{x_{i+1}} \frac{ds}{a\left(\frac{s}{\epsilon}\right)}}, \\
\varphi_i^{\epsilon}(x) &= \frac{\int_{x}^{x_{i+1}} \frac{ds}{a\left(\frac{s}{\epsilon}\right)}}{\int_{x_i}^{x_{i+1}} \frac{ds}{a\left(\frac{s}{\epsilon}\right)}}.
\end{aligned}$$

Then, in general,

$$\varphi_i^{\epsilon}(x) = \begin{cases} \left[\int_{x_{i-1}}^{x_i} \frac{ds}{a\left(\frac{s}{\epsilon}\right)}\right]^{-1} \left[\int_{x_{i-1}}^{x} \frac{ds}{a\left(\frac{s}{\epsilon}\right)}\right], & x \in [x_{i-1}, x_i]; \\ \left[\int_{x_i}^{x_{i+1}} \frac{ds}{a\left(\frac{s}{\epsilon}\right)}\right]^{-1} \left[\int_{x}^{x_{i+1}} \frac{ds}{a\left(\frac{s}{\epsilon}\right)}\right], & x \in (x_i, x_{i+1}]; \\ 0, & \text{otherwise}. \end{cases}$$

Discrete Error Analysis of the One-Dimensional MsFEM. Consider a uniform partition on the interval $I = [0,1]$,

$$P : 0 = x_0 < x_1 < \ldots < x_N = 1,$$

with mesh size $h = 1/N$. Further, let $I_i = [x_i, x_{i+1}]$. We define the discrete l_2 and l_∞ norms as follows,

$$\begin{aligned}
\|f\|_{l_2} &= \left(\sum_{i=0}^{N} |f(x_i)|^2\right)^{1/2}, \\
\|f\|_{l_\infty} &= \max_{i=0,\ldots,N} |f(x_i)|.
\end{aligned}$$

In this section, we will show that the l_∞ error for one-dimensional MsFEM is zero, and in particular, the l_2 error for one-dimensional MsFEM is zero as well.

The stiffness matrix is given by

$$\begin{aligned}
A_{ij}^h &= a\left(\varphi_i^{\epsilon}, \varphi_j^{\epsilon}\right) \\
&= -\int_0^1 a\left(\frac{x}{\epsilon}\right) \nabla\varphi_i^{\epsilon} \nabla\varphi_j^{\epsilon} dx \\
&= \begin{cases} -\int_{x_{i-1}}^{x_{i+1}} a\left(\frac{x}{\epsilon}\right) \partial_x \varphi_i^{\epsilon} \partial_x \varphi_j^{\epsilon} dx, & j = i-1, i, i+1; \\ 0, & \text{otherwise}. \end{cases}
\end{aligned}$$

Since $\varphi_{i-1}^{\epsilon}+\varphi_i^{\epsilon}\equiv 1$ in I_{i-1} for all i, we have, $\partial_x\varphi_{i-1}^{\epsilon}+\partial_x\varphi_i^{\epsilon}\equiv 0$ in I_{i-1}, and hence,

$$\begin{aligned}
A_{ii}^h &= -\int_{I_{i-1}} a\left(\frac{x}{\epsilon}\right)\partial_x\varphi_i^{\epsilon}\partial_x\varphi_i^{\epsilon}dx - \int_{I_i} a\left(\frac{x}{\epsilon}\right)\partial_x\varphi_i^{\epsilon}\partial_x\varphi_i^{\epsilon}dx \\
&= -\int_{I_{i-1}} a\left(\frac{x}{\epsilon}\right)\partial_x\varphi_i^{\epsilon}\left(-\partial_x\varphi_{i-1}^{\epsilon}\right)dx - \int_{I_i} a\left(\frac{x}{\epsilon}\right)\partial_x\varphi_i^{\epsilon}\left(-\partial_x\varphi_{i+1}^{\epsilon}\right)dx \\
&= -\left(-\int_{I_{i-1}+I_{i-2}} a\left(\frac{x}{\epsilon}\right)\partial_x\varphi_i^{\epsilon}\partial_x\varphi_{i-1}^{\epsilon}dx - \int_{I_i+I_{i+1}} a\left(\frac{x}{\epsilon}\right)\partial_x\varphi_i^{\epsilon}\partial_x\varphi_{i+1}^{\epsilon}dx\right) \\
&= -\left(A_{ii-1}^h + A_{ii+1}^h\right),
\end{aligned}$$

where the second to last equality is because $\operatorname{supp}\left(\partial_x\varphi_i^{\epsilon}\partial_x\varphi_{i-1}^{\epsilon}\right)\subset I_{i-1}$.

We note further that $a(\cdot,\cdot)$ is a symmetric bilinear form, and consequently,

$$A_{ij}^h = A_{ji}^h.$$

Let us define $B_i^h\equiv A_{ii-1}^h$, and therefore, $A_{ii+1}^h = A_{i+1,i}^h = B_{i+1}^h$. This allows us to conclude that

$$\begin{aligned}
\left(A^hU^h\right)_i &= A_{ij}^hU_j^h \\
&= A_{ii+1}^hU_{i+1}^h + A_{ii}^hU_i^h + A_{ii-1}^hU_{i-1}^h \\
&= A_{ii+1}^hU_{i+1}^h - \left(A_{ii+1}^h + A_{ii-1}^h\right)U_i^h + A_{ii-1}^hU_{i-1}^h \\
&= A_{ii+1}^h\left(U_{i+1}^h - U_i^h\right) - A_{ii-1}^h\left(U_i^h - U_{i-1}^h\right) \\
&= D^+\left(A_{ii-1}^h\left(U_i^h - U_{i-1}^h\right)\right) \\
&= D^+\left(B_i^h\left(U_i^h - U_{i-1}^h\right)\right) \\
&= D^+\left(B_i^hD^-U_i^h\right),
\end{aligned}$$

where the forward and backward difference operators D^+ and D^- are defined by

$$\begin{aligned}
D^+\left(f\left(u_i\right)\right) &= f\left(u_{i+1}\right) - f\left(u_i\right), \\
D^-\left(f\left(u_i\right)\right) &= f\left(u_i\right) - f\left(u_{i-1}\right).
\end{aligned}$$

The MsFEM equation is given by

$$A_{ij}^hU_j^h = f_i^h\,,$$

where $f_i^h = \int_0^1 f(x)\,\varphi_i(x)\,dx$. In particular,

$$f_i^h = \int_0^1 f(x)\,\varphi_i(x)\,dx$$

$$= \left[\int_{x_i}^{x_{i+1}} \frac{dx}{a\left(\frac{x}{\epsilon}\right)} \right]^{-1} \int_{x_i}^{x_{i+1}} f(x) \left[\int_{x}^{x_{i+1}} \frac{dx}{a\left(\frac{x}{\epsilon}\right)} \right] dx$$

$$+ \left[\int_{x_{i-1}}^{x_i} \frac{dx}{a\left(\frac{x}{\epsilon}\right)} \right]^{-1} \int_{x_{i-1}}^{x_i} f(x) \left[\int_{x_{i-1}}^{x} \frac{dx}{a\left(\frac{x}{\epsilon}\right)} \right] dx$$

$$= \left[\int_{x_i}^{x_{i+1}} \frac{dx}{a\left(\frac{x}{\epsilon}\right)} \right]^{-1} \left[\int_{x_i}^{x_{i+1}} \frac{F(x)}{a\left(\frac{x}{\epsilon}\right)} dx - \frac{\int_0^1 \frac{F(x)}{a\left(\frac{x}{\epsilon}\right)} dx}{\int_0^1 \frac{dx}{a\left(\frac{x}{\epsilon}\right)}} \int_{x_i}^{x_{i+1}} \frac{dx}{a\left(\frac{x}{\epsilon}\right)} \right]$$

$$- \left[\int_{x_{i-1}}^{x_i} \frac{dx}{a\left(\frac{x}{\epsilon}\right)} \right]^{-1} \left[\int_{x_{i-1}}^{x_i} \frac{F(x)}{a\left(\frac{x}{\epsilon}\right)} dx - \frac{\int_0^1 \frac{F(x)}{a\left(\frac{x}{\epsilon}\right)} dx}{\int_0^1 \frac{dx}{a\left(\frac{x}{\epsilon}\right)}} \int_{x_i-1}^{x_i} \frac{dx}{a\left(\frac{x}{\epsilon}\right)} \right],$$

where we performed an integration by parts to obtain the last equality. We will further rewrite the expression above using the difference operators.

$$f_i^h = D^+ \left(\left[\int_{x_{i-1}}^{x_i} \frac{dx}{a\left(\frac{x}{\epsilon}\right)} \right]^{-1} \left[\int_{x_{i-1}}^{x_i} \frac{F(x)}{a\left(\frac{x}{\epsilon}\right)} dx - \frac{\int_0^1 \frac{F(x)}{a\left(\frac{x}{\epsilon}\right)} dx}{\int_0^1 \frac{dx}{a\left(\frac{x}{\epsilon}\right)}} \int_{x_i-1}^{x_i} \frac{dx}{a\left(\frac{x}{\epsilon}\right)} \right] \right)$$

$$= D^+ \left(\left[\int_{x_{i-1}}^{x_i} \frac{dx}{a\left(\frac{x}{\epsilon}\right)} \right]^{-2} \left[\int_{x_{i-1}}^{x_i} \frac{1}{a\left(\frac{x}{\epsilon}\right)} dx \right] \left(u^\epsilon(x_i) - u^\epsilon(x_{i-1}) \right) \right)$$

$$= D^+ \left(- \left(\int_{x_{i-1}}^{x_i} a\left(\frac{x}{\epsilon}\right) \left(\left[\int_{x_{i-1}}^{x_i} \frac{dx}{a\left(\frac{x}{\epsilon}\right)} \right]^{-1} \frac{1}{a\left(\frac{x}{\epsilon}\right)} \right) \left(\left[\int_{x_{i-1}}^{x_i} \frac{dx}{a\left(\frac{x}{\epsilon}\right)} \right]^{-1} \frac{-1}{a\left(\frac{x}{\epsilon}\right)} \right) dx \right) D^- u^\epsilon(x_i) \right) \tag{C.0.1}$$

Recall from our analytical expression for the MsFEM shape functions that

$$\varphi_i^\epsilon(x) = \begin{cases} \left[\int_{x_{i-1}}^{x_i} \frac{ds}{a\left(\frac{s}{\epsilon}\right)} \right]^{-1} \left[\int_{x_{i-1}}^{x} \frac{ds}{a\left(\frac{s}{\epsilon}\right)} \right], & x \in [x_{i-1}, x_i]\,; \\ \left[\int_{x_i}^{x_{i+1}} \frac{ds}{a\left(\frac{s}{\epsilon}\right)} \right]^{-1} \left[\int_{x}^{x_{i+1}} \frac{ds}{a\left(\frac{s}{\epsilon}\right)} \right], & x \in (x_i, x_{i+1}]\,; \\ 0\,, & \text{otherwise}\,, \end{cases}$$

and hence,

$$\partial_x \varphi_i^\epsilon(x) = \begin{cases} \left[\int_{x_{i-1}}^{x_i} \frac{ds}{a\left(\frac{s}{\epsilon}\right)} \right]^{-1} \frac{1}{a\left(\frac{x}{\epsilon}\right)}, & x \in [x_{i-1}, x_i]\,; \\ \left[\int_{x_i}^{x_{i+1}} \frac{ds}{a\left(\frac{s}{\epsilon}\right)} \right]^{-1} \frac{-1}{a\left(\frac{x}{\epsilon}\right)}, & x \in (x_i, x_{i+1}]\,; \\ 0\,, & \text{otherwise}\,. \end{cases}$$

We therefore recognize two of the terms in Equation C.0.1 as $\partial_x \varphi_i^\epsilon$ and $\partial_x \varphi_{i-1}^\epsilon$. Consequently, we have that

$$
\begin{aligned}
f_i^h &= D^+ \left(- \left(\int_{x_{i-1}}^{x_i} a\left(\frac{x}{\epsilon}\right) \partial_x \varphi_i^\epsilon \partial_x \varphi_{i-1}^\epsilon dx \right) D^- u^\epsilon \left(x_i\right) \right) \\
&= D^+ \left(A_{ii-1}^h D^- u^\epsilon \left(x_i\right) \right) \\
&= D^+ \left(B_i^h D^- u^\epsilon \left(x_i\right) \right) .
\end{aligned}
$$

Hence,

$$
A_{ij}^h u^\epsilon \left(x_j\right) = D^+ \left(B_i^h D^- u^\epsilon \left(x_i\right) \right) = f_i = A_{ij}^h U_j^h \, .
$$

Since the matrix A^h is invertible, we can conclude that

$$
U_i^h = u^\epsilon \left(x_i\right) .
$$

This implies that one-dimensional MsFEM is exact at the nodal points, and in particular,

$$
\left\| u^\epsilon - u_h \right\|_{l_2} = 0 \, ,
$$

and

$$
\left\| u^\epsilon - u_h \right\|_{l_\infty} = 0 \, .
$$

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Symbols

$\mathbb{F}L$, *see* Legendre transform

$\mathbb{F}L_d$, *see* Legendre transform, discrete

J, *see* momentum map

J_L, *see* momentum map, Lagrangian

J_d, *see* momentum map, discrete

L_d, *see* Lagrangian, discrete

$\hat{R}^\mu$, *see* Routhian

$\mathfrak{X}_d(K)$, *see* vector field, primal

$\mathfrak{X}_d(\star K)$, *see* vector field, dual

Δ, *see* Laplace–Beltrami

div, *see* divergence

$\Omega_d^k(K)$, *see* form, primal

$\Omega_d^k(\star K)$, *see* form, dual

$*$, *see* Hodge star

$\boldsymbol{\delta}$, *see* codifferential

$\flat$, *see* flat

κ, *see* causality sign

$\sharp$, *see* sharp

$\star$, *see* circumcentric, duality operator

$\wedge$, *see* wedge product

$\mathbf{d}$, *see* exterior derivative

$\mathbf{i}_X$, *see* contraction

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Vita

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