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Geometric Variational Integrators for Multisymplectic PDEs and Adjoint Systems

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Geometric Variational Integrators for Multisymplectic PDEs and Adjoint Systems

A dissertation submitted in partial satisfaction of the
requirements for the degree of Doctor of Philosophy

in

Mathematics with Specialization in Computational Science

by

Brian Kha Tran

Committee in charge:

Professor Melvin Leok, Chair
Professor Albert Chern
Professor Michael Holst
Professor John McGreevy
Professor Jeffrey Rabin

2023

The dissertation of Brian Kha Tran is approved, and it is acceptable in quality and form for publication on microfilm and electronically.

University of California San Diego

2023

DEDICATION

I dedicate this dissertation

To my parents, Tuan and Huong, for your undying love and support, and for the many sacrifices you have made to ensure opportunities for your children.

To my siblings, Steven, Ken, Anh and Ann, for your patience, support, love and guidance throughout my life.

To my best friends, Chris, Lucille, Lucia, Steven and Dobie, for always having my back and pushing me forward in difficult times.

To my dearest friends and family, for your constant source of inspiration and love, and for always being there for me.

EPIGRAPH

In mathematical language, the integral called action, instead of being always a minimum, is often a maximum; and often it is neither the one nor the other: though it has always a certain stationary property, of a kind which has been already alluded to, and which will soon be more fully explained. We cannot, therefore, suppose the economy of this quantity to have been designed in the divine idea of the universe: though a simplicity of some high kind may be believed to be included in that idea. And though we may retain the name of action to denote the stationary integral to which it has become appropriated–which we may do without adopting either the metaphysical or (in optics) the physical opinions that first suggested the name–yet we ought not (I think) to retain the epithet least: but rather to adopt the alteration proposed above, and to speak, in mechanics and in optics, of the Law of Stationary Action.

Sir William Rowan Hamilton

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Chapter 2, in full, is a reprint of the material as it appears in ”Multisymplectic Hamiltonian Variational Integrators” (2022). Tran, Brian; Leok, Melvin, *International Journal of Computer Mathematics (Special Issue on Geometric Numerical Integration, Twenty-Five Years Later)*, 99(1), 113-157. The dissertation author was the primary investigator and first author of this paper.

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ABSTRACT OF THE DISSERTATION

Geometric Variational Integrators for Multisymplectic PDEs and Adjoint Systems

by

Brian Kha Tran

Doctor of Philosophy in Mathematics with Specialization in Computational Science

University of California San Diego, 2023

Professor Melvin Leok, Chair

Variational integrators are a class of geometric structure-preserving numerical integrators that are based on a discretization of Hamilton's variational principle. We construct, analyze and investigate the applications of variational integrators to multisymplectic partial differential equations and to adjoint systems.

The variational structure of multisymplectic PDEs encodes both the conservation laws admitted by these systems via Noether's theorem and multisymplecticity, a covariant spacetime generalization of symplecticity. We develop variational integrators for these systems which preserve these properties at the discrete level, in both the Lagrangian and Hamiltonian settings. In the Lagrangian setting, we utilize compatible finite element spaces to develop these variational

integrators and utilize their preservation of the de Rham complex to define discrete geometric structures associated to these integrators and naturally relate them to their continuous counterparts. In the Hamiltonian setting, we utilize a discrete Type II variational principle, based on the notion of a Type II generating functional for multisymplectic PDEs, to construct structure-preserving variational integrators for multisymplectic Hamiltonian PDEs.

Adjoint systems are ubiquitous in optimization and optimal control theory since they allow for efficient computation of sensitivities of cost functionals in optimization problems and arise as necessary conditions for optimality in optimal control problems via Pontryagin's maximum principle. Adjoint systems admit a fundamental quadratic conservation law which is at the heart of the method of adjoint sensitivity analysis; this conservation law arises from the symplectic geometry of these systems. We develop a geometric theory for continuous and discrete adjoint systems associated to ordinary differential equations and differential-algebraic equations, by investigating their underlying symplectic and presymplectic structures, respectively. We develop a Type II variational principle for such systems at the continuous level. Subsequently, we discretize this variational principle to construct variational integrators for adjoint systems which preserve the quadratic conservation law at the discrete level and thus, allow for sensitivities of cost functions to be computed exactly. We further extend this framework to the Lie group setting and develop a variational integrator based on novel continuous and discrete Type II variational principles on cotangent bundles of Lie groups.

Introduction

In this dissertation, we explore the construction, analysis, and application of variational integrators to the numerical simulation of multisymplectic PDEs and adjoint systems. Multisymplectic PDEs are a class of geometric partial differential equations arising in classical field theories of physics; the multisymplectic geometry is an integral part of such theories, as it encodes symmetries and conservation laws covariantly. Adjoint systems are widely used in dynamically-constrained optimization and optimal control; the symplectic geometry of these systems leads to a quadratic conservation law which allows one to compute sensitivities of cost functions. A major theme in this thesis is to understand, at the continuous level, the relation of the geometry of these systems with their associated conservation laws. By understanding these relations at the continuous level, we elucidate the construction of structure-preserving discretizations of these systems, in order to preserve these relations at the discrete level.

This dissertation can be broadly divided into two parts. In Chapters 1 and 2, we study structure-preserving discretizations of multisymplectic PDEs, in the Lagrangian and Hamiltonian frameworks, respectively. In Chapters 3 and 4, we study structure-preserving discretizations of adjoint systems, on vector spaces and on Lie groups, respectively. The chapters in this dissertation can be read mostly independently; however, the material in Chapter 4 is built upon the material in Chapter 3, so it is recommended to read Chapter 3 before Chapter 4. Furthermore, although the two parts study different types of systems (multisymplectic PDEs and adjoint systems), they do share a common thread in the construction of the methods used in this dissertation; in particular, Chapters 2, 3, and 4 all develop Type II variational principles in order to construct geometric variational integrators.

Chapter 1

Variational Structures in Cochain Projection Based Variational Discretizations of Lagrangian PDEs

1.1 Introduction

The problem of structure-preservation in numerical discretizations of partial differential equations has primarily been studied in two disjoint stages, the first involving the semi-discretization of the spatial degrees of freedom, and the second having to do with the time-integration of the resulting coupled system of ordinary differential equations. Implicit in such an approach is the use of tensor product meshes in spacetime. In the context of spatial semi-discretization, the notion of structure-preservation is focused on compatible discretizations (see Arnold [6], and references therein), that preserve in some manner the functional and geometric relationships between the different function spaces that arise in the partial differential equation, and in the context of time-integration, geometric numerical integrators (see Hairer et al. [51], and references therein) aim to preserve geometric invariants like the symplectic or Poisson structure, energy, momentum, and the nonlinear manifold structure of the configuration spaces, like its Lie group, homogeneous space, or Riemannian structure.

Lagrangian partial differential equations are an important class of partial differential equations that exhibit geometric structure, and they can benefit from numerical discretizations that preserve such geometric structure. This can either be viewed as an infinite-dimensional Lagrangian system with time as the independent variable, or a finite-dimensional Lagrangian multisymplectic field theory [87] with space and time as independent variables. Lagrangian variational integrators [84; 85] are a popular method for systematically constructing symplectic integrators of arbitrarily high-order, and satisfy a discrete Noether's theorem that relates group-invariance with momentum conservation. A group-invariant (and hence momentum-preserving) variational integrator can be constructed from group-equivariant interpolation spaces [40].

In this paper, we will demonstrate how compatible discretization, multisymplectic variational integrators, and group-equivariant interpolation spaces can be combined to yield a natural geometric structure-preserving discretization framework for Lagrangian field theories.

1.1.1 Multisymplectic Formulation of Classical Field Theories

The variational principle for Lagrangian PDEs involve a multisymplectic formulation [85; 87]. The base space X consists of independent variables, denoted by $(x^0,\dots,x^n) \equiv (t,x)$, where $x^0 \equiv t$ is time, and $(x^1,\dots,x^n) \equiv x$ are space variables. The dependent field variables, $(y^1,\dots,y^m) \equiv y$, form a fiber over each spacetime basepoint. The independent and field variables form the configuration bundle, $\pi : Y \to X$. The configuration of the system is specified by a section of Y over X, which is a continuous map $\phi : X \to Y$, such that $\pi \circ \phi = 1_X$. This means that for every $(t,x) \in X$, $\phi((t,x))$ is in the fiber $\pi^{-1}((t,x))$ over (t,x).

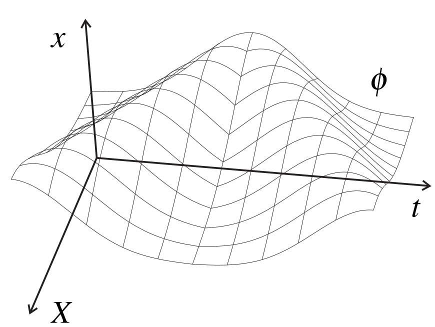


Figure 1.1. A section of the configuration bundle: the horizontal axes represent spacetime, and the vertical axis represent dependent field variables. The section ϕ gives the value of the field variables at every point of spacetime.

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

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

which is a section of the fiber bundle J^1Y over X. We refer to sections of J^1Y of the form $j^1\phi$, where ϕ is a section of Y, as holonomic. The configuration space is the space of sections of Y and the velocity phase space is the space of holonomic sections of J^1Y. The Lagrangian density is a bundle map $\mathscr{L} : J^1Y \to \wedge^{n+1}(T^*X)$ and hence, induces a map on the space of sections $\mathscr{L} : \Gamma(J^1Y) \to \Omega^{n+1}(X)$. Thus, we can define the action functional $S : \Gamma(Y) \to \mathbb{R}$ by $S[\phi] = \int_X \mathscr{L}(j^1\phi)$. Hamilton's principle states that $\delta S = 0$, subject to compactly supported variations. As we will see, this is the basis of Lagrangian multisymplectic variational integrators [85].

The variational structure of a Lagrangian field theory is given by the Cartan form, which in coordinates has the expression

$$\Theta_{\mathscr{L}} = \frac{\partial L}{\partial v^a_\mu} dy^a \wedge d^n x_\mu + \left(L - \frac{\partial L}{\partial v^a_\mu} v^a_\mu\right) d^{n+1}x. \tag{1.1}$$

This can be defined intrinsically as the pullback of the canonical $(n+1)$-form on the dual jet bundle by the covariant Legendre transform $\mathbb{F}\mathscr{L} : J^1Y \to J^1Y^*$. Then, the action can be expressed as $S[\phi] = \int_X \mathscr{L}(j^1\phi) = \int_X (j^1\phi)^*\Theta_{\mathscr{L}}$. The variation of the action is then expressed as

$$dS[\phi]\cdot V = -\int_X (j^1\phi)^*(j^1V \lrcorner\, \Omega_{\mathscr{L}}) + \int_{\partial X} (j^1\phi)^*(j^1V \lrcorner\, \Theta_{\mathscr{L}}),$$

where $\Omega_{\mathscr{L}} = -d\Theta_{\mathscr{L}}$ defines the multisymplectic form and j^1V denotes the jet prolongation of the vector field V (for details, see Gotay et al. [44]). Hence, the variation of the action is completely specified by the Cartan form; we will show that a finite element discretization of the variational principle gives rise to a discrete form and subsequently we will express variational properties of the discrete system in terms of the discrete Cartan form.

In this paper, we will take the fields to be elements of $H\Lambda^k(X)$, the space of square integrable $k-$forms on X with square integrable exterior derivative. In this setting, the appropriate analogue of the configuration space is $H\Lambda^k$ and the appropriate analogue of the velocity phase space is $J^1_{H\Lambda^k} := H\Lambda^k \times dH\Lambda^k$, where the jet extension of a field $\phi \in H\Lambda^k$, only depending on the exterior derivative, is $j^1_d\phi \equiv (x, \phi, d\phi)$, i.e., we consider Lagrangian theories that depend on the exterior derivative of the field and not depending more generally on all first-order derivatives; for scalar fields, $k = 0$, these are equivalent. We refer to $j^1_d : H\Lambda^k \to J^1_{H\Lambda^k}$ as the exterior jet extension.

1.1.2 Finite Element Exterior Calculus

The notion of compatible discretization is a research area that has garnered significant interest and activity in the finite element community, motivated by the seminal work of Arnold et al. [7] on finite element exterior calculus that provides a broad generalization of Hiptmair's work on mixed finite elements for electromagnetism [54]. This arises from the fundamental role that the de Rham complex of exterior differential forms plays in mixed formulations of elliptic partial differential equations, and the realization that many of the most successful mixed finite element spaces, such as Raviart–Thomas and Nédélec elements, can be viewed as finite element subspaces of the de Rham complex that satisfy a bounded cochain projection property, so that the set of mixed finite elements form a subcomplex that provides stable approximations of the original problem.

1.1.3 Group-equivariant interpolation

The study of group-equivariant approximation spaces [40] for functions taking values on manifolds is motivated by the applications to geometric structure-preserving discretization of Lagrangian and Hamiltonian PDEs with symmetries. In particular, when the Lagrangian density for a Lagrangian PDE with symmetry is discretized using a Lagrangian multisymplectic variational integrator constructed from an approximation space that is equivariant with respect to the symmetry group, the resulting numerical method automatically preserves the momentum map associated with the symmetry of the PDE. In essence, such variational discretizations exhibit a discrete analogue of Noether's theorem, which connects symmetries of the Lagrangian with momentum conservation laws.

Many intrinsic geometric flows such as the Ricci flow and the Einstein equations involves computing the evolution of a Riemannian or pseudo-Riemannian metric on spacetime. Additionally, these intrinsic geometric flows can often be formulated variationally, so it is natural to consider group-equivariant approximation spaces taking values on Riemannian or pseudo-Riemannian metrics with a view towards constructing variational discretizations that preserve the associated momentum maps.

A now standard approach to constructing an approximation space for functions taking values on a Riemannian manifold that is equivariant with respect to Riemannian isometries is the method of geodesic finite elements introduced independently by Sander [105] and Grohs [48]. Given a Riemannian manifold (M,g), the geodesic finite element $\varphi : \Delta^n \to M$ associated with a set of linear space finite elements $\{v_i : \Delta^n \to \mathbb{R}\}_{i=0}^n$ is given by the Fréchet (or Karcher) mean,

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

where the optimization problem involved can be solved using optimization algorithms developed for matrix manifolds (see Absil et al. [2], and references therein). The spatial derivatives of the geodesic finite element can be computed in terms of an associated optimization problem. The advantage of the geodesic finite element approach is that it inherits the approximation properties of the underlying linear space finite element, but it can be expensive to compute, since it entails solving an optimization problem on a manifold.

An alternative approach to group-equivariant interpolation for functions taking values on symmetric spaces was introduced in Gawlik and Leok [40], which, in particular, is applicable to the interpolation of Riemannian and pseudo-Riemannian metrics. It uses the generalized polar decomposition [91] to construct a local diffeomorphism between a symmetric space and a Lie triple system, and thereby lift a scalar-valued interpolant to a symmetric space-valued interpolant.

1.1.4 Lagrangian Variational Integrators

Variational integrators (see [84], and references therein) are a class of geometric structure-preserving numerical integrators that are based on a discretization of Hamilton's principle. They are particularly appropriate for the simulation of Lagrangian and Hamiltonian ODEs and PDEs, as they automatically preserve many geometric invariants, including the symplectic structure, momentum maps associated with symmetries of the system, and exhibit bounded energy errors for exponentially long times.

In the case of Lagrangian ODEs, variational integrators are based on constructing computable approximations $L_d : Q \times Q \to \mathbb{R}$ of the exact discrete Lagrangian,

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

which can be viewed as Jacobi's solution of the Hamilton–Jacobi equation. Given a discrete Lagrangian L_d, one introduces the discrete action sum $\mathbb{S}_d = \sum_{k=0}^{n-1} L_d(q_k, q_{k+1})$, and then the discrete Hamilton's principle states that $\delta \mathbb{S}_d = 0$, for fixed boundary conditions q_0 and q_n. This leads to the discrete Euler–Lagrange equations,

$$D_2L_d(q_{k-1},q_k)+D_1L_d(q_k,q_{k+1})=0,$$

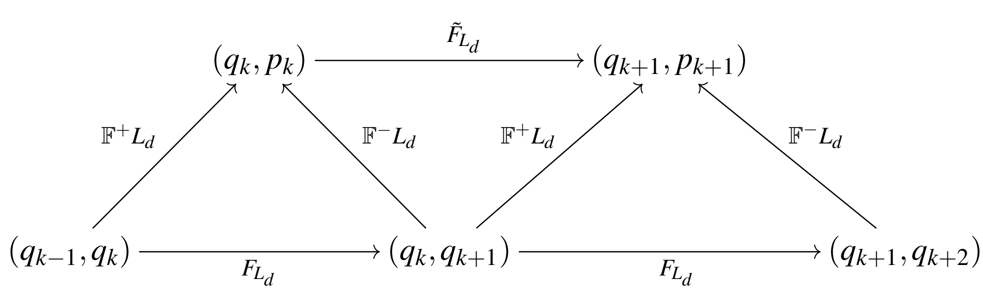
where D_i denotes the partial derivative with respect to the i-th argument. This implicitly defines the discrete Lagrangian map $F_{L_d}:(q_{k-1},q_k)\mapsto(q_k,q_{k+1})$ for initial conditions (q_{k-1},q_k) that are sufficiently close to the diagonal of $Q\times Q$. It is also equivalent to the implicit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

$$p_k=-D_1L_d(q_k,q_{k+1}),\qquad p_{k+1}=D_2L_d(q_k,q_{k+1}),$$

which implicitly defines the discrete Hamiltonian map $\tilde{F}_{L_d}:(q_k,p_k)\mapsto(q_{k+1},p_{k+1})$, which is automatically symplectic. This clearly follows from the fact that these equations are precisely the characterization of a symplectic map in terms of a Type I generating function. The two equations in the implicit discrete Euler–Lagrange equations can be used to define the discrete Legendre transforms, $\mathbb{F}^{\pm}L_d:Q\times Q\to T^*Q$:

$$\begin{aligned}\mathbb{F}^{+}L_d&:(q_0,q_1)\to(q_1,p_1)=(q_1,D_2L_d(q_0,q_1)),\\ \mathbb{F}^{-}L_d&:(q_0,q_1)\to(q_0,p_0)=(q_0,-D_1L_d(q_0,q_1)).\end{aligned}$$

The following commutative diagram illustrates the relationship between the discrete Hamiltonian flow map, discrete Lagrangian flow map, and the discrete Legendre transforms,



If the discrete Lagrangian is invariant under the diagonal action of a Lie group G, i.e., $L_d(q_0,q_1) = L_d(gq_0,gq_1)$, for all $g \in G$, then the discrete Noether's theorem states that there is a discrete momentum map that is automatically preserved by the variational integrator. The bounded energy error of variational integrators can be understood by performing backward error analysis [11; 49], which then shows that the discrete flow map is approximated with exponential accuracy by the exact flow map of the Hamiltonian vector field of a modified Hamiltonian. Similarly, backward error analysis for Lagrangian variational integrators is considered in [117].

1.1.5 Multisymplectic Hamiltonian Variational Integrators.

For Hamiltonian PDEs (see, for example, Marsden and Shkoller [83]) the action is a functional on the field and multimomenta values (more precisely, sections of the restricted dual jet bundle),

$$S[\phi,p] = \int [p^\mu \partial_\mu \phi - H(\phi,p)] d^{n+1}x,$$

where the integration is over some $(n+1)$-dimensional region of spacetime. The variational principle gives the De Donder–Weyl equations $\partial_\mu p^\mu = -\partial H/\partial \phi$, $\partial_\mu \phi = \partial H/\partial p^\mu$. Defining $z = (\phi, p^0, \dots, p^n)$ and K^μ as the $(n+2)\times(n+2)$ skew-symmetric matrix with value -1 in the $(0,\mu+1)$ entry, 1 in the $(\mu+1,0)$ entry, and 0 in every other entry (with indexing from 0 to $n+1$), the De Donder–Weyl equations can be written in the form

$$K^0 \partial_0 z + \cdots + K^n \partial_n z = \nabla_z H.$$

This formulation of Hamiltonian PDEs was studied in Bridges [18]; in particular, it was shown that such a system admits a multisymplectic conservation law of the form $\partial_\mu \omega^\mu(V,W) = 0$, where the ω^μ are two-forms corresponding to K^μ and the conservation law holds when evaluated on first variations V, W. For discretizing such equations, multisymplectic integrators have been developed which admit a discrete analogue of this multisymplectic conservation law (see, for example, Bridges and Reich [22]). Such multisymplectic integrators have traditionally not been approached from a variational perspective.

However, in Tran and Leok [112], we developed a systematic method for constructing variational integrators for multisymplectic Hamiltonian PDEs which automatically admit a discrete multisymplectic conservation law and a discrete Noether's theorem by virtue of the discrete variational principle. The construction is based on a discrete approximation of the boundary Hamiltonian that was introduced in Vankerschaver et al. [116],

$$H_{\partial U}(\varphi_A, \pi_B) = \text{ext}\left[\int_B p^\mu \phi d^n x_\mu - \int_U (p^\mu \partial_\mu \phi - H(\phi, p)) d^{n+1}x\right],$$

where $\partial U = A \sqcup B$, boundary conditions are placed on the field value ϕ on A and normal momenta value on B, and one extremizes over the sections (ϕ, p) over U satisfying the specified boundary conditions. The boundary Hamiltonian is a generating functional in the sense that the Type II variational principle generates the normal momenta value along A and the field value along B,

$$\frac{\delta H_{\partial U}}{\delta \varphi_A} = -p^n|_A, \quad \frac{\delta H_{\partial U}}{\delta \pi_B} = \phi|_B.$$

A variational integrator is then constructed by first approximating the boundary Hamiltonian using a finite-dimensional function space and quadrature, and subsequently enforcing the Type II variational principle. For example, with particular choices of function spaces and quadrature, Tran and Leok [112] recover the class of multisymplectic partitioned Runge–Kutta methods.

In this paper, we take a different approach in several regards. First, we focus on Lagrangian field theories as opposed to Hamiltonian field theories. For Hamiltonian field theories, the momenta are related to the field and its derivative by the Legendre transform; this falls out from the variational principle so one does not need to enforce it beforehand. Thus, in this sense, the momenta and field values can be considered as independent before enforcing the variational principle. On the other hand, for Lagrangian field theories, the Lagrangian depends on both the field value and its first derivative, so one cannot naïvely treat the two as independent; that is, the

Lagrangian depends on holonomic sections of the jet bundle. As we will see, this will mean that we need to pay particular attention to the holonomic condition when discretizing via a finite element projection. Furthermore, as opposed to constructing variational integrators from a generating functional (the analogue in the Lagrangian framework would be the boundary Lagrangian, see Vankerschaver et al. [116]), in this paper, we instead investigate directly discretizing the variational principle $\delta S = 0$ utilizing projections into finite-dimensional subspaces. Finally, for simplicity, we do not utilize any quadrature approximations of the various integrals which we encounter; for strong nonlinearities in the Lagrangian, one generally has to utilize quadrature to construct an efficient discretization. However, the theory that we outline is also applicable to the case of quadrature approximation by first applying the quadrature approximation of the action before enforcing the variational principle, so that the resulting discretization is still variational; we will elaborate on this in Remark 1.2.5. For this reason, we will assume exact integration in order to keep the exposition simple.

Main Contributions. This paper studies the variational finite element discretization of Lagrangian field theories from two perspectives; we begin by investigating directly discretizing the full variational principle over the full spacetime domain, which we refer to as the "covariant" approach, and subsequently study semi-discretization of the instantaneous variational principle on a globally hyperbolic spacetime, which we refer to as the "canonical" approach. This paper can be considered a discrete analogue to the program initiated in Gotay et al. [44, 45], which lays the foundation for relating the covariant and canonical formulations of Lagrangian field theories through their (multi)symplectic structures and momentum maps. One of the goals of understanding the relation between these two different formulations is to systematically relate the covariant gauge symmetries of a gauge field theory to its initial value constraints. This is seen, for example, in general relativity, where the diffeomorphism gauge invariance gives rise to the Einstein constraint equations over the initial data hypersurface (see, for example, Gourgoulhon [46]). When one semi-discretizes such gauge field theories, the discrete initial data must satisfy an associated discrete constraint. We aim to make sense of the discrete geometric structures in the covariant and canonical discretization approaches as a foundation for understanding the discretization of gauge field theories.

In Section 1.2, we begin by formulating a discrete variational principle in the covariant approach, utilizing the finite element construction to appropriately project the variational principle. We show that a cochain projection from the underlying de Rham complex onto the finite element spaces yields a natural discrete variational principle that is compatible with the holonomic jet structure of a Lagrangian field theory. In Section 1.2.2, we then show that discretizing by cochain projections leads to a naturality relation between the continuous variational problem and the discrete variational problem; this naturality then implies that discretization and the variational principle commute and also, that discretizing at the level of the configuration bundle or at the level of the jet bundle are equivalent. Subsequently, by decomposing the finite element spaces into boundary and interior components, we define a discrete weak Cartan form in analogy with the continuum weak Cartan form which will, in a sense, encode the discrete variational structure. With particular choices of finite element spaces, this discrete weak Cartan form recovers the notion of the discrete Cartan form introduced by Marsden et al. [85]. However, we note that our notion of a discrete weak Cartan form is more general and furthermore, since our discrete variational problem is naturally related to the continuum variational problem, we are able to explicitly discuss in what sense the discrete weak Cartan form converges to the continuum weak Cartan form. Using this discrete weak Cartan form, in Sections 1.2.3 and 1.2.4, we state and prove discrete analogues of the multisymplectic form formula and Noether's theorem. In Section 1.2.5, we reinterpret and concisely summarize the preceding sections by interpreting the discrete variational structures as elements of a discrete variational complex. In Section 1.2.6, we provide an example of a multisymplectic integrator for the scalar Poisson equation and prove the convergence of the discrete weak Cartan form to the weak Cartan form.

In Section 1.3, we study the semi-discretization of the canonical formulation of a Lagrangian field theory on a globally hyperbolic spacetime. In Section 1.3.1, we discretize the instantaneous variational principle utilizing cochain projections onto finite element spaces over a Cauchy surface, which gives rise to a semi-discrete Euler–Lagrange equation. In Section 1.3.2, we relate this semi-discrete Euler–Lagrange equation to a Hamiltonian flow on a symplectic semi-discrete phase space. We will discuss in what sense the symplectic structure on the semi-discrete phase space arises from a symplectic structure on the continuum phase space. Subsequently, we will investigate the energy-momentum map structure associated to the semi-discrete phase space in Section 1.3.3, and discuss how, under appropriate equivariance conditions on the projection, the energy-momentum map structure on the semi-discrete phase space arises as the pullback of the energy-momentum map structure on the continuum phase space. This lays a foundation for understanding initial value constraints when discretizing field theories with gauge symmetries. Finally, in Section 1.3.4, we relate the covariant and canonical discretization approaches in the case of tensor product finite element spaces.

The underlying theme of this paper is that, when one discretizes the variational principle utilizing compatible discretization techniques, the associated (covariant or canonical) discretization inherits discrete variational structures which can be viewed as pullbacks or projections of the associated continuum variational structures. These discrete variational structures allow one to investigate structure-preservation under discretization of important physical properties, such as momentum conservation, symplecticity, and (gauge) symmetries.

1.2 Covariant Discretization of Lagrangian Field Theories

In this section, we discretize the covariant Euler–Lagrange equations which arise from the variational principle $\delta S[\phi] = 0$ for the action $S : \phi \mapsto \int_X \mathscr{L}(j^1_d \phi)$ where $\phi \in H\Lambda^k$ is an element of the configuration space and $j^1_d \phi = (x, \phi, d\phi)$. To utilize the finite element method, we take our base space X to be a bounded $(n+1)-$dimensional polyhedral domain with boundary ∂X, equipped with a finite element triangulation $\mathscr{T}_h$. We will assume X has a Riemannian or Lorentzian metric. For this discretization, we perform the variation over a finite element space, and subsequently study how the multisymplectic and covariant momentum map structures are affected by discretization. In particular, we show how these structures are preserved for particular choices of finite element spaces, namely spaces whose projections are cochain maps or group-equivariant interpolation spaces. To begin, we first discuss the weak formulation of Lagrangian field theory.

1.2.1 Weak Lagrangian Field Theory

In this section, we formulate a weak version of Lagrangian field theory on the Hilbert space $H\Lambda^k$. Since we wish to work in the Sobolev space setting, it does not make sense to consider pointwise values of (e.g., square integrable) sections. However, we will assume that the Lagrangian density makes sense as a map on sections, $\mathscr{L} : J^1_{H\Lambda^k} \to \Omega^{n+1}(X)$, i.e., given a section $\phi \in H\Lambda^k$, the quantity $\mathscr{L}(j^1_d \phi)$ is a top-dimensional form on X. Hence, we can define the action $S : H\Lambda^k \to \mathbb{R}$ via $S[\phi] = \int_X \mathscr{L}(j^1_d \phi)$. Thus, from our perspective, a weak Lagrangian field theory is defined by a Lagrangian density $\mathscr{L} : J^1_{H\Lambda^k} \to \Omega^{n+1}(X)$ with associated action $S : H\Lambda^k \to \mathbb{R}$.

We derive the weak Euler–Lagrange equations in the Hilbert space setting, where the velocity phase space is $J^1_{H\Lambda^k} = H\Lambda^k \times dH\Lambda^k$. Fixing the trace of ϕ on ∂X, the variational principle is to find $\phi \in H\Lambda^k$ such that $\delta S[\phi] \cdot v = 0$ for all $v \in \mathring{H}\Lambda^k \equiv \{v \in H\Lambda^k : \mathrm{Tr}(v) = 0\}$. This yields the weak Euler–Lagrange equations

$$\begin{aligned} 0 = \delta S[\phi] \cdot v &= \int_X \Big(\delta_2 \mathscr{L}(j^1_d \phi) \cdot v + \delta_3 \mathscr{L}(j^1_d \phi) \cdot dv \Big) \\ &= (\partial_2 \mathscr{L}(j^1_d \phi), v)_{L^2\Lambda^k} + (\partial_3 \mathscr{L}(j^1_d \phi), dv)_{L^2\Lambda^{k+1}} \\ &= (\partial_2 \mathscr{L}(j^1_d \phi), v)_{L^2\Lambda^k} + (d^* \partial_3 \mathscr{L}(j^1_d \phi), v)_{L^2\Lambda^k}, \end{aligned} \tag{2.1}$$

where δ_i denotes the variation with respect to the i^{th} argument, the codifferential d^* is interpreted in the weak sense, and in the second line we apply the Riesz representation theorem to express the linear functional $v \in L^2\Lambda^k \mapsto \int_X \delta_2 \mathscr{L}(j^1_d \phi) \cdot v$ as an element $\partial_2 \mathscr{L}(j^1_d \phi)$ of $L^2\Lambda^k$ and similarly, the linear functional $w \in L^2\Lambda^{k+1} \mapsto \int_X \delta_3 \mathscr{L}(j^1_d \phi) \cdot w$ as an element $\partial_3 \mathscr{L}(j^1_d \phi)$ of $L^2\Lambda^{k+1}$, assuming that these linear functionals are bounded.

Remark 1.2.1. *As mentioned above, the linear functionals $v \in L^2\Lambda^k \mapsto \int_X \delta_2 \mathscr{L}(j^1_d\phi)\cdot v$ and $w \in L^2\Lambda^{k+1} \mapsto \int_X \delta_3 \mathscr{L}(j^1_d\phi)\cdot w$ should be bounded in order to represent them as elements of $L^2\Lambda^k$ and $L^2\Lambda^{k+1}$, respectively. We give some examples of classes of Lagrangian densities for which this holds.*

Consider a Lagrangian density containing at most quadratic terms in ϕ and $d\phi$, of the form

$$\mathscr{L}(j^1_d\phi) = \frac{1}{2}a_1 d\phi \wedge *d\phi + \frac{1}{2}a_2\phi\wedge *\phi + a_3 f\wedge *d\phi + a_4 g\wedge *\phi,$$

where $a_i \in L^\infty, f \in L^2\Lambda^{k+1}, g \in L^2\Lambda^k$ are given. The variation of the associated action can be computed

$$\delta S[\phi]\cdot v = \int_X \Big((a_2\phi + a_4 g)\wedge *v + (a_1 d\phi + a_3 f)\wedge *dv \Big).$$

We see that the functional $v \in L^2\Lambda^k \mapsto \int_X \delta_2\mathscr{L}(j^1_d\phi)\cdot v = \int_X (a_2\phi + a_4 g)\wedge *v$ is bounded, since

$$\begin{aligned}\Big| \int_X (a_2\phi + a_4 g)\wedge *v \Big| &= (a_2\phi, v)_{L^2\Lambda^k} + (a_4 g, v)_{L^2\Lambda^k} \\ &\leq (\|a_2\|_{L^\infty}\|\phi\|_{L^2\Lambda^k} + \|a_4\|_{L^\infty}\|g\|_{L^2\Lambda^k})\|v\|_{L^2\Lambda^k}.\end{aligned}$$

Thus, we can represent this functional as an element of $L^2\Lambda^k$; explicitly, $\partial_2\mathscr{L}(j^1_d\phi) = a_2\phi + a_4 g$. Similarly, $w \in L^2\Lambda^{k+1} \mapsto \int_X \delta_3\mathscr{L}(j^1_d\phi)\cdot w = \int_X (a_1 d\phi + a_3 f)\wedge *w$ is bounded and $\partial_3\mathscr{L}(j^1_d\phi) = a_1 d\phi + a_3 f$.

One can also consider nonlinearities, given sufficient control on the nonlinearity. For example, with $k = 0$ (for simplicity; one could consider $k \geq 1$ with the nonlinearities acting on the components of ϕ), consider a Lagrangian density which contains a term of the form $V(\phi)\, d^{n+1}x$, where $V \in C^1(\mathbb{R},\mathbb{R})$ has bounded derivative $V' \in L^\infty(\mathbb{R},\mathbb{R})$. The variation of this *term in the associated action gives the linear functional*

$$v \in L^2 \mapsto \int_X V'(\phi) v \, d^{n+1}x.$$

Since the domain X is bounded, we have the continuous embedding $L^2 \hookrightarrow L^1$ with $\|v\|_{L^1} \le C\|v\|_{L^2}$. Hence, the above linear functional is bounded, since

$$\left| \int_X V'(\phi) v \, d^{n+1}x \right| \le \|V'\|_{L^\infty} \|v\|_{L^1} \le C\|V'\|_{L^\infty} \|v\|_{L^2}.$$

An example of such a nonlinearity occurs in the sine–Gordon Lagrangian density, which contains a term of the form $V(\phi)\, d^{n+1}x = \cos(\phi)\, d^{n+1}x$.

We now define a weak analogue of the Cartan form (1.1), relative to a region $U \subset X$. If we only assume $H\Lambda$ regularity on the fields and variations, we define the weak Cartan form, at a solution of the weak Euler–Lagrange equations, to be the variation of the action

$$\Theta_U(\phi) \cdot v \equiv dS[\phi] \cdot v;$$

note that this is in general nonzero since we are not assuming that v has vanishing trace on the boundary. In some sense, the weak Cartan form encodes the contribution of the boundary term to the variation of the action. To see this explicitly, we need to assume higher regularity.

To make sense of such a boundary term, we require higher regularity, at least locally on U; namely, since the trace acts as a bounded operator $\mathrm{Tr} : H\Lambda^m(U) \to H^{-1/2}\Lambda^m(\partial U)$ ([7]) and as a bounded operator $\mathrm{Tr} : H^1\Lambda^m(U) \to H^{1/2}\Lambda^m(\partial U)$, the solution ϕ and the Lagrangian have to have enough regularity so that $\partial_3 \mathscr{L}(j^1_d \phi)$ is in $H^1\Lambda^{k+1}(U)$. For example, in the first class of Lagrangians discussed in Remark 1.2.1, if the solution ϕ has H^2 regularity and the given f has H^1 regularity, then this is satisfied. Assuming this higher regularity, the weak Cartan form is defined to be the boundary term which arises for a variation v with generally nonzero boundary trace. That is,

$$\Theta_U(\phi)\cdot v \equiv \int_{\partial U} v \wedge *\partial_3 \mathscr{L}(j^1_d\phi). \tag{2.2}$$

We refer to this as the weak Cartan form since it involves integration, whereas (in the smooth setting) the Cartan form is the integrand of the above expression. With this definition, the variation of the action with respect to $v \in H\Lambda^k$ can be expressed

$$\delta S[\phi]\cdot v = \mathrm{EL}(\phi)\cdot v + \Theta(\phi)\cdot v,$$

where $\mathrm{EL}(\phi)\cdot v \equiv (\partial_2\mathscr{L}(j^1_d\phi), v)_{L^2\Lambda^k} + (d^*\partial_3\mathscr{L}(j^1_d\phi), v)_{L^2\Lambda^k}$ is the weak Euler–Lagrange form which, by definition, vanishes for a solution ϕ of the weak Euler–Lagrange equations.

It will also be useful to think of variations as vector fields over the configuration space. With the identification $T(H\Lambda^k) \cong H\Lambda^k \times H\Lambda^k$, we can view a vector field $V \in \mathfrak{X}(H\Lambda^k)$ as a map $V : H\Lambda^k \to H\Lambda^k$. Thus, we define the weak Cartan form and weak Euler–Lagrange form, acting on vector fields, as

$$\boldsymbol{\Theta}(\phi)\cdot V \equiv \Theta(\phi)\cdot V(\phi),$$
$$\mathbf{EL}(\phi)\cdot V \equiv \mathrm{EL}(\phi)\cdot V(\phi).$$

The variation of the action with respect to V can then be expressed $dS[\phi]\cdot V = \mathbf{EL}(\phi)\cdot V + \boldsymbol{\Theta}(\phi)\cdot V$. With the above notation, we now derive weak analogues of the multisymplectic form formula and Noether's theorem.

Weak Multisymplectic Form Formula. Let V, W be first variations of a solution ϕ of the weak Euler–Lagrange equations, i.e., their respective flows on ϕ still satisfy the weak Euler–Lagrange equation. Then, one has the weak multisymplectic form formula

$$d\Theta(\phi)\cdot(V,W) = 0. \tag{2.3}$$

The proof follows from $d^2S(\phi)\cdot(V,W)=0$. We will perform the proof in the discrete setting in Theorem 1.2.1, where the computation is analogous.

Weak Noether's Theorem. Suppose there is a Lie group action of a Lie group G on $H\Lambda^k$, which we denote by $g\cdot\phi$ for $g\in G, \phi\in H\Lambda^k$. For a Lie algebra element $\xi\in \mathrm{Lie}(G)$, we denote by $\widetilde{\xi}$ its associated infinitesimal generator, which is a vector field on $H\Lambda^k$ defined by

$$\widetilde{\xi}(\phi)=\lim_{t\to 0}\frac{e^{t\xi}\cdot\phi-\phi}{t}.$$

Furthermore, suppose that the action $S_U : H\Lambda^k\to\mathbb{R}$ is G-invariant for any region $U\subset X$, i.e., $S_U[g\cdot\phi]=S[\phi]$ for all $g\in G,\phi\in H\Lambda^k$. Thus, $S_U[e^{t\xi}\cdot\phi]=S_U[\phi]$ for all $\xi\in\mathrm{Lie}(G)$. By differentiating, this gives the expression

$$dS_U[\phi]\cdot\widetilde{\xi}=0 \text{ for all } \xi\in\mathrm{Lie}(G).$$

Explicitly, one has

$$\begin{aligned}0=dS_U[\phi]\cdot\widetilde{\xi}&=(\partial_2\mathscr{L}(j^1_d\phi),\widetilde{\xi}(\phi))_{L^2\Lambda^k(U)}+(\partial_3\mathscr{L}(j^1_d\phi),d\widetilde{\xi}(\phi))_{L^2\Lambda^{k+1}(U)}\\&=(\partial_2\mathscr{L}(j^1_d\phi),\widetilde{\xi}(\phi))_{L^2\Lambda^k}+(d^*\partial_3\mathscr{L}(j^1_d\phi),\widetilde{\xi}(\phi))_{L^2\Lambda^{k+1}(U)}+\int_{\partial U}\widetilde{\xi}(\phi)\wedge\star\partial_3\mathscr{L}(j^1_d\phi).\end{aligned}$$

The first two terms in the second line above vanish by the weak Euler–Lagrange equation, so that

$$0=\int_{\partial U}\widetilde{\xi}(\phi)\wedge\star\partial_3\mathscr{L}(j^1_d\phi)=\Theta_U(\phi)\cdot\widetilde{\xi}.$$

Thus, Noether's theorem in the weak setting states that the integrated Cartan form paired with an infinitesimal generator of a G action vanishes, $\Theta_U(\phi)\cdot\widetilde{\xi}=0$, if the action is G-invariant. In the smooth setting, by applying Stokes' theorem and noting that U is arbitrary, one has the stronger statement that the exterior derivative of the integrand above vanishes (Marsden et al. [85]).

1.2.2 Variational Discretization

To formulate a discrete variational principle, let $\{\Lambda_h^m\}_{m=0}^{n+1}$ be a subcomplex of finite element spaces approximating $\{H\Lambda\}$ with projections $\pi_h^m : H\Lambda^m \to \Lambda_h^m$. This provides an approximation of $J^1_{H\Lambda^k} = H\Lambda^k \times dH\Lambda^k$ by $\pi_h^k H\Lambda^k \times \pi_h^{k+1}(dH\Lambda^k)$. Consider the degenerate Lagrangian density $\mathscr{L}_h : J^1_{H\Lambda^k} \to \Omega^{n+1}(X)$, $\mathscr{L}_h(j^1_d\phi) \equiv \mathscr{L}(x, \pi_h^k\phi, \pi_h^{k+1}d\phi)$ and the associated degenerate action $S_h : H\Lambda^k \to \mathbb{R}$ defined by

$$S_h[\phi] = \int_X \mathscr{L}(x, \pi_h^k\phi, \pi_h^{k+1}d\phi). \tag{2.4}$$

We refer to these as degenerate since the projections have nontrivial kernels, as projections from infinite-dimensional spaces to finite-dimensional subspaces.

The variational principle associated to the degenerate action S_h is to find $\phi \in H\Lambda^k$ such that

$$0 = \delta S_h[\phi]\cdot v = (\partial_2\mathscr{L}_h(j^1_d\phi), \pi_h^k v)_{L^2\Lambda^k} + (\partial_3\mathscr{L}_h(j^1_d\phi), \pi_h^{k+1}dv)_{L^2\Lambda^{k+1}}, \text{ for all } v \in \mathring{H}\Lambda^k. \tag{2.5}$$

The issue with (2.5) is that the in the second term on the right hand side, the projection $\pi_h^{k+1}dv$ occurs after taking the exterior derivative, so one cannot in general integrate by parts to obtain a boundary term, which is necessary in the continuous theory to define the Cartan form (which, recall, is defined to be the boundary term induced by a variation which does not vanish on the boundary).

On the other hand, one can produce the desired boundary term if one instead utilizes a different degenerate action defined by $\widetilde{S}_h \equiv S \circ \pi_h^k$,

$$\widetilde{S}_h[\phi] = \int_X \mathscr{L}(x, \pi_h^k\phi, d\pi_h^k\phi), \tag{2.6}$$

since the associated variational principle is to find $\phi \in H\Lambda^k$ such that

$$\begin{aligned} 0 &= \delta\widetilde{S}_h[\phi] \\ &= (\partial_2\mathscr{L}(x,\pi_h^k\phi,d\pi_h^k\phi),\pi_h^k v)_{L^2\Lambda^k} + (\partial_3\mathscr{L}(x,\pi_h^k\phi,d\pi_h^k\phi),d\pi_h^k v)_{L^2\Lambda^k}, \text{ for all } v \in \mathring{H}\Lambda^k. \end{aligned} \tag{2.7}$$

One can now integrate by parts in the second term, since the exterior derivative is taken after the projection. However, the issue with the latter degenerate action, $\widetilde{S}_h$, is that there is in general no associated degenerate Lagrangian density, i.e., there is in general no map $\widetilde{\mathscr{L}_h}$: $J^1_{H\Lambda^k} \to \Omega^{n+1}(X)$ such that $\widetilde{\mathscr{L}_h}(j^1_d\phi) = \mathscr{L}(x,\pi_h^k\phi,d\pi_h^k\phi)$. One would want there to be an associated degenerate Lagrangian density, in order to compare to the continuous theory, e.g., when examining convergence.

Thus, the degenerate action S_h has the issue that one cannot in general extract a boundary term in the variation, whereas the degenerate action $\widetilde{S}_h$ has the issue that one cannot in general associate to it a degenerate Lagrangian density. Both of these issues are resolved with the assumption that the projections commute with the exterior derivative, $\pi_h^{k+1}d\phi = d\pi_h^k\phi$, since then $\widetilde{S}_h = S_h$. We will henceforth assume this through the paper.

Assumption 1.2.1 (Cochain Projections)**.** *The projections $\pi_h^m : H\Lambda^m \to \Lambda_h^m$ are cochain projections, i.e., $\pi_h^{k+1}d = d\pi_h^k$.*

Furthermore, we will generally denote the projections as π_h, where the degree of the differential forms that they act on are suppressed for notational convenience.

With this assumption, the two variational principles (2.5) and (2.7) are equivalent. However, even ignoring issues of degeneracy of the Lagrangian density itself, e.g., due to gauge freedom, these equivalent variational principles are underdetermined due to the nontrivial kernels of the projections. As such, the action is constant on fibers of the projection, which corresponds to a symmetry of the action. Thus, instead of enforcing the variational principle over the full field space, the finite-dimensional reduction to the problem is given by enforcing the variational principle over the discrete space: find $\phi \in \Lambda_h^k$ such that $\delta S[\phi] \cdot v = 0$ for all $v \in \Lambda_h^k$ with vanishing trace on the boundary; we denote the space of such v by $\mathring{\Lambda}_h^k$. The variational principle thus yields a discrete weak form of the Euler–Lagrange equation: find $\phi \in \Lambda_h^k$ such that

$$0 = \delta S[\phi] \cdot v = \big(\partial_2 \mathscr{L}(j_d^1 \phi), v\big)_{L^2\Lambda^k} + \big(\partial_3 \mathscr{L}(j_d^1 \phi), dv\big)_{L^2\Lambda^{k+1}}, \text{ for all } v \in \mathring{\Lambda}_h^k. \tag{2.8}$$

Integrating by parts, this gives

$$0 = \big(\partial_2 \mathscr{L}(j_d^1 \phi), v\big)_{L^2\Lambda^k} + \big(d^* \partial_3 \mathscr{L}(j_d^1 \phi), v\big)_{L^2\Lambda^k} + \int_{\partial X} v \wedge * \partial_3 \mathscr{L}(j_d^1 \phi), \text{ for all } v \in \mathring{\Lambda}_h^k, \tag{2.9}$$

where the codifferential d^* is interpreted in the weak sense. Note the boundary term vanishes since $v \in \mathring{\Lambda}_h^k$, but we include it explicitly since it will be necessary in the formulation of the multisymplectic form formula and Noether's theorem, where one generally has nonzero variations on the boundary.

We refer to these equivalent equations, (2.8) and (2.9), as the discrete Euler–Lagrange equations (DEL). Fixing a basis of shape functions $\{v_i\}$ for $\mathring{\Lambda}_h^k$, expressing $\phi = \phi^j v_j$, and choosing $v = v_i$, (2.8) is equivalent to a (generally nonlinear) system of equations for the unknown components ϕ^i. Letting $[i]$ denote the set of indices j such that $\operatorname{supp}(v_j) \cap \operatorname{supp}(v_i)$ has positive measure, the system of equations can be written as

$$\big(\partial_2 \mathscr{L}(j_d^1(\sum_{j\in[i]} \phi^j v_j)), v_i\big)_{L^2\Lambda^k} + \big(\partial_3 \mathscr{L}(j_d^1(\sum_{j\in[i]} \phi^j v_j)), dv_i\big)_{L^2\Lambda^{k+1}} = 0, \; i = 1, \dots, \dim \mathring{\Lambda}_h^k.$$

In order to provide local statements of the multisymplectic form formula and Noether's theorem, we now localize the DEL. For a region $U \subset X$, we say that a node i is an interior point of U if U contains all simplices touching i. Denote $\bar{U}$ as the union of all simplices touching interior nodes i of U; we say that U is regular if $U = \bar{U}$. We define the admissible variations with respect to a regular region U as the space of all $v \in \mathring{\Lambda}_h^k$ such that $v|_U \in \mathring{\Lambda}_h^k(U)$. We define the localized action $S_U[\phi] = \int_U \mathscr{L}(j^1_d\phi)$ and the associated localized DEL,

$$\begin{aligned} 0 = \delta S_U[\phi]\cdot v &= \big(\partial_2\mathscr{L}(j^1_d\phi), v\big)_{L^2\Lambda^k(U)} + \big(\partial_3\mathscr{L}(j^1_d\phi), dv\big)_{L^2\Lambda^{k+1}(U)} \\ &= \big(\partial_2\mathscr{L}(j^1_d\phi), v\big)_{L^2\Lambda^k(U)} + \big(d^*\partial_3\mathscr{L}(j^1_d\phi), v\big)_{L^2\Lambda^k(U)} + \int_{\partial U} v\wedge *\partial_3\mathscr{L}(j^1_d\phi), \end{aligned} \tag{2.10}$$

which is enforced for all regular U and admissible v. As before, the boundary term vanishes for admissible v, but we write it explicitly as it will arise later.

Proposition 1.2.1. *The localized DEL (2.10), ranging over all regular U and admissible v, are equivalent to the DEL (2.9).*

Proof. To see that the localized DEL imply the DEL, choose $U = X$ which is trivially regular; the space of admissible variations with respect to X is then just $\mathring{\Lambda}^k_h$. To see that the DEL imply the localized DEL, let U be regular and v be admissible. Since $\text{supp}(v) \subset U$, the integrals over X in the DEL can be replaced by integrals over U. □

In this section, we aim to elucidate the variational structure that arises from discretizing the variational principle utilizing cochain projections. Recalling that the Cartan form (1.1) encodes the variational structure of a Lagrangian field theory, we will construct a discrete analogue of the Cartan form, which will naturally encode the variational structure of the discretized theory.

We first show that the restricted variational principle over the finite-dimensional subspace $\mathring{\Lambda}^k_h$ can be interpreted as a Galerkin variational integrator. Restricting the configuration space to $\mathring{\Lambda}^k_h$, we can view the action as a function of the components ϕ^i in the expansion $\phi = \phi^i v_i$.

$$S[\phi^i] = \int \mathscr{L}(x, \phi^i v_i, \phi^i dv_i).$$

Taking the variation of S with respect to ϕ^j,

$$\begin{aligned}\frac{\delta S[\phi^i]}{\delta \phi^j} &= \int \Big(\frac{\delta \mathscr{L}}{\delta \phi} \cdot \frac{\delta(\phi^i v_i)}{\delta \phi^j} + \frac{\delta \mathscr{L}}{\delta(d\phi)} \cdot \frac{\delta(\phi^i dv_i)}{\delta \phi^j} \Big) = \int \Big(\frac{\delta \mathscr{L}}{\delta \phi} \cdot v_j + \frac{\delta \mathscr{L}}{\delta(d\phi)} \cdot dv_j \Big) \\ &= (\partial_2 \mathscr{L}, v_j) + (\partial_3 \mathscr{L}, dv_j),\end{aligned}$$

which shows that the conditions $\delta S/\delta \phi^j = 0$ is equivalent to the DEL (2.9). Similarly, the localized DEL (2.10) is equivalent to the conditions $\delta S_U/\delta \phi^j = 0$ for all interior nodes j. That is, the DEL can be interpreted as a Galerkin variational integrator. From this viewpoint of the DEL, we see that given appropriate choices of function spaces (and possibly a choice of quadrature rule), our discrete Euler–Lagrange equation reproduces multisymplectic variational integrators based on finite differences or nodal value finite element spaces (e.g., as discussed in Marsden et al. [85] and Chen [30]). However, the discrete variational principle in the form $\delta S[\phi] \cdot v = 0$, for $\phi \in \Lambda_h^k$ and $v \in \mathring{\Lambda}_h^k$, is expressed explicitly at the level of function spaces and hence, will allow us to examine the discrete variational structure more directly. Along with allowing more general approximating finite element spaces, this also has the advantage of stating properties of the discrete variational principle at the level of function spaces. Consequently, as we will see, properties such as multisymplecticity and Noether's theorem can be stated in a geometric way, which makes no explicit reference to finite differencing or quadrature.

By the above, we can view the Lagrangian structure associated to the equations (2.8) as the restriction of the full Lagrangian structure to the discrete space. The next natural question to ask would be: is there some sense in which the discrete equations, which arises as a restriction of the variational principle, can instead be viewed as a variational principle on the full configuration bundle? Since we assume that the projection maps $\pi_h : H\Lambda^m \to \Lambda_h^m$ are cochain projections on the Hilbert de Rham complex, there is a natural relation between the dynamics of the restricted Lagrangian structure and variations on the full space of the degenerate Lagrangian. To see this, recall that we view the Lagrangian density as a map on the space of sections, $\mathscr{L} : J^1_{H\Lambda^k} \to \Omega^{n+1}(X)$. Furthermore, recall the degenerate Lagrangian density, $\mathscr{L}_h : J^1_{H\Lambda^k} \to \Omega^{n+1}(X)$ given by $\mathscr{L}_h(j^1_d\phi) = \mathscr{L}(x, \pi_h\phi, \pi_h d\phi)$ with associated degenerate action $S_h[\phi] = \int_X \mathscr{L}_h(j^1_d\phi)$. In the case of a cochain projection, we can then view the variations of S restricted to Λ^k_h as variations of S_h on the full configuration bundle.

Proposition 1.2.2. ***(Naturality of Discrete Variational Structure)***

The restricted variational structures are related to the degenerate variational structures by

$$\mathscr{L}(j^1_d\pi_h\phi) = \mathscr{L}_h(j^1_d\phi), \tag{2.11}$$

$$\delta S[\pi_h\phi] \cdot \pi_h v = \delta S_h[\phi] \cdot v, \tag{2.12}$$

for $\phi \in H\Lambda^k$ and $v \in H\Lambda^k$.

Proof. For (2.11), since π_h is a cochain projection,

$$\mathscr{L}(j^1_d\pi_h\phi) = \mathscr{L}(x, \pi_h\phi, d\pi_h\phi) = \mathscr{L}(x, \pi_h\phi, \pi_h d\phi) = \mathscr{L}_h(x, \phi, d\phi) = \mathscr{L}_h(j^1_d\phi).$$

Thus, it follows that $S[\pi_h\phi] = S_h[\phi]$.

Then, (2.12) follows similarly using the cochain property,

$$\begin{aligned} \delta S[\pi_h\phi] \cdot \pi_h v = \frac{d}{d\varepsilon}\Big|_{\varepsilon=0} S[\pi_h\phi + \varepsilon\pi_h v)] &= \frac{d}{d\varepsilon}\Big|_{\varepsilon=0} S[\pi_h(\phi + \varepsilon v)] \\ = \frac{d}{d\varepsilon}\Big|_{\varepsilon=0} S_h[\phi + \varepsilon v] &= \delta S_h[\phi] \cdot v. \end{aligned}$$

□

Remark 1.2.2. *The above proposition is subtle, in that there are two degenerate actions that one could define, recalling S_h and $\widetilde{S}_h$ defined by* (2.5) *and* (2.7)*, respectively. which are both maps from $H\Lambda^k \to \mathbb{R}$. As discussed previously, the latter is not, without the cochain projection assumption, holonomic in the sense that it does not implicitly depend on ϕ through its exterior jet extension, $j^1_d\phi = (x, \phi, d\phi)$, while the former is. Thus, the former degenerate action is the* *more suitable degenerate action when comparing the discrete theory to the continuous theory, due to its holonomic dependence on $j^1_d\phi$. On other hand, as previously remarked, the former action has the issue that, without the cochain property, one cannot make sense of a boundary term in the variation (which we will need to make sense of a discrete Cartan form), whereas one can in the latter. Assuming a cochain projection, these respective issues of the two degenerate actions are both solved simultaneously, since $S_h = S \circ \pi_h$.*

The naturality equations (2.11) and (2.12) reveal that the process of discretization of the variational principle, i.e., by restricting the action and its variations to a finite-dimensional subspace, with the assumption of cochain projections for discretization, is itself associated to an action which arises from a holonomic Lagrangian density on the full field space. Simply put, the discretization is compatible with the structure of a Lagrangian theory. A corollary is that equation (2.8) can be seen as either arising from the discrete variation of the full action S at a discrete field $\pi_h\phi$, or as from the full variation of the discrete action S_h at the full field ϕ. This shows that the variations associated to S_h on the full field space are degenerate, since they are equivalently given by the variations of S on the projected space. Thus, the finite-dimensionality of the restricted variational principle on S can be interpreted as the degeneracy of the variational principle of S_h on the full space, where two fields are equivalent if their difference is in $\ker(\pi_h)$. In other words, our finite-dimensional variational problem on the discrete space arises as a degenerate (symmetric) variational problem over the infinite-dimensional space, where the set of equivalence classes forms a finite-dimensional space, with the canonical representative $i_h\pi_h\phi$ for the equivalence class of ϕ, where $i_h : \Lambda^k_h \hookrightarrow H\Lambda^k$ is the inclusion map.

Furthermore, the above naturality relation shows that projecting the equations obtained from the variational principle applied to the continuum action is equivalent to first discretizing the action through the projection and subsequently applying the variational principle. Thus, when discretizing via cochain projections, the variational principle and discretization commute:

$$\begin{array}{ccc} S : H\Lambda^k \to \mathbb{R} & \xrightarrow{\text{Discretize}} & S_h : \Lambda_h^k \to \mathbb{R} \\ \Big\downarrow {\scriptstyle \text{Variational Principle}} & & \Big\downarrow {\scriptstyle \text{Variational Principle}} \\ \text{Weak EL} & \xrightarrow{\text{Discretize}} & \text{Discrete EL}\,. \end{array}$$

This generalizes the result of Leok [73] where it was shown that discretization via discrete exterior calculus and the variational principle commute in the case of electromagnetism. In particular, the result of Leok [73] follows from the above, since one can view discrete exterior calculus in the framework of finite element exterior calculus as a particular low-order example; namely, through the use of Whitney forms.

As a final remark on the above naturality relation, a more fundamental issue for discretization is whether one should discretize at the level of the configuration bundle or the jet bundle. One can discretize the field first via $\phi \mapsto \pi_h \phi$ and take the argument of the Lagrangian density to be $j^1_d \pi_h \phi = (x, \pi_h \phi, d\pi_h \phi)$, or one can take the argument of the Lagrangian density to be $(x, \pi_h \phi, \pi_h d\phi)$; in general, these methods are not equivalent. However, in the case of cochain projections, these two discretization processes are equivalent, i.e., the following diagram commutes

$$\begin{array}{ccc} \phi & \xmapsto{\pi_h^k} & \pi_h \phi \\ \Big\downarrow {\scriptstyle j^1_d} & & \Big\downarrow {\scriptstyle j^1_d} \\ j^1 \phi & \xmapsto{\pi_h^k \times \pi_h^{k+1}} & j^1_d(\pi_h \phi), \end{array}$$

so there is no ambiguity as to which discretization procedure to use. Furthermore, regarding Assumption 1.2.1, the above diagram shows that we only need the existence of the space Λ_h^{k+1} and the projection π_h^{k+1} such that the above diagram commutes and thus, one can perform the discretization solely using Λ_h^k and π_h^k, without reference or implementation of Λ_h^{k+1} and π_h^{k+1}. In particular, as discussed in, for example, Arnold et al. [7, 8] and Arnold [6], there is a large class of classical finite element spaces for which such cochain projections exist, so the discussion is broadly applicable.

In order to state discrete analogues of the multisymplectic form formula and Noether's theorem, we will have to consider variations with nonzero boundary trace with respect to a regular region U. To do this, let U be a regular region and let $v \in \Lambda^k_h$, and consider v restricted to U. In general, since we no longer assume that v is an admissible variation relative to U, v may have nonzero trace along ∂U. Decompose $v = v_\partial + v_{in}$ where v_∂ denotes the boundary component of v consisting of the expansion of v with respect to all shape functions which have nonzero trace on ∂U and $v_{in} = v - v_\partial$ corresponds to the expansion of v into shape functions with vanishing trace on the boundary. Let $\mathscr{T}[\partial U]$ denote the set of all top-dimensional elements in $\mathscr{T}_h$ on which shape functions with nonvanishing trace on ∂U are supported.

Remark 1.2.3. *If one considers Lagrange polynomial nodal shape functions (corresponding to point value degrees of freedom), then the shape functions which are nonzero on the boundary are those associated to the nodes on ∂U. In this case, $\mathscr{T}[\partial U]$ consists of those top-dimensional elements touching the boundary, i.e., the one-ring of the boundary ∂U. For general (local) shape functions, internal nodes may give rise to shape functions which are nonzero on the boundary, so $\mathscr{T}[\partial U]$ will generally consist of the elements touching ∂U and the elements touching those elements, i.e., the two-ring of the boundary ∂U. In any case, we consider discretization by the finite element method due to the local support property of the shape functions, which will allow the discrete Cartan form defined below to be localized on $\mathscr{T}[\partial U]$.*

We can now consider variations with nonvanishing trace on ∂U. In particular, we compute for a solution ϕ_h of the discrete Euler–Lagrange equation and for a variation v,

$$\delta S_U[\phi_h] \cdot v = \sum_{T \in \mathscr{T}[\partial U]} \int_T (\partial_2 \mathscr{L}(j^1\phi_h) \wedge * v_\partial + \partial_3 \mathscr{L}(j^1\phi_h) \wedge \star dv_\partial) = \delta S_U[\phi_h] \cdot v_\partial,$$

i.e., for a solution of the DEL, $\delta S_U[\phi_h] \cdot v = \delta S_U[\phi_h] \cdot v_\partial$, since $\delta S_U[\phi_h] \cdot v_{in} = 0$ by the DEL.

This boundary variation formula will be our candidate for a discrete weak Cartan form, as it encodes the contribution to the action from V nonvanishing on and near the boundary, and will allow us to state discrete analogues of the multisymplectic form formula and Noether's theorem. We refer to it as "weak", since its definition involves integration and it is not a pointwise-defined quantity. Note that, unlike the weak Cartan form (2.2), which required the higher regularity assumption $\partial_3\mathscr{L}(j^1_d\phi) \in H^1$, the above makes sense even when $\phi, v \in H\Lambda^k$. However, if the finite element subspace does have enough regularity to make sense of the pairing of the traces on the boundary, the above can be rewritten as

$$\delta S_U[\phi_h]\cdot v = \int_{\partial U} v \wedge *\partial_3\mathscr{L}(j^1\phi_h) + \sum_{T\in\mathscr{T}[\partial U]}\int_T (\partial_2\mathscr{L}(j^1\phi_h) + d^*\partial_3\mathscr{L}(j^1\phi_h)) \wedge \star v_\partial.$$

Definition 1.2.1 (Discrete Weak Cartan Form)**.** *The discrete weak Cartan form on a regular region U, evaluated at a field $\phi \in \Lambda^k_h$ and a variation v, is defined by*

$$\Theta^h_U(\phi)\cdot v \equiv \delta S_U[\phi]\cdot v_\partial. \tag{2.13}$$

Remark 1.2.4. *Analogous to our discussion of the weak Cartan form in Section 1.2.1, we can instead think of the discrete weak Cartan form as acting on vector fields. We make identification $T\Lambda^k_h \cong \Lambda^k_h \times \Lambda^k_h$, so that a vector field can be viewed as a map $V : \Lambda^k_h \to \Lambda^k_h$. Hence, the action of the discrete weak Cartan form on V can be expressed as*

$$\boldsymbol{\Theta}^h_U(\phi)\cdot V = \Theta^h_U(\phi)\cdot V(\phi).$$

This identification will be useful when we prove the discrete multisymplectic form formula, since we will view first variations as vector fields on Λ^k_h whose flow preserves the DEL.

Even though the weak Cartan form only involves integration on ∂U whereas the discrete weak Cartan form involves integration on ∂U and over regions $T \in \mathscr{T}[\partial U]$, this is the appropriate definition in the discrete setting because it encodes the boundary variation of the action, i.e., it equals the variation of the action when the discrete Euler–Lagrange equations are imposed.

Remark 1.2.5 (Quadrature)**.** *Although, in our exposition, we have assumed that with the given Lagrangian and choice of finite element space, one can evaluate the integrals involved exactly, one can more generally utilize quadrature to approximate the action before enforcing the variational principle. For a regular region U, let us consider quadrature nodes $\{c_a \in U\}$ and associated quadrature weights $\{b_a\}$. With finite element shape functions $\{v_j\}$ and expressing the density as $\mathscr{L} = Ld^{n+1}x$, the associated discrete action is given by applying quadrature,*

$$\mathbb{S}_U[\{\phi^j\}] = \sum_a b_a L(j^1_d(\phi^i v_i))|_{c_a}. \tag{2.14}$$

The variation in the direction $w = w^k v_k$ is given by

$$\delta \mathbb{S}_U[\{\phi^j\}] \cdot \{w^k\} = \sum_a b_a \frac{\partial}{\partial \phi^k} \Big[L(j^1_d(\phi^i v_i))\big|_{c_a} \Big] w^k. \tag{2.15}$$

The associated discrete Euler–Lagrange equation is given by enforcing the variational principle for variations w with vanishing trace on ∂U. Then, the discrete Cartan form with quadrature (at a solution of the discrete Euler–Lagrange equation), is defined by taking an arbitrary variation and removing the term on the interior which vanishes by the discrete Euler–Lagrange equation. In particular, it is given by summing over all a such that c_a is contained in the support of some shape function with nonvanishing trace on the boundary; we denote the set of all such a by $\mathscr{I}[\partial U]$. Hence, the discrete Cartan form with quadrature is given by

$$\Theta^h_U(\phi) \cdot w = \sum_{a \in \mathscr{I}[\partial U]} b_a \frac{\partial}{\partial \phi^k} \Big[L(j^1_d(\phi^i v_i))\big|_{c_a} \Big] w^k.$$

Using this discrete Cartan form, an analogous statement of discrete multisymplecticity that we state below holds in this setting, with the caveat that the first variations are defined *relative to the discrete Euler–Lagrange equations with quadrature. Similarly, an analogous statement to the discrete Noether's theorem below also holds in this setting, with the caveat that the group action leaves the discrete action with quadrature, equation (2.14), invariant. This is a direct consequence of the fact that the formulation with quadrature is still variational, since we applied the quadrature rule to the action, before enforcing the variational principle (see Section 1.2.5). In general, if one applies quadrature after enforcing the variational principle, i.e., to the equations of motion (2.9), the system is not variational. To see this, we compute the variation of the action first,*

$$\delta S_U[\phi^j v_j]\cdot(w^k v_k) = \int_X [\partial_2 \mathscr{L}(j_d^1(\phi^i v_i)) + d^*\partial_3 \mathscr{L}(j_d^1(\phi^i v_i))] \wedge \star w^k v_k,$$

(for w with vanishing trace on ∂U) and subsequently apply quadrature, so that the above becomes

$$\sum_a b_a \Big[* \Big([\partial_2 \mathscr{L}(j_d^1(\phi^i v_i)) + d^*\partial_3 \mathscr{L}(j_d^1(\phi^i v_i))] \wedge \star w^k v_k \Big) \Big] \Big|_{c_a}.$$

In general, this is not equal to (2.15), except when ϕ a scalar field, using nodal interpolating shape functions and quadrature points at those nodes, in which case they are the same. Thus, for a variational formulation, one should generally apply quadrature before enforcing the variational principle. For the rest of the paper, we will revert to the assumption that one can evaluate the various integrals exactly, but keeping in mind that similar results hold in the case of quadrature.

We make several additional remarks regarding this candidate (2.13) for a discrete Cartan form. We defined the discrete Cartan form as the variation of the action, for variations that may be nonvanishing on the boundary, at a solution of the discrete Euler–Lagrange equations. Even though this functional involves integration over top-dimensional regions $T \in \mathscr{T}[\partial U]$, it only depends on the degrees of freedom which contribute to the nonzero value of V on ∂U and so makes sense as a candidate for a discrete Cartan form. In the continuum variational problem, boundary variations can be supported arbitrarily close to ∂U, whereas in the finite element variational problem, this is not the case, so the discrete Cartan form, which encodes the contribution of the variation of the action by boundary variations, should indeed contain the additional terms involving integration over the elements of $\mathscr{T}[\partial U]$. These terms shrink relative to the integral over ∂U in the following heuristic sense. The terms involving $\mathscr{T}[\partial U]$ are $O(h)$ smaller than the term over ∂U: the cardinality of $\mathscr{T}[\partial U]$ scales like the number of boundary faces in ∂U, which is $O(h^{-n})$; on the other hand, the size of T is $O(h^{n+1})$, so the terms in the discrete Cartan form involving the sum over $\mathscr{T}[\partial U]$ is $O(h)$, whereas the first term is $O(1)$ for a fixed region U. Thus, as $h \to 0$, for a fixed region U, the Cartan form formally only involves the first contribution, as expected. In other words, as we refine the mesh, ∂U stays (roughly) the same, while the region containing only elements touching ∂U shrinks, and a similar remark applies to the discrete multisymplectic form formula and the additional terms involving the sum over $\mathscr{T}[\partial U]$, so that the multisymplectic form formula is formally recovered in the limit. This can be combined with bounds on the integrands to show convergence more rigorously. More precisely, to show that the discrete weak Cartan form converges to the weak Cartan form, we would aim to show that for a solution ϕ_h of the DEL and a solution ϕ of the weak Euler–Lagrange equations and a variation v,

$$\left|\Theta_U^h(\phi_h) \cdot \pi_h v - \Theta_U(\phi) \cdot v\right| \to 0,$$

as $h \to 0^+$. This error can be decomposed as

$$\begin{aligned}\left|\Theta_U^h(\phi_h) \cdot \pi_h v - \Theta_U(\phi) \cdot v\right| \leq &\left|\left(\Theta_U^h(\phi_h) - \Theta_U^h(\pi_h \phi)\right) \cdot \pi_h v\right| \\ &+ \left|\Theta_U(\phi) \cdot (v - \pi_h v)\right| + \left|\left(\Theta_U(\phi) - \Theta_U^h(\pi_h \phi)\right) \cdot \pi_h v\right|.\end{aligned}$$

The first term on the right hand side can be shown to converge with an appropriate quasi-optimatility bound between the discrete solution ϕ_h and the projected weak solution $\pi_h \phi$, and assuming the projection π_h is bounded. The second term can be shown to converge if $\|v - \pi_h v\|$

converges in some appropriate norm. The third term can be shown to converge with an appropriate quasi-optimality bound between the projected weak solution and the weak solution, and again assuming the projection is bounded. Here, "appropriate" qualifies the fact that the above terms involve the Cartan form which is defined in terms of derivatives of the Lagrangian density and hence, will be dependent on the particular theory under consideration. We provide an example in Section 1.2.6.

We now show that Definition 2.7 recovers the notion of the discrete Cartan form introduced in Marsden et al. [85] and further examined in Chen [30], in the case that the degrees of freedom are the nodal values of the field with nodal interpolating shape functions. As previously remarked, in this case, the shape functions which are nonzero on ∂U are those associated to nodes on ∂U. Consider a single node i on ∂U and let v_i be the shape function associated to the degree of freedom on the node. Note that v_i (restricted to U) is supported in some $T_i \in \mathscr{T}[\partial U]$ and denote $F_i = \partial T_i \cap \partial U$. Consider a variation of the form $V_i v_i$ ($V_i \in \mathbb{R}$). Marsden et al. [85] and Chen [30] define the discrete Cartan form associated to this node as $\frac{\delta S_U[\phi^j v_j]}{\delta \phi^i} V_i$ (no summation over i), viewing the action as a function of the components in the expansion of $\phi = \phi^j v_j$. Then, compute

$$\begin{aligned}\frac{\delta S_U[\phi^j v_j]}{\delta \phi^i} V_i &= \int_U \Big(\frac{\delta \mathscr{L}}{\delta \phi} \cdot \frac{\delta(\phi^j v_j)}{\delta \phi^i} V_i + \frac{\delta \mathscr{L}}{\delta (d\phi)} \cdot \frac{\delta(\phi^j d v_j)}{\delta \phi^i} V_i \Big) \\ &= \int_U \Big(\frac{\delta \mathscr{L}}{\delta \phi} \cdot V_i v_i + \frac{\delta \mathscr{L}}{\delta (d\phi)} \cdot V_i d v_i \Big) = \int_U \Big(\partial_2 \mathscr{L} \wedge \star V_i v_i + \partial_3 \mathscr{L} \wedge \star V_i d v_i \Big).\end{aligned}$$

Summing over all such variations on each node on ∂U, one recovers our discrete Cartan form, equation (2.13). There are several generalizations which our discrete Cartan form makes relative to the discrete Cartan form of Marsden et al. [85] and Chen [30]. First, note that their Cartan form is defined in terms of the nodal values of the field, which implicitly suppresses the fact that the Cartan form involves integration over both ∂U and elements of $\mathscr{T}[\partial U]$. Our explicit formula for the discrete Cartan form lends itself more easily to showing convergence to the continuum Cartan form, as we sketched heuristically above and will discuss further when discussing Noether's theorem. That the discrete Cartan form involves integration over elements neighboring the boundary is inevitable, since a variation of the field value on the boundary induces changes to the field values on elements of $\mathscr{T}[U]$. Furthermore, since we allow for general finite element spaces, we immediately obtain several generalizations. First, note that the dimension of the spacetime is arbitrary in our formulation, so this discrete Cartan form holds beyond the $1+1$ spacetime dimensions that they utilize explicitly in their framework (although this is not a fundamental restriction in their theory). Furthermore, our framework allows for differential forms of arbitrary degree, as opposed to just scalar fields. In particular, the degrees of freedom associated to the boundary variations need not be nodal values, but can be determined by more general degrees of freedom, such as moments or flux type degrees of freedom, e.g., when considering a theory involving vector fields, which one can identify with $1-$forms via the metric. Furthermore, these degrees of freedom determining the boundary variations may be close to, i.e., in $\mathscr{T}[\partial U]$, but not necessarily on ∂U.

In the next two sections, we will utilize the discrete Cartan form to state discrete analogues of multisymplecticity and Noether's theorem. We will see that these statements, involving Θ_U^h, will be in direct analogy to the continuum theorems, involving Θ_U.

1.2.3 Discrete Multisymplectic Form Formula

We now state a discrete analogue of the multisymplectic form formula, which generalizes the preservation of the symplectic form under the flow of a symplectic vector field. In the smooth setting, if ϕ is a solution to the Euler–Lagrange equations and V, W are first variations at ϕ, i.e., their respective flows on ϕ are still solutions, then

$$\int_{\partial U} (j^1\phi)^* \left(j^1 V \lrcorner\, j^1 W \lrcorner\, \Omega_{\mathscr{L}} \right) = 0, \tag{2.16}$$

where $U \subset X$ is a submanifold with smooth closed boundary (Marsden et al. [85]). The multisymplectic form formula encompasses many physical conservation laws appearing in Lagrangian field theories. For example, viewing a Lagrangian field theory in the instantaneous canonical formulation, multisymplecticity gives rise to the usual field-theoretic notion of symplecticity (Marsden et al. [85]). Furthermore, multisymplecticity encompasses the notion of reciprocity in many physical systems, relating the infinitesimal perturbation of a system by a source and the associated infinitesimal perturbation of the response by the system (see, for example, Vankerschaver et al. [116] for Lorenz reciprocity in electromagnetism and McLachlan and Stern [90] for reciprocity in semilinear elliptic PDEs, within the context of multisymplecticity). Additionally, for wave propagation problems, multisymplecticity provides a geometric formulation for the conservation of wave action (Bridges [18, 19]). Since multisymplecticity is an important property of Lagrangian field theories encompassing many natural physical conservation laws, we will investigate multisymplecticity within our discretization framework.

In the literature, integrators which admit a discrete analogue of this formula are referred to as "multisymplectic integrators". We show that our discrete system (2.9) admits a discrete multisymplectic form formula. The main idea of the derivation for the multisymplectic form formula is to look at second variations of the action at ϕ with respect to first variations V and W, $d^2S[\phi]\cdot(V,W)=0$. More specifically, one decomposes the variation of the action into two functionals, corresponding to interior and boundary variations:

$$dS[\phi]\cdot V = \underbrace{-\int_U (j^1\phi)^*(j^1V \lrcorner \Omega_{\mathscr{L}})}_{\equiv \mathrm{EL}_U(\phi)\cdot V} + \underbrace{\int_{\partial U} (j^1\phi)^*(j^1V \lrcorner \Theta_{\mathscr{L}})}_{=\Theta_U(\phi)\cdot V}.$$

Then, $0=d^2S[\phi]\cdot(V,W)=d\mathrm{EL}_U(\phi)\cdot(V,W)+d\Theta_U(\phi)\cdot(V,W)$. The term $d\mathrm{EL}_U(\phi)\cdot(V,W)$ vanishes from the first variation property, so the multisymplectic form formula can be expressed as

$$d\Theta_U(\phi)\cdot(V,W)=0,$$

which is equivalent to equation (2.16).

In our construction, the first difference is that we are working in the weak setting, as discussed in Section 1.2.1. Furthermore, in the discretized theory, the main impediment for a discrete analogue of the multisymplectic form formula is that a solution of the discrete equation (2.9) does not in general satisfy an Euler–Lagrange equation locally (i.e., for arbitrary U) but rather integrated over a regular region U. Additionally, there is an additional contribution from the boundary components of the variation in the elements neighboring the boundary $T \in \mathscr{T}[\partial U]$. It is in this restricted setting that we have a discrete multisymplectic form formula.

To prepare for the proof of the discrete multisymplectic form formula, we will express variations in terms of vector fields. As briefly discussed in Remark 1.2.4, we can express the action of the Cartan form in terms of vector fields, instead of variations, which follows from the identification $T(\Lambda_h^k) \cong \Lambda_h^k \times \Lambda_h^k$ and thus, a vector field $V \in \mathfrak{X}(\Lambda_h^k)$ can be viewed as a map $V : \Lambda_h^k \to \Lambda_h^k$. Similarly, for a vector field V, the variation of the action can be expressed as

$$dS[\phi] \cdot V = \delta S[\phi] \cdot V(\phi).$$

Furthermore, we decompose a vector field into its interior and boundary components,

$$V_{in} : \phi \mapsto (V(\phi))_{in},$$
$$V_{\partial} : \phi \mapsto (V(\phi))_{\partial}.$$

Theorem 1.2.1. ***(Discrete Multisymplectic Form Formula)*** *Let U be a regular region and let ϕ_h be a solution of the local DEL (2.10) and $V, W \in \mathfrak{X}(\Lambda_h^k)$ be first variations for ϕ_h, i.e., their flow on ϕ_h still satisfies the DEL, but for arbitrary boundary variations, then*

$$d\mathbf{\Theta}_U^h(\phi_h) \cdot (V, W) = 0. \tag{2.17}$$

Proof. Decompose the variation of the action into interior and boundary variations,

$$dS_U[\phi_h]\cdot V = \underbrace{dS_U[\phi_h]\cdot V_{in}}_{\equiv \mathbf{EL}^h_U(\phi_h)\cdot V} + \underbrace{dS[\phi_h]\cdot V_\partial}_{=\mathbf{\Theta}^h_U(\phi_h)\cdot V}.$$

so that $dS[\phi_h]\cdot V = \mathbf{EL}^h_U(\phi_h)\cdot V + \mathbf{\Theta}^h_U(\phi_h)\cdot V$. Observe that, by definition of $\mathbf{EL}^h_U$, the DEL is equivalent to the statement that $\mathbf{EL}^h_U(\phi_h)\cdot V = 0$ for all $V \in \mathfrak{X}(\Lambda^k_h)$. Thus, we define a first variation W as a vector field which preserves the DEL, $d(\mathbf{EL}^h_U(\phi_h)\cdot V)\cdot W = 0$. Thus, we have

$$0 = d^2 S_U[\phi_h]\cdot(V,W) = d\mathbf{EL}^h_U(\phi_h)\cdot(V,W) + d\mathbf{\Theta}^h_U(\phi_h)\cdot(V,W).$$

Then, express

$$d\mathbf{EL}^h_U(\phi_h)\cdot(V,W) = d(\mathbf{EL}^h_U(\phi_h)\cdot V)\cdot W - d(\mathbf{EL}^h_U(\phi_h)\cdot W)\cdot V - \mathbf{EL}^h_U(\phi_h)\cdot[V,W].$$

The first two terms on the right hand side of the above equation vanish by the definition of first variation; furthermore, the third term vanishes by the DEL. Hence, $d\mathbf{EL}^h_U(\phi_h)\cdot(V,W) = 0$. Thus, we have

$$d\Theta^h_U(\phi_h)\cdot(V,W) = d^2 S_U[\phi_h]\cdot(V,W) = 0.$$

□

Remark 1.2.6. *Although we immediately see that the discrete multisymplectic form formula $d\mathbf{\Theta}^h_U(\phi_h)\cdot(V,W) = 0$ is in direct analogy with the continuum multisymplectic form formula $d\Theta_U(\phi)\cdot(V,W) = 0$, if we write the discrete formula using the definition of the discrete Cartan form, we see that there is an additional contribution corresponding to the integration over elements $T \in \mathscr{T}[\partial U]$. Although we will not write this out explicitly, we see that this additional contribution involves a sum-integral of the form $\sum_{T\in\mathscr{T}[\partial U]}\int_T$, which is $O(h)$ as discussed previously. As such, we only need control of the residual associated to the linearized equations* *to formally show convergence of the discrete multisymplectic form formula to the continuum multisymplectic form formula.*

We note that the aforementioned convergence is formal since it must also be combined appropriately with convergence of the discrete solution to a continuum weak solution using bounds on the projection. One possible method for combining these is the following observation. Since, by assumption, the projections are cochain projections, we have that

$$d^2S_h[\phi]\cdot(V,W) = d^2(\pi_h^* S)[\phi]\cdot(V,W) = d^2S[\pi_h\phi]\cdot(T\pi_h\cdot V, T\pi_h\cdot W).$$

In particular, for first variations $V,W \in \mathfrak{X}(Y)$ for the degenerate action, $T\pi_h\cdot V, T\pi_h\cdot W$ correspond to first variations of the discrete Euler–Lagrange equations, and the discrete multisymplectic form formula can be reinterpreted as the multisymplectic form formula for the degenerate action. Note also that for cochain projections, a simple calculation shows that $j^1(T\pi_h\cdot V) = T(\pi_h^k \times \pi_h^{k+1})\cdot j^1V$, so that the terms in the integrand of the discrete multisymplectic form formula, (2.17), are in the image of the (tangent) projections. This allows us to formulate the discrete multisymplectic formula in terms of the projection and its tangent lift, and hence more directly determine in what sense the discrete multisymplectic form formula converges as $h \to 0$.

Of course, without specifying a particular field theory and finite element spaces, we cannot proceed further to show convergence. We aim to investigate more rigorous convergence results for particular field theories in future work. See also the discussion below regarding convergence of the discrete Noether theorem to its continuum analogue.

Remark 1.2.7. *As noted before, the discrete Cartan form, in the case of nodal interpolating shape functions, gives precisely the discrete notion of Cartan form introduced in Marsden et al. [85]. In this case, our discrete multisymplectic form formula $d\mathbf{\Theta}_U^h(\phi_h)\cdot(V,W) = 0$ (for first variations V,W) gives precisely the discrete multisymplectic form formula derived in Marsden et al. [85].*

1.2.4 Discrete Noether's Theorem

In this section, we establish a discrete analogue of the weak Noether's theorem as discussed in Section 1.2.1.

To derive a discrete analogue, we first must restrict to regular regions instead of allowing arbitrary regions, analogous to the discussion of the discrete multisymplectic form formula. Furthermore, we must make sense of a group action on the discrete space $\Lambda_h^k \subset H\Lambda^k$. In general, one cannot expect the group action $G \times H\Lambda^k \to H\Lambda^k$ to restrict to a group action $G \times \Lambda_h^k \to \Lambda_h^k$, i.e., the group orbit $G \cdot \Lambda_h^k$ is not necessarily contained in Λ_h^k. However, suppose there exists a Lie group homomorphism $\psi_h : G \to G$ such that

$$\psi_h(g) \cdot \pi_h \phi = \pi_h(g \cdot \phi), \text{ for all } g \in G, \phi \in H\Lambda^k.$$

In such a case, we say that the projection π_h is G-equivariant with intertwining homomorphism ψ_h.

Remark 1.2.8. *In essence, the motivation behind this definition is that when one discretizes a theory, a symmetry group of the original theory may be reduced to a smaller subgroup. This is encoded in the homomorphism ψ_h, where the smaller subgroup is $\psi_h(G) \cong G/\ker \psi_h$. We will see some examples of this after proving a discrete Noether's theorem.*

We are now ready to state a discrete Noether's theorem.

Theorem 1.2.2. *Let U be a regular region. Suppose the action S is G-invariant and the projection is G-equivariant with intertwining homomorphism ψ_h. Then, for a solution $\phi_h \in \Lambda_h^k$ of the DEL,*

$$\boldsymbol{\Theta}_U^h(\phi_h) \cdot T\pi_h(\widetilde{\xi}) = 0, \tag{2.18a}$$

or, equivalently,

$$\boldsymbol{\Theta}_U^h(\phi_h) \cdot \widetilde{(\psi_h)_*\xi} = 0, \tag{2.18b}$$

where $(\psi_h)_*$ *is the induced Lie algebra homomorphism.*

Proof. Since $\phi_h \in \Lambda_h^k$ and $\pi_h : H\Lambda^k \to \Lambda_h^k$ is surjective, there exists some $\phi \in H\Lambda^k$ such that $\phi_h = \pi_h \phi$. Then, for any $g \in G$,

$$S_U[\pi_h(g \cdot \phi)] = S_U[\psi_h(g) \cdot \pi_h \phi] = S_U[\pi_h \phi],$$

where G-equivariance of the projection was used in the first equality and G-invariance of the action was used in the second equality. The above holds for all g and in particular, for $\xi \in \mathrm{Lie}(G)$, one has that

$$S_U \circ \pi_h[e^{t\xi} \cdot \phi] = S_U \circ \pi_h[\phi].$$

Differentiating the above yields

$$0 = d(S_U \circ \pi_h)[\phi] \cdot \widetilde{\xi} = \pi_h^* dS_U[\phi] \cdot \widetilde{\xi} = dS_U[\pi_h \phi] \cdot T\pi_h \widetilde{\xi} = dS_U[\phi_h] \cdot T\pi_h \widetilde{\xi}.$$

Finally, we decompose the variation of the action as

$$0 = dS_U[\phi_h] \cdot T\pi_h \widetilde{\xi} = \mathbf{EL}_U^h(\phi_h) \cdot T\pi_h \widetilde{\xi} + \mathbf{\Theta}_U^h(\phi_h) \cdot T\pi_h \widetilde{\xi}.$$

The term $\mathbf{EL}_U^h(\phi_h) \cdot T\pi_h \widetilde{\xi}$ vanishes since ϕ_h satisfies the DEL and $T\pi_h \widetilde{\xi}$ is a vector field on Λ_h^k. Thus, equation (2.18a) follows.

To see that this is equivalent to equation (2.18b), it suffices to show

$$T\pi_h \widetilde{\xi}(\phi) = \widetilde{(\psi_h)_* \xi}(\phi_h).$$

To see this, recall that

$$\widetilde{\xi}(\phi) = \lim_{t \to 0} \frac{e^{t\xi} \cdot \phi - \phi}{t}.$$

Thus, the pushforward can be computed as

$$\begin{aligned} T\pi_h \widetilde{\xi}(\phi) &= \lim_{t\to 0} \frac{\pi_h(e^{t\xi}\cdot\phi) - \pi_h\phi}{t} \\ &= \lim_{t\to 0} \frac{\psi_h(e^{t\xi})\cdot\pi_h\phi - \pi_h\phi}{t} \\ &= \widetilde{(\psi_h)_*\xi}, \end{aligned}$$

where G-equivariance was used in the second equality and the third equality is simply the definition of an infinitesimal generator. □

Remark 1.2.9. *Note that the proof above is still valid if one weakens the notion of G-equivariance to only hold infinitesimally up to $o(t)$, i.e.,*

$$\psi_h(e^{t\xi})\cdot\pi_h\phi = \pi_h(e^{t\xi}\cdot\phi) + o(t), \text{ for all } \xi \in Lie(G), \phi \in H\Lambda^k.$$

We give two simple examples of group-equivariant cochain projections and subsequently remark on how one might construct more general group-equivariant cochain projections.

Example 1.2.1 (Global Linear Group Action)**.** *First, note that although we took our field configuration bundle to be $\Lambda^k(X)$, we could have more generally taken our fields to be vector-valued forms, corresponding to the bundle $\Lambda^k(X)\otimes V$ for some finite-dimensional vector space V. With a basis $\{e_i\}$ for V, the only modification to the discrete Euler–Lagrange (2.9) equation is that there are* $\dim(V)$ *equations corresponding to each component of the field $\phi^i \in \Lambda^k(X)$ in the expansion $\phi(x) = \sum_i \phi_i(x)\otimes e_i$.*

Suppose that a Lagrangian with such a configuration bundle is invariant under the global action by a group representation $D: G \to GL(V)$. That is, D acts on $\phi \in \Lambda^k(X)\otimes V$ as $1_{\Lambda^k(X)}\otimes D$:

$$D(g)\phi(x) = \sum_i \phi_i(x)\otimes(D(g)e_i),$$

where $D(g)$ is independent of x.

Let $\pi_h^k : H\Lambda^k \to \Lambda_h^k$ *and* $\pi_h^{k+1} : H\Lambda^{k+1} \to \Lambda_h^k$ *be cochain projections, i.e., they satisfy* $\pi_h^{k+1} d = d\pi_h^k$*. We can extend these to cochain projections on vector-valued forms by* $\tilde{\pi}_h = \pi_h \otimes 1_V$*. Furthermore, group-equivariance follows from linearity of the group action and the above definitions,*

$$
\begin{aligned}
D(g)\tilde{\pi}_h\phi = D(g)\tilde{\pi}_h\left(\sum_i \phi_i \otimes e_i\right) &= D(g)\sum_i \pi_h(\phi_i)\otimes e_i = \sum_i \pi_h(\phi_i)\otimes D(g)e_i \\
&= \tilde{\pi}_h\left(\sum_i \phi_i \otimes D(g)e_i\right) = \tilde{\pi}_h\left(D(g)\sum_i \phi_i \otimes e_i\right) = \tilde{\pi}_h D(g)\phi.
\end{aligned}
$$

Thus, the discrete Noether's theorem holds in this case, where the intertwining homomorphism is just the identity.

A simple example of such a theory is the Schrödinger equation with $V = \mathbb{C}$*,* $G = U(1)$*, and the group representation given by the fundamental representation of* $U(1)$ *in* $GL(\mathbb{C})$*. The corresponding Noether conservation law is conservation of mass in the* L^2 *norm.*

Example 1.2.2 (Yang–Mills Theory)**.** *As an example of a non-global (but still linear) group action, consider Yang–Mills theories with a structure group G. In this setting, the field* $A \in \Lambda^1(X)\otimes\mathfrak{g}$*, i.e., A is valued in the Lie algebra* $\mathfrak{g}$ *associated to G. More precisely, the field is valued in the adjoint representation of the Lie algebra. This class of theories is invariant under the linear action of* $\Lambda^0(X)\otimes\mathfrak{g}$*, viewed as a group under addition, on* $\Lambda^1(X)\otimes\mathfrak{g}$ *given by*

$$
\alpha \cdot A \equiv A + d\alpha,
$$

for any $\alpha \in \Lambda^0(X)\otimes\mathfrak{g}$*. Unlike the previous example, this action is local in the sense that* $D(\alpha)$ *depends on the position in spacetime.*

Now, suppose that we have cochain projections for the sequence $H\Lambda^0 \xrightarrow{d} H\Lambda^1 \xrightarrow{d} H\Lambda^2$*, i.e.,* $\pi_h^2 d = d\pi_h^1, \pi_h^1 d = d\pi_h^0$*. Extend these to projections* $\tilde{\pi}_h$ *on* $H\Lambda\otimes\mathfrak{g}$ *as in the previous example. The relation* $\tilde{\pi}_h^2 d = d\tilde{\pi}_h^1$ *is required for naturality of the variational structure. On the other hand,* *the relation* $\tilde{\pi}_h^1 d = d\tilde{\pi}_h^0$ *gives group equivariance in the following sense,*

$$\tilde{\pi}_h^1(\alpha \cdot A) = \tilde{\pi}_h^1(A + d\alpha) = \tilde{\pi}_h^1 A + \tilde{\pi}_h^1 d\alpha = \tilde{\pi}_h^1 A + d\tilde{\pi}_h^0 \alpha = \tilde{\pi}_h^0(\alpha) \cdot \tilde{\pi}_h^1 A.$$

Thus, the discrete Noether's theorem holds where the intertwining homomorphism is $\psi_h = \tilde{\pi}_h^0$.

In the continuum Hilbert space setting, the associated conservation law is the weak Gauss' law, where Gauss' law holds tested against any element of the Hilbert space. In the discrete setting, the discrete Noether's theorem gives a discrete Gauss' law, where Gauss' law holds tested against any element of the finite-dimensional subspace.

The previous two examples were simple in the sense that they had a linear or global group action. Although the second example was local, the acting group is contained in the Hilbert complex of forms and group-equivariance arose from having cochain projections.

To construct group-equivariant cochain projections for more general actions, one possible method would be to utilize group-equivariant interpolation [40; 74] in constructing the projection. One method to construct cochain projections from interpolants is to place an intermediate sequence between the sequence of Hilbert spaces and the sequence of finite-dimensional subspaces,

$$\begin{array}{ccc} H\Lambda^k & \xrightarrow{\quad d \quad} & H\Lambda^{k+1} \\ \downarrow{\scriptstyle \sigma^k} & & \downarrow{\scriptstyle \sigma^{k+1}} \\ C^k & \xrightarrow{\quad D \quad} & C^{k+1} \\ \downarrow{\scriptstyle \mathscr{I}^k} & & \downarrow{\scriptstyle \mathscr{I}^{k+1}} \\ \Lambda_h^k & \xrightarrow{\quad d \quad} & \Lambda_h^{k+1}, \end{array}$$

where $\{\sigma^m\}$ are the degrees of freedom mapping into the coefficient spaces $\{C^m\}$, $\{\mathscr{I}^m\}$ are interpolants from the coefficient spaces into the finite-dimensional subspaces, D realizes d in the coefficient space, and the projections are defined by $\pi_h = \mathscr{I} \circ \sigma$. The degrees of freedom must be unisolvent when restricted to the image of the interpolants. Constructing cochain projections amounts to ensuring that the top diagram commutes. Then, fixing group-equivariant interpolants $\mathscr{I}^k, \mathscr{I}^{k+1}$, group-equivariant cochain projections could be achieved by choosing the degrees of freedom such that they are unisolvent for this choice of interpolants and ensuring that the top diagram commutes. We will pursue such a construction in future work.

1.2.5 A Discrete Variational Complex

The variational bicomplex is a double complex on the spaces of differential forms over the jet bundle of a configuration bundle used to study the variational structures of Lagrangian field theories defined on this bundle (see, for example, Anderson [4]). The differential forms arising in Lagrangian field theory, such as the Lagrangian density, the Cartan form, and the multisymplectic form, can be interpreted as elements of this variational bicomplex. The cochain maps in this double complex are the horizontal and vertical exterior derivatives on the jet bundle, which give a geometric interpretation to the variations encountered in Lagrangian field theories. The variational bicomplex has also been extended to problems with symmetry in Kogan and Olver [63], and to the discrete setting for difference equations corresponding to discretizing Lagrangian field theories on a lattice in Hydon and Mansfield [56].

In this section, we interpret and summarize the results from the previous sections in terms of a discrete variational complex which arises naturally in our discrete construction and, in a sense, resembles the vertical direction of the variational bicomplex.

In our previous discussion, we saw a complex which arises from the space of discrete forms,

$$\Lambda_h^0 \xrightarrow{d} \Lambda_h^1 \xrightarrow{d} \cdots \xrightarrow{d} \Lambda_h^n \xrightarrow{d} \Lambda_h^{n+1},$$

which forms a complex due to the cochain projection property. Now, consider instead the following "vertical" complex; consider the spaces of smooth forms on Λ_h^k, which we denote $\Omega(\Lambda_h^k)$, with the "vertical" exterior derivative $d_v : \Omega^m(\Lambda_h^k) \to \Omega^{m+1}(\Lambda_h^k)$ being the usual exterior derivative over the base manifold Λ^k_h (which is a vector space). This gives a discrete variational complex:

$$\begin{array}{c} \Omega^{\dim(\Lambda^k_h)}(\Lambda^k_h) \\ d_v \Big\uparrow \\ \vdots \\ d_v \Big\uparrow \\ \Omega^1(\Lambda^k_h) \\ d_v \Big\uparrow \\ \Omega^0(\Lambda^k_h)\ . \end{array}$$

Note that in the previous sections, we used d to denote both the exterior derivative corresponding to the de Rham complex and the vertical exterior derivative, e.g., the multisymplectic form formula $d\mathbf{\Theta}^h_U(V,W) = 0$ is more precisely $d_v\mathbf{\Theta}^h_U(V,W) = 0$, where it was understood which was meant by the spaces where the relevant quantities were defined. However, we will distinguish the two in this section to be more precise. We call the above a vertical complex for two reasons: first, the vertical exterior derivative corresponds to differentiation with respect to the fiber values as we will see below. Furthermore, it resembles the vertical direction of the variational bicomplex. However, in our construction, there is no horizontal direction, since in the discrete setting, we are considering transgressed forms, i.e., forms integrated over a region, so the horizontal direction collapses.

Examples of forms in the discrete variational complex include the restricted action $S \in \Omega^0(\Lambda^k_h)$, the discrete weak Cartan form $\mathbf{\Theta}^h \in \Omega^1(\Lambda^k_h)$, and the discrete multisymplectic form $d_v\mathbf{\Theta}^h \in \Omega^2(\Lambda^k_h)$. Let $\{v_i\}$ be a basis for Λ^k_h; we then coordinatize the vector space Λ^k_h by the components of the expansion of any $\phi = \sum_i \phi^i v_i \in \Lambda^k_h$, which we denote as a vector

$(\phi^i) = (\phi^0, \dots, \phi^{\dim(\Lambda_h^k)}) \in \Lambda_h^k$. For example, the vertical exterior derivative of the action is

$$d_v S[\phi] = \sum_j \frac{\partial S[(\phi^i)]}{\partial \phi^j} d_v \phi^j.$$

The naturality of the variational principle and the interpretation of the weak Euler–Lagrange equations as a Galerkin variational integrator, discussed in Section 1.2.2, relate the vertical exterior derivative of S to the variation of the degenerate action S_h. Now, let Π_i be the projection onto the i^{th} coordinate ϕ^i and let $\mathscr{I}[\partial U]$ denote the set of indices i such that v_i has nonvanishing trace on ∂U. Then, for $v = (v^i) \in \Lambda_h^k$, we have that

$$\begin{aligned} v_\partial &= \sum_{i \in \mathscr{I}[\partial U]} \Pi_i(v), \\ v_{in} &= v - v_\partial = \sum_{i \notin \mathscr{I}[\partial U]} \Pi_i(v). \end{aligned}$$

Recall that we can view vector fields $V \in \mathfrak{X}(\Lambda_h^k)$ as maps $V : \Lambda_h^k \to \Lambda_h^k$, and we extend this to the vector fields $V_\partial(\phi) \equiv (V(\phi))_\partial$ and $V_{in}(\phi) \equiv (V(\phi))_{in}$. In particular, the discrete weak Cartan form in this notation is given by

$$\mathbf{\Theta}^h(\phi) \cdot V = d_v S[\phi] \cdot V_\partial.$$

The variation of the action can then be expressed as

$$d_v S[\phi] \cdot V = \mathbf{EL}^h(\phi) \cdot V + \mathbf{\Theta}^h(\phi) \cdot V.$$

More explicitly, these can be expressed as

$$\boldsymbol{\Theta}^h(\phi) = \sum_{j \in \mathscr{I}[\partial U]} \frac{\partial S[(\phi^i)]}{\partial \phi^j} d_v \phi^j,$$
$$\mathbf{EL}^h(\phi) = \sum_{j \notin \mathscr{I}[\partial U]} \frac{\partial S[(\phi^i)]}{\partial \phi^j} d_v \phi^j.$$

In particular, the discrete Euler–Lagrange equations are given by the null Euler–Lagrange condition, $\mathbf{EL}(\phi) = 0$, i.e., $\mathbf{EL}(\phi) \cdot V = 0$ for all V. Assuming a solution ϕ of the null Euler–Lagrange condition, we immediately see that

$$d_v S[\phi] \cdot V = \boldsymbol{\Theta}^h(\phi) \cdot V,$$

and in particular, for a symmetry of the action $d_v S[\phi] \cdot \tilde{\xi} = 0$, we have the discrete Noether's theorem $\boldsymbol{\Theta}^h(\phi) \cdot \tilde{\xi} = 0$. By taking the second exterior derivative of the action, we have that

$$0 = d_v^2 S[\phi] = d_v \mathbf{EL}(\phi) + d_v \boldsymbol{\Theta}^h(\phi).$$

The space of first variations at ϕ is precisely the kernel of the quadratic form $d_v \mathbf{EL}(\phi)$, so this gives the discrete multisymplectic form formula $d_v \boldsymbol{\Theta}^h(\phi)(\cdot, \cdot) = 0$ when evaluated on first variations. Thus, the results of the previous sections can be concisely summarized in terms of the structure given by the discrete variational complex.

Furthermore, this framework also encompasses the discrete variational principle with quadrature, as discussed in Remark 1.2.5. Namely, from the discrete viewpoint, a discrete action is an element of $\Omega^0(\Lambda_h^k)$ and in particular, the discrete action with quadrature $\mathbb{S}$ from (2.14) is an element of $\Omega^0(\Lambda_h^k)$. Then, the variation of $\mathbb{S}$ can be decomposed into interior and boundary one-forms as before,

$$
\begin{aligned}
d_v\mathbb{S}[(\phi)] &= \mathbb{EL}(\phi) + \Theta^h(\phi), \\
\Theta^h(\phi) &= \sum_{j \in \mathscr{I}[\partial U]} \frac{\partial \mathbb{S}[(\phi^i)]}{\partial \phi^j} d_v\phi^j, \\
\mathbb{EL}(\phi) &= \sum_{j \notin \mathscr{I}[\partial U]} \frac{\partial \mathbb{S}[(\phi^i)]}{\partial \phi^j} d_v\phi^j.
\end{aligned}
$$

The discrete Euler–Lagrange equations with quadrature are given by the null Euler–Lagrange condition $\mathbb{EL}(\phi) = 0$, and subsequently, the discrete Noether's theorem and discrete multisymplectic form formula (in the case of quadrature) then follow analogously to before, where symmetries are with respect to $\mathbb{S}$ and the space of first variations at ϕ is the kernel of the quadratic form $d_v\mathbb{EL}(\phi)$.

1.2.6 Numerical Example

We consider the scalar Poisson equation in $(1+1)$-spacetime dimensions on a rectangular domain, $X = [a,b] \times [c,d]$,

$$
\partial_t^2\phi + \partial_x^2\phi = f(x,y).
$$

The Lagrangian is given by $L = \frac{1}{2}(\partial_t\phi)^2 + \varepsilon\frac{1}{2}(\partial_x\phi)^2 + f(x,y)\phi$, or equivalently, the Lagrangian density is given by

$$
\mathscr{L} = \frac{1}{2} d\phi \wedge \star d\phi + f \wedge *\phi.
$$

Compute $\partial_3\mathscr{L}(j_d^1\phi) = d\phi$, $\partial_2\mathscr{L}(j_d^1\phi) = f$, where we assume $f \in L^2\Lambda^0$, so the discrete Euler–Lagrange equation reads: find $\phi \in \Lambda_h^0$ such that

$$
(d\phi, dv)_{L^2} = (f,v)_{L^2}, \text{ for all } v \in \mathring{\Lambda}_h^0.
$$

We subdivide X into a regular rectangular mesh and use a tensor-product basis of hat functions $\psi_{ij}(t,x) = \chi_i(t)\xi_j(x)$ subordinate to this mesh.

Expressing $\phi = \phi^{ij}\psi_{ij}$ and taking $v = \psi_{mn}$, the above equation reads as

$$\sum_{ij\in[mn]}\Big(\phi^{ij}(\chi_i'(t),\chi_m'(t))_{L^2}(\xi_j(x),\xi_n(x))_{L^2}+\phi^{ij}(\chi_i(t),\chi_m(t))_{L^2}(\xi_j'(x),\xi_n'(x))_{L^2}\Big)=(f,\psi_{mn})_{L^2}.$$

Since $[m] = \{m-1, m, m+1\}$, this gives a nine-point stencil on the interior elements of the mesh. Explicitly, we compute the stiffness and mass matrix elements

$$\{(\chi_i'(t),\chi_m'(t))_{L^2}\}_{i\in[m]} = \frac{1}{\Delta t}\{-1,2,-1\},$$
$$\{(\chi_i(t),\chi_m(t))_{L^2}\}_{i\in[m]} = \Delta t\left\{\frac{1}{6},\frac{2}{3},\frac{1}{6}\right\},$$

and similarly for the x direction. This gives

$$\frac{\phi^{m+1\tilde{n}}-2\phi^{m\tilde{n}}+\phi^{m-1\tilde{n}}}{\Delta t^2}+\frac{\phi^{\tilde{m}n+1}-2\phi^{\tilde{m}n}+\phi^{\tilde{m}n-1}}{\Delta x^2}+\frac{1}{\Delta t\Delta x}(f,\psi_{mn}),$$

where $\phi^{m\tilde{n}} = \frac{1}{6}(\phi^{mn+1}+4\phi^{mn}+\phi^{mn-1})$ and $\phi^{\tilde{m}n} = \frac{1}{6}(\phi^{m+1n}+4\phi^{mn}+\phi^{m-1n})$. Noting that $(N'(\phi),\psi_{mn}) = \delta\mathscr{N}/\delta\phi^{mn}$, where $\mathscr{N} = \int N(\phi)dt\wedge dx$, this reproduces the nine-point variational integrator derived by Chen [30]. As was shown in Chen [30], using mid-point quadrature, this method reduces to the multisymplectic integrator derived by Marsden et al. [85].

Now, we consider the discrete Cartan form for this example. Consider a regular region $U \subset X$; for simplicity, we take U to be a rectangular region $U = [t_0,t_M]\times[x_0,x_N]$, without loss of generality, since any regular region on a rectangular mesh is a union of such rectangular regular regions, where the vertices of U are given by $\{(t_i,x_j)\}_{i,j=0}^{M,N}$ where $t_i = t_0 + i\Delta t, x_j = x_0 + j\Delta x$. We index the piecewise linear nodal interpolating shape functions $\psi_{ij}(t,x) = \chi_i(t)\xi_j(x)$ by the node (t_i,x_j) which it interpolates, i.e., $\psi_{ij}(t_k,x_l) = \chi_i(t_k)\xi_j(x_l) = \delta_{ik}\delta_{jl}$. Let

$$\phi_h = \sum_{i,j=0}^{M,N}\phi_h^{ij}\psi_{ij}$$

be a solution of the associated discrete Euler–Lagrange equation, restricted to U.

Recall the definition of the discrete weak Cartan form as the variation of the action by $w \in \Lambda_h^0(U)$, with generally nonvanishing trace on ∂U. Letting $w = w_{in} + w_\partial \in \Lambda_h^0(U)$ and $W \in \mathfrak{X}(\Lambda_h^0)$ such that $W(\phi_h) = w$, we have $\delta S_U[\phi_h] \cdot w_{in} = 0$ and hence,

$$\begin{aligned} \Theta_U^h(\phi_h) \cdot W &= \delta S_U[\phi_h] \cdot w = \delta S_U[\phi_h] \cdot (w - w_{in}) = \delta S_U[\phi_h] \cdot w_\partial \\ &= \sum_{T \in \mathscr{T}[\partial U]} \int_T d\phi_h \wedge * dw_\partial. \end{aligned} \tag{2.19}$$

As discussed above, in the case where the degrees of freedom are the nodal values and the finite-dimensional function space is given by nodal interpolating shape functions, the discrete weak Cartan form reproduces the discrete Cartan form in Marsden et al. [85] and Chen [30]. However, we will now explicitly show this for this example. We express the action as a function of the components ϕ_h^{ij}:

$$S_U[\{\phi_h^{ij}\}] = \int_U [d\phi_h \wedge * d\phi_h - N(\phi_h) dt \wedge dx] = \int_U \left[\frac{1}{2} \sum_{i,j} \sum_{k,l} \phi_h^{ij} \phi_h^{kl} d\psi_{ij} \wedge * d\psi_{kl} \right].$$

Let $ij \in \mathscr{I}[\partial U]$, i.e., the index corresponds to a node on ∂U, consisting of indices ij such that either $i = 0$ or M or $j = 0$ or N. Marsden et al. [85] and Chen [30] define the discrete Cartan form associated to this node to be

$$\frac{\partial S_U[\{\phi_h^{kl}\}]}{\partial \phi_h^{ij}} d\phi_h^{ij}, \tag{2.20}$$

where d is the vertical exterior derivative along the fiber and not the exterior derivative on the base space. Compute

$$\frac{\partial S_U[\{\phi_h^{kl}\}]}{\partial \phi_h^{ij}} = \int_U \left[\sum_{k,l} \phi_h^{kl} d\psi_{ij} \wedge * d\psi_{kl} \right].$$

With coordinates ϕ_h^{ij} on Λ_h^0, we can express the vector field $W = \sum_{k,l} W^{kl} \partial / \partial \phi_h^{kl}$ and hence $W^{kl}(\phi_h) = w^{kl}$. Pairing (2.20) with W and summing over all $ij \in \mathscr{I}[\partial U]$, we see that this gives

(2.19), since $w_\partial = \sum_{ij\in\mathscr{I}[\partial U]} w^{ij}\psi_{ij}$ and ψ_{ij} for $ij \in \mathscr{I}[\partial U]$ are supported on $\cup_{T\in\mathscr{T}[\partial U]} T$.

Finally, we now discuss in what sense the discrete weak Cartan form for this example converges to the weak Cartan form. Consider a node $ij \in \mathscr{I}[\partial U]$ along, say, the $\{t = t_0\}$ edge of ∂U, so that $i = 0$. We compute part of the discrete Cartan form for a boundary variation w^{0j} associated to this node. Namely, we compute the part associated to the derivative in the t direction, since this is the normal direction along this edge. This is given by

$$\begin{aligned}\int_U \sum_{k,l} \phi_h^{kl}\chi_k'(t)\xi_l(x)w^{0j}\chi_0'(t)\xi_j(x)dt\wedge dx &= \int_U \sum_{k=0}^{1}\sum_{l=j-1}^{j+1} \phi_h^{kl}\chi_k'(t)\xi_l(x)w^{0j}\chi_0'(t)\xi_j(x)dt\wedge dx \\ &= \sum_{l=j-1}^{j+1} \frac{\phi_h^{0l}-\phi_h^{1l}}{\Delta t}(\xi_l,\xi_j)_{L^2}w^{0j}.\end{aligned}$$

Since $(\xi_l,\xi_j)_{L^2}$ for $l = j-1, j, j+1$ has total mass Δx, this formally converges to $\int \frac{\partial\phi}{\partial n} w\, dx$, where we note that the normal vector on this edge is $-\hat{t}$. Repeating this over all nodes on ∂U, the discrete Cartan form formally converges to

$$\int_{\partial U} \frac{\partial \phi}{\partial n} w\, dl,$$

where dl is the codimension one measure on ∂U, which is the weak Cartan form for a solution ϕ of the weak Euler–Lagrange equation.

To be more rigorous about the convergence of the discrete weak Cartan form to the weak Cartan form, we have the bound

$$\begin{aligned}&\left|\Theta_U^h(\phi_h)\cdot\pi_h v - \Theta_U(\phi)\cdot v\right| \\ &\quad\le \left|\Big(\Theta_U^h(\phi_h)-\Theta_U^h(\pi_h\phi)\Big)\cdot\pi_h v\right| + \left|\Theta_U(\phi)\cdot(v-\pi_h v)\right| + \left|\Big(\Theta_U(\phi)-\Theta_U^h(\pi_h\phi)\Big)\cdot\pi_h v\right| \\ &\quad\le C|\phi_h-\pi_h\phi|_{H^1}\|\pi_h v\|_{H^1} + C|\phi_h|_{H^1}\|v-\pi_h\phi\|_{H^1} + C|\phi-\pi_h\phi|_{H^1}\|\pi_h v\|_{H^1} \\ &\quad\le hC(\phi,f),\end{aligned}$$

where $C(\phi, f)$ is independent of h, and we have applied standard estimates for piecewise-linear elements applied to the Poisson equation (see, e.g., Larsson and Thomée [66]). Thus, we expect linear convergence of the discrete weak Cartan form to the weak Cartan form.

As a numerical example, we take $U = X = [0,1] \times [0,1]$ with $f(x,y) = -\pi^2 \sin(\pi x) - \pi^2 \sin(\pi y)$, $v(x,y) = e^x + e^y$, and $\Delta t = \Delta x = h$ for various values of h. Since we have the analytic solution $\phi(x,y) = \sin(\pi x) + \sin(\pi y)$, we can directly compute the error

$$\mathrm{E}(h) = \left| \Theta_U^h(\phi_h) \cdot \pi_h v - \Theta_U(\phi) \cdot v \right|.$$

The linear convergence, i.e.,

$$\left| \Theta_U^h(\phi_h) \cdot \pi_h v - \Theta_U(\phi) \cdot v \right| \leq \mathscr{O}(h),$$

is shown in Figure 1.2.

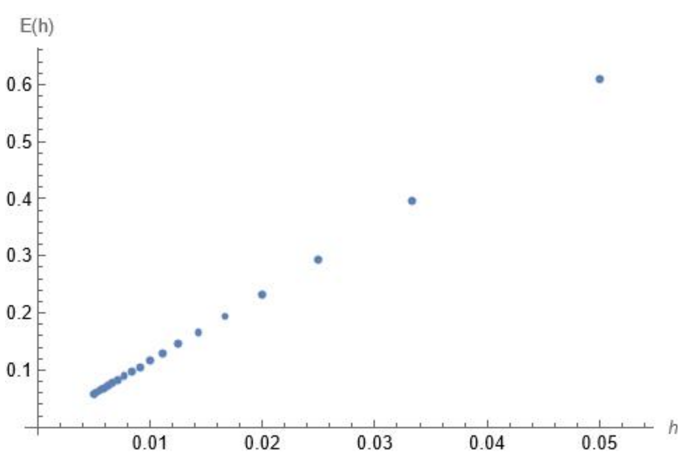


Figure 1.2. Linear Convergence of the discrete weak Cartan form to the weak Cartan form.

1.3 Canonical Semi-discretization of Lagrangian Field Theories

Turning now to the canonical formalism of field theories, we assume that our $(n+1)$-dimensional spacetime X is globally hyperbolic, i.e., X contains a smooth Cauchy hypersurface Σ such that every infinite causal curve intersects Σ exactly once. It was shown in Bernal and Sánchez [14] that a globally hyperbolic spacetime is diffeomorphic to the product, $X \cong \mathbb{R} \times \Sigma$. Identifying X with the product, we have a slicing of the spacetime. Taking an interval $I \subseteq \mathbb{R}$, we have the spacelike embeddings

$$i_t : \Sigma \to X,$$

for each $t \in I$, such that the images $\{\Sigma_t := i_t(\Sigma)\}_{t\in I}$ form a foliation of X.

We will assume our Lagrangian depends on time-dependent fields as $\mathscr{L}(x^\mu, \varphi, \dot{\varphi}, d\varphi)$, where the field $\varphi(t) \in H\Lambda^k(\Sigma_t)$, denoted by φ as opposed to the full field ϕ, and the exterior derivative acts on $\Lambda^k(\Sigma_t)$ for each t.

Remark 1.3.1. *There is a slight subtlety here when comparing to the covariant theory on the full spacetime X. In the covariant theory, we consider k-forms on X, $\Lambda^k X$, whereas here we are considering k-forms on Σ, $\Lambda^k(\Sigma)$. Letting $\pi_1 : \mathbb{R}\times\Sigma \to \mathbb{R}, \pi_2 : \mathbb{R}\times\Sigma\to\Sigma$ be the projections, we have pointwise,*

$$\wedge^k(T^*X) = \wedge^k T^*(\mathbb{R}\times\Sigma) \cong \Big(\pi_1^*(\wedge^0 T^*\mathbb{R}) \wedge \pi_2^*(\wedge^k T^*\Sigma)\Big) \oplus \Big(\pi_1^*(\wedge^1 T^*\mathbb{R}) \wedge \pi_2^*(\wedge^{k-1} T^*\Sigma)\Big).$$

This congruence does not hold at the level of sections: to see this in coordinates (t,x) on $\mathbb{R}\times\Sigma$, we have forms which look like $f(t)g(x)dx^{j_1}\wedge\cdots\wedge dx^{j_k}, f(t)dt\wedge g(x)dx^{j_1}\wedge\cdots\wedge dx^{j_{k-1}}$ which cannot give a form which looks like, e.g., $h(t,x)dt\wedge dx^{j_1}\wedge\cdots\wedge dx^{j_{k-1}}$ where h is some function that cannot be expressed as a product $f(t)g(x)$. However, we are assuming time-dependent fields $\varphi : t\mapsto H\Lambda^k(\Sigma)$ so we do have the forms which look like $\varphi(t) = g(t,x)dx^{j_1}\wedge\cdots\wedge dx^{j_k}$. Thus, we only need to consider multiple fields to obtain full generality $\varphi_1 : t\mapsto H\Lambda^k(\Sigma), \varphi_2 : t\mapsto H\Lambda^{k-1}(\Sigma)$.

Here, we are identifying $\Lambda^1(I) \cong \Lambda^0(I)$, so by $\varphi_2(t)$ we really mean $\varphi_2(t)dt$. Of course, this issue does not arise for scalar functions; however, for $k > 0$, one needs to consider multiple fields.

To be more precise regarding this decomposition, consider first the case $k = 0$. Since the exterior derivative on scalar functions on $I \times \Sigma$ splits into $d = d_t + d_\Sigma$, where, in terms of vector field proxies, $d_t = \partial_t, d_\Sigma = \nabla_\Sigma$, one does not need to consider multiple fields. In this case, one has

$$H\Lambda^0(I \times \Sigma) = H\Lambda^0(I, L^2(\Sigma)) \cap L^2(I, H\Lambda^0(\Sigma)).$$

For the case $k > 0$, we first begin with a formal calculation. For any k-form ϕ on $I \times \Sigma$, we can express ϕ as

$$\phi = \underbrace{\sum_{I \in I_t^{k-1}} \psi_I(t,x) dt \wedge dx^I}_{\equiv \psi} + \underbrace{\sum_{J \in I_\Sigma^k} \varphi_J(t,x) dx^J}_{\equiv \varphi},$$

where I and J are multi-indices of size $k-1$ and k, respectively, and for a multi-index $I = (i_1, \dots, i_m)$ of size m, $dx^I \equiv dx^{i_1} \wedge \cdots \wedge dx^{i_m}$. The multi-index set I_t^{k-1} is defined as the set of all multi-indices $(i_1, \dots, i_{k-1})$ such that $i_1 < \cdots < i_{k-1}$ and such that each of the indices are non-zero, where we adopt the convention that $dx^0 = dt$. The multi-index set I_Σ^k is defined as the set of all multi-indices $(i_1, \dots, i_k)$ such that $i_1 < \cdots < i_k$ and such that each of the indices are non-zero. Note that φ and ψ are orthogonal with respect to the $L^2\Lambda^k(I \times \Sigma)$ inner product, so square integrability of ϕ is equivalent to square integrability of both φ and ψ. For the square integrability of $d\phi$, we compute the exterior derivative of ϕ

$$d\phi = \sum_{I \in I_t^{k-1}} d_\Sigma \psi_I(t,x) \wedge dt \wedge dx^I + \sum_{J \in I_\Sigma^k} \frac{\partial}{\partial t} \varphi_J(t,x) dt \wedge dx^J + \sum_{J \in I_\Sigma^k} d_\Sigma \varphi_J(t,x) \wedge dx^J.$$

Thus, for square integrability of ϕ and $d\phi$, it suffices to have $\psi \in L^2\Lambda^1(I, H\Lambda^{k-1}(\Sigma))$ and $\varphi \in H^1\Lambda^0(I, L^2\Lambda^k(\Sigma)) \cap L^2\Lambda^0(I, H^1\Lambda^k(\Sigma))$. Thus, in the covariant picture, we can view a field ϕ as splitting into two fields φ and ψ. We will treat the case where $\psi = 0$, i.e., we consider *theories depending only on k-forms of the form*

$$\phi = \sum_{J \in I_\Sigma^k} \varphi_J(t,x) dx^J.$$

In this case, the exterior derivative splits into temporal and spatial derivatives, so we have the identification $(\phi, d\phi) \cong (\varphi, \dot{\varphi}, d_\Sigma \varphi)$. *We will subsequently refer to the spatial exterior derivative* d_Σ *simply as* d.

We will discuss how a semi-discretization of the variational principle gives rise to finite-dimensional Lagrangian and Hamiltonian dynamical systems (see, for example, Abraham and Marsden [1]) and subsequently discuss how the energy-momentum map structure of a canonical field theory (see Gotay et al. [45]) is affected by semi-discretization.

1.3.1 Semi-discrete Euler–Lagrange Equations

In this section, we formally derive the semi-discrete Euler–Lagrange equations. Given our $\Lambda^{n+1}(X)$-valued Lagrangian density, we can produce an instantaneous density by contracting with the generator of the slicing $\partial/\partial t$, and pulling back by the inclusion of Σ_t into X. This gives a $\Lambda^n(\Sigma_t)$-valued density, which we will still call $\mathscr{L}$. In coordinates where the density is $L\, dt \wedge V(t)$ and $V(t)$ restricts to a volume form on Σ_t, $\mathscr{L} = i_t^* LV(t)$. The action in the canonical framework is given by

$$S[\varphi] = \int_I dt \int_{\Sigma_t} \mathscr{L}(x^\mu, \varphi, \dot{\varphi}, d\varphi), \tag{3.1}$$

where $(x^\mu) = (t, x^1, \ldots, x^n) = (t,x)$, and $x = (x^i)$ denotes spatial coordinates.

To derive a semi-discrete formulation of the Euler–Lagrange equations, instead of looking at arbitrary variations of the form $v(t,x)$, we instead consider variations of the form $u(t)v(x)$ where $v \in H\Lambda^k(\Sigma)$ and $u \in C_0^2(I, \mathbb{R})$. The basic idea of the semi-discrete formulation is to allow u to be arbitrary but restrict v to a finite-dimensional subspace Λ_h^k. As in the covariant case, in order to compute the variations formally without going through the Hamilton–Pontryagin principle, we will assume that the projections are cochain projections, with respect to the spatial exterior derivative d on Σ.

Assumption 1.3.1. *The projections* $\pi_h^m : H\Lambda^m(\Sigma) \to \Lambda_h^m(\Sigma)$ *are cochain projections, i.e.,*

$$\pi_h^{k+1} d = d\pi_h^k,$$

with respect to $d : \Lambda^m(\Sigma) \to \Lambda^{m+1}(\Sigma)$.

Remark 1.3.2. *Note that we assume a finite element discretization* Λ_h^k *of the fields on the reference space* $H\Lambda^k(\Sigma)$*, with associated projection* π_h*. There are two ways to view the variations with respect to our slicing* $\{\Sigma_t\}$*. On the one hand, the field variation on the reference space* $v \in \Lambda_h^k \subset H\Lambda^k(\Sigma)$ *is pulled back to a field variation on a time slice* $(i_t^{-1})^* v \in H\Lambda^k(\Sigma_t)$*, where we restrict the embedding to its image* $i_t : \Sigma \to \Sigma_t$*. On the other hand, we can pull back forms on* Σ_t *to forms on* Σ *via* i^**, e.g., the Lagrangian density and its derivatives, and perform any relevant integration over the reference space* Σ*. We will utilize the latter since in computation it is preferable to work on one reference space. For simplicity, we will not explicitly write the pullbacks* i_t^* *but rather implicitly incorporate it into the spacetime dependence of the Lagrangian.*

Theorem 1.3.1. *The semi-discrete Euler–Lagrange equations corresponding to the variational principle* $\delta S[\varphi] \cdot (uv) = 0$ *for all* $v \in \Lambda_h^k$ *and* $u \in C_0^2(I, \mathbb{R})$ *are given by*

$$\frac{d}{dt}(\partial_3 \mathscr{L}, v)_{L^2\Lambda^k(\Sigma)} - (\partial_2 \mathscr{L}, v)_{L^2\Lambda^k(\Sigma)} - (\partial_4 \mathscr{L}, dv)_{L^2\Lambda^{k+1}(\Sigma)} = 0, \text{ for all } v \in \Lambda_h^k \text{ and } t \in I, \quad (3.2)$$

where $\mathscr{L}$ *is evaluated at* $(x^\mu, \varphi, \dot{\varphi}, d\varphi)$.

Proof. With $\mathscr{L}$ evaluated at $(x^\mu, \varphi, \dot{\varphi}, d\varphi)$, compute

$$\begin{aligned}
0 = \delta S[\varphi]\cdot(uv) &= \frac{d}{d\varepsilon}\Big|_{\varepsilon=0} S[\phi+\varepsilon uv] \\
&= \int_I dt \int_\Sigma \Big[\partial_2\mathscr{L}\wedge\star u(t)v + \partial_3\mathscr{L}\wedge\star\dot{u}(t)v + \partial_4\mathscr{L}\wedge\star u(t)dv\Big] \\
&= \int_I dt \Big[\int_\Sigma \Big(\partial_3\mathscr{L}\wedge\star v\Big)\dot{u}(t) + \int_\Sigma \Big(\partial_2\mathscr{L}\wedge\star v + \partial_4\mathscr{L}\wedge\star dv\Big)u(t)\Big] \\
&= \int_I dt \Big[(\partial_3\mathscr{L}, v)_{L^2}\dot{u}(t) + (\partial_2\mathscr{L}, v)_{L^2}u(t) + (\partial_4\mathscr{L}, dv)_{L^2}u(t)\Big] \\
&= -\int_I dt \Big[\frac{d}{dt}(\partial_3\mathscr{L}, v)_{L^2} - (\partial_2\mathscr{L}, v)_{L^2} - (\partial_4\mathscr{L}, dv)_{L^2}\Big]u(t).
\end{aligned}$$

Since $u \in C_0^2(I,\mathbb{R})$ is arbitrary, the terms in the brackets vanish, which gives (3.2). □

Remark 1.3.3. *Similar to our discussion of the covariant case, there is a naturality relation in the variational principle when using spatial cochain projections for the semi-discrete theory. In particular,*

$$S[\pi_h\varphi] = \int_I dt \int_\Sigma \mathscr{L}(x^\mu, \pi_h\varphi, \pi_h\dot{\varphi}, d\pi_h\varphi) = \int_I dt \int_\Sigma \mathscr{L}(x^\mu, \pi_h\varphi, \pi_h\dot{\varphi}, \pi_h d\varphi) =: S_h[\varphi],$$

so that the restricted variational principle can be realized as a full variational principle on a degenerate action, $\delta S[\pi_h\phi]\cdot(u\,\pi_h v) = \delta S_h[\phi]\cdot(uv)$. *Analogous to the discussion in the covariant case, the cochain property additionally removes the ambiguity of how one should discretize the spatial derivative of the field, i.e., whether one should project before or after taking the spatial derivative.*

We now show that the semi-discrete Euler–Lagrange equation (3.2) arises from an instantaneous Lagrangian. To do this, let $\{v_i\}$ be a basis for Λ_h^k. We define the instantaneous semi-discrete Lagrangian to be

$$L_h(t, \varphi^i, \dot{\varphi}^i) = \int_\Sigma \mathscr{L}(x^\mu, \varphi^i v_i, \dot{\varphi}^i v_i, \varphi^i dv_i), \tag{3.3}$$

where $\varphi = \varphi^i(t)v_i \in C^2(I,\Lambda_h^k)$ and the associated action $S_h[\{\varphi^i\}] = \int_I dt L_h(t,\varphi^i,\dot{\varphi}^i)$. We enforce the variational principle over curves $u = u^i(t)v_i \in C_0^2(I,\Lambda_h^k)$. The variational principle yields

$$0 = dS_h[\{\varphi^i\}]\cdot\{u^j\} = \frac{d}{d\varepsilon}\Big|_0 S_h[\{\varphi^i+\varepsilon u^j\}] = \sum_j \int_I dt\Big(\frac{\partial L_h}{\partial \varphi^j}(t,\varphi^i,\dot{\varphi}^i)u^j + \frac{\partial L_h}{\partial \dot{\varphi}^j}(t,\varphi^i,\dot{\varphi}^i)\dot{u}^j\Big)$$
$$= \sum_j \int_I dt\Big[\frac{\partial L_h}{\partial \varphi^j}(t,\varphi^i,\dot{\varphi}^i) - \frac{d}{dt}\frac{\partial L_h}{\partial \dot{\varphi}^j}(t,\varphi^i,\dot{\varphi}^i)\Big]u^j.$$

This holds for arbitrary $u^j \in C_0^2(I,\mathbb{R})$, so the term in the brackets,

$$\frac{\partial L_h}{\partial \varphi^j}(t,\varphi^i,\dot{\varphi}^i) - \frac{d}{dt}\frac{\partial L_h}{\partial \dot{\varphi}^j}(t,\varphi^i,\dot{\varphi}^i) = 0, \tag{3.4}$$

vanishes for each j by the fundamental lemma of the calculus of variations. Expressing the derivatives of L_h in terms of $\mathscr{L}$,

$$\frac{\partial L_h}{\partial \varphi^j} = (\partial_2\mathscr{L}, v_j)_{L^2\Lambda^k(\Sigma)} + (\partial_2\mathscr{L}, dv_j)_{L^2\Lambda^{k+1}(\Sigma)}, \tag{3.5a}$$
$$\frac{\partial L_h}{\partial \dot{\varphi}^j} = (\partial_3\mathscr{L}, v_j)_{L^2\Lambda^k(\Sigma)}. \tag{3.5b}$$

Substituting these expressions into equation (3.4), we see that this is equation (3.2) with the choice $v = v_j$. This holds for each basis form v_j and hence for arbitrary $v \in \Lambda_h^k$.

We will now introduce a Hamiltonian structure associated with the semi-discretization and show that, in the hyperregular case, this instantaneous Lagrangian system is equivalent to an instantaneous Hamiltonian system.

1.3.2 Symplectic Structure of Semi-discrete Dynamics and Hamiltonian Formulation

Having derived the semi-discrete Euler–Lagrange equation (3.2), we now relate the symplectic structure on the cotangent space of the full field space $T^*H\Lambda^k(\Sigma)$ to a symplectic structure on the discretized space $T^*\Lambda_h^k$, and show that the semi-discrete Euler–Lagrange equations are equivalent to a Hamiltonian flow on $T^*\Lambda_h^k$ if the Lagrangian is hyperregular.

We work with the reference space Σ, since via the diffeomorphism $i_t : \Sigma \to \Sigma_t$, we can pullback forms on Σ to Σ_t or vice versa, or forms on iterated exterior bundles, such as the symplectic form which is an element of $\Lambda^2(T^*H\Lambda^k(\Sigma))$. On the full phase space $T^*H\Lambda^k(\Sigma)$, the canonical one-form $\theta \in \Lambda^1(T^*H\Lambda^k(\Sigma))$ is given in coordinates by

$$\theta\big|_{(\varphi,\pi)} = \int_\Sigma \pi_A d\varphi^A \otimes d^n x_0, \tag{3.6}$$

and the corresponding symplectic form $\omega = -d\theta$ is given by

$$\omega\big|_{(\varphi,\pi)} = \int_\Sigma (d\varphi^A \wedge d\pi_A) \otimes d^n x_0.$$

Using the projection map $\pi_h : H\Lambda^k(\Sigma) \to \Lambda_h^k$, we have the pullback $\pi_h^* : T^*\Lambda_h^k \to T^*H\Lambda^k(\Sigma)$ and the twice iterated pullback $\pi_h^{**} : \Lambda^p(T^*H\Lambda^k(\Sigma)) \to \Lambda^p(T^*\Lambda_h^k)$ for any p. We define $\theta_h \equiv \pi_h^{**}\theta$ and $\omega_h \equiv \pi_h^{**}\omega = -d\theta_h \in \Lambda^2(T^*\Lambda_h^k)$. To find an expression for θ_h and ω_h, we will introduce global coordinates on $T^*\Lambda_h^k$. Let $\{v_i\}$ be a finite element basis for Λ_h^k; we will use the components φ^i of the basis expansion $\varphi = \varphi^i v_i$ as the coordinates on Λ_h^k. Similarly, if we identify $T\Lambda_h^k \cong \Lambda_h^k \times \Lambda_h^k$, then we have a basis for $T_\varphi^*\Lambda_h^k$ consisting of $v^i := (\cdot, v_i)_{L^2}$. This gives the trivialization $T^*\Lambda_h^k \cong \Lambda_h^k \times (\Lambda_h^k)^*$ with global coordinates $(\varphi, \pi) \sim (\varphi^i, \pi_i)$ where $\varphi = \varphi^i v_i$ and $\pi = \pi_i v^i$. We will denote these coordinates using vector notation $\vec{\varphi} = (\varphi^i)$, $\vec{\pi} = (\pi_i)$.

Proposition 1.3.1. *The* 1*-form θ_h is given in the above coordinates by*

$$\theta_h = v^j(v_i)\pi_j d\varphi^i = d\vec{\varphi}^T M \vec{\pi}, \tag{3.7}$$

where the mass matrix M has components $M_i{}^j := v^j(v_i) = \int_\Sigma v_i v_j d^n x_0$. Furthermore, the 2*-form $\omega_h = -d\theta_h$ is a symplectic form on $T^*\Lambda_h^k$ with coordinate expression*

$$\omega_h = d\varphi^i \wedge v^j(v_i) d\pi_j = d\vec{\varphi}^T \wedge M d\vec{\pi}. \tag{3.8}$$

Proof. Let $(\varphi,\pi) \in T^*\Lambda_h^k$ and $U \in T_{(\varphi,\pi)}(T^*\Lambda_h^k)$, with coordinate expression

$$U(\varphi,\pi) = \Phi^i \frac{\partial}{\partial \varphi^i} + \Pi_i \frac{\partial}{\partial \pi_i}.$$

Note that $\theta|_{(\varphi',\pi')}(V)$ gives the canonical pairing between the $\partial/\partial\varphi'$ component of V and π' by equation (3.6). Then, since $\pi_h^* : T^*\Lambda_h^k \hookrightarrow T^*H\Lambda^k(\Sigma)$ is an inclusion, $T\pi_h^*$ is an inclusion on the corresponding tangent space, which gives

$$\theta_h|_{(\varphi,\pi)}(U) = \theta|_{\pi_h^*(\varphi,\pi)}(T\pi_h^* U) = \langle \Phi, \pi \rangle = \Phi^i \pi_j \int_\Sigma v_i v_j d^n x_0 = v^j(v_i)\pi_j \Phi^i = v^j(v_i)\pi_j d\varphi^i(U).$$

Equation (3.8) then follows from taking (minus) the exterior derivative of equation (3.7).

The nondegeneracy and closedness of ω_h clearly follow from the (global) coordinate expression (3.8) above. In particular, since the mass matrix M is invertible (hence nondegenerate), ω_h is nondegenerate. Closedness follows from

$$d\omega_h = d^2\vec{\varphi}^T \wedge Md\vec{\pi} - d\vec{\varphi}^T \wedge dM \wedge d\vec{\pi} - d\vec{\varphi}^T \wedge Md^2\vec{\pi} = 0.$$

Alternatively, ω_h is closed as the pullback of a closed form ω. □

Remark 1.3.4. *Under a change of basis, ω_h can be seen as a canonical symplectic form on $T^*\Lambda_h^k$. To see ω_h in canonical form, we change basis. Let Q be an orthogonal matrix which diagonalizes the symmetric mass matrix M, i.e., $QMQ^T = D$. Define coordinates $\vec{q} = Q\vec{\varphi}$ and $\vec{p} = DQ\vec{\pi}$; then*

$$\omega_h = d\vec{\varphi}^T \wedge Md\vec{\pi} = d\vec{\varphi}^T \wedge Q^T DQd\vec{\pi} = d(Q\vec{\varphi})^T \wedge d(DQ\vec{\pi}) = d\vec{q}^T \wedge d\vec{p}.$$

However, we will work with the form of ω_h corresponding to the finite element basis (3.8) since it is more directly applicable to our discretization. Also, if we chose the dual basis l^j to be different from the basis $v^j = (\cdot, v_j)$, M would not necessarily be symmetric but would still define *a symplectic form. This follows from the fact that, for a finite element method to be consistent, one requires that the matrix with components $l^j(v_i)$ is invertible. Hence, it is more natural to work with the coordinates $(\vec{\varphi}, \vec{\pi})$.*

Let $H_d : T^*\Lambda_h^k \to \mathbb{R}$ be a given semi-discrete Hamiltonian, expressed in our global coordinates as $H_d(\vec{\varphi}, \vec{\pi})$. Later, we will choose the semi-discrete Hamiltonian induced by the semi-discrete Lagrangian. The dynamics of the Hamiltonian system (ω_h, H_d) is given by the flow generated by the Hamiltonian vector field X_{H_d} satisfying $X_{H_d} \lrcorner\, \omega_h = dH$, or with vector field components $X_{H_d} = (\dot{\varphi}^i, \dot{\pi}_i)$,

$$\begin{cases} M^j_{\ k}\dot{\varphi}^k = \frac{\partial H_d}{\partial \pi_j}, \\ M_j^{\ k}\dot{\pi}_k = -\frac{\partial H_d}{\partial \varphi^j}. \end{cases} \tag{3.9}$$

Remark 1.3.5. *In the above, we denote row j and column k of M as $M_j^{\ k}$ and for M^T as $M^j_{\ k}$, which allows for the more general case where M is asymmetric that was discussed previously. If we define $\vec{z}$ as the concatenation of $\vec{\varphi}$ and $\vec{\pi}$, the equations (3.9) can be written in skew-symmetric form,*

$$\frac{d}{dt}\vec{z} = J_M \nabla_{\vec{z}} H_d,$$

where $J_M = \begin{pmatrix} 0 & (M^{-1})^T \\ -M^{-1} & 0 \end{pmatrix}$.

Remark 1.3.6. *In our discussion of the covariant discretization of Lagrangian field theories, we saw that the variation of the discretized action on the discrete space can be naturally related to the variation of a degenerate action on the full space. In the semi-discrete setting, an analogous statement can be made in terms of the semi-discrete symplectic structure and a presymplectic structure on the full space. Namely, we have the symplectic form $\omega_h \in \Lambda^2(T^*\Lambda_h^k)$. Now, consider the presymplectic form $\tilde{\omega}_h \in \Lambda^2(T^*H\Lambda^k)$ defined by $\tilde{\omega}_h = i_h^{**}\omega_h$ where $i_h = (\pi_h)^\dagger : \Lambda_h^k \hookrightarrow H\Lambda^k$ is the inclusion. Clearly, $\tilde{\omega}_h$ is closed as the pullback of a closed form. To see that it is degenerate,* *observe that for any $V,W \in \mathfrak{X}(T^*H\Lambda^k)$, we have,*

$$\tilde{\omega}_h(V,W) = (i_h^{**}\pi_h^{**}\omega)(V,W) = \omega(T(\pi_h^* i_h^*)V, T(\pi_h^* i_h^*)W).$$

Since $i_h\pi_h$ has a nontrivial kernel, so does $T(\pi_h^* i_h^*) = T(i_h\pi_h)^*$ and hence $\tilde{\omega}_h$ is degenerate. The flow of a vector field in the kernel of $\tilde{\omega}_h$, projected back to the semi-discrete space, corresponds to equivalent states in the semi-discrete setting. Quotienting the presymplectic manifold $(T^*H\Lambda^k, \tilde{\omega}_h)$ by the orbits of the flow of vector fields in the kernel of $\tilde{\omega}_h$ gives the symplectic manifold $(T^*\Lambda_h^k, \omega_h)$. This relates a symplectic flow on $(T^*\Lambda_h^k, \omega_h)$ to an equivalence class of presymplectic flows on $(T^*H\Lambda^k, \tilde{\omega}_h)$, where the equivalence class is formed by orbits of the flow of vector fields in the kernel of $\tilde{\omega}_h$.

We also allow our semi-discrete Hamiltonian to explicitly depend on time, $H_d : I \times T^*\Lambda_h^k \to \mathbb{R}$, i.e., the domain of H_d is the extended phase space $I \times T^*\Lambda_h^k$. The dynamics are now given by any vector field X_{H_d} on the extended phase space such that $X_{H_d} \lrcorner (\omega_h + dH_d \wedge dt) = 0$, where ω_h is extended to the full phase space by pulling back along the projection $I \times T^*\Lambda_h^k \to T^*\Lambda_h^k$. If we consider the vertical component $X_{H_d}^V$ of X_{H_d} with respect to the trivial bundle $I \times \Lambda_h^k \to I$, then the above is equivalent to $X_{H_d}^V \lrcorner\, \omega_h = d_v H_d$ holding for all times. This is given again by equation (3.9) but with explicit time dependence in H_d. Here, $d_v H_d$ is the vertical exterior derivative of H_d with coordinate expression $d_v H_d(t,\varphi,\pi) = \frac{\partial H_d}{\partial \varphi^i} d\varphi^i + \frac{\partial H_d}{\partial \pi_j} d\pi_j$. We could also allow explicit time dependence in M, but since we pullback our integration to Σ, we view M as constant and absorb the time dependence into H_d.

Now, we would like to relate the semi-discrete Euler–Lagrange equations (3.2) to the Hamiltonian dynamics of ω_h by making a particular choice of semi-discrete Hamiltonian. The first step is to produce a Hamiltonian associated to the instantaneous Lagrangian

$$L(t,\varphi,\dot{\varphi}) = \int_\Sigma \mathscr{L}(x^\mu, \varphi, \dot{\varphi}, d\varphi).$$

To do this, we use the Legendre transform, which takes the form $\pi = \partial L / \partial \dot{\varphi}$. The pairing of π with a tangent vector field with components (φ, v) is given by computing the variation

$$\langle \pi, v \rangle = \left\langle \frac{\partial L}{\partial \dot{\varphi}}, v \right\rangle = \frac{d}{d\varepsilon}\Big|_{\varepsilon=0} L(t, \varphi, \dot{\varphi} + \varepsilon v) = (\partial_3 \mathscr{L}, v)_{L^2\Lambda^k}.$$

The instantaneous Hamiltonian is given by

$$H(t, \varphi, \pi) = \langle \pi, \dot{\varphi} \rangle - L(t, \varphi, \dot{\varphi}),$$

where the $\dot{\varphi}$ dependence is removed either by extremizing over $\dot{\varphi}$ or, assuming L is hyperregular, by inverting the Legendre transform to obtain $\dot{\varphi}$ as a function of (φ, π). Restricting to our finite element space $T^*\Lambda_h^k$ gives a semi-discrete Hamiltonian H_h, defined by

$$H_h(t, \varphi^i, \pi_i) = H(t, \varphi^i v_i, \pi_i v^j) = \langle \pi_j v^j, \dot{\varphi}^i v_i \rangle - L(t, \varphi^i v_i, \dot{\varphi}^i v_i) = M_i{}^j \pi_j \dot{\varphi}^i - L(t, \varphi^i v_i, \dot{\varphi}^i v_i).$$

Note that H_h corresponds to the Legendre transform of the semi-discrete Lagrangian (3.3), where we recall the duality pairing between $(\varphi^j, \pi_j) \in T^*\Lambda_h^k$ and $(\varphi^i, \dot{\varphi}^i) \in T\Lambda_h^k$ is given by $M_i{}^j \pi_j \dot{\varphi}^i$.

Proposition 1.3.2. *Assume that L_h is hyperregular, then the dynamics associated with the Hamiltonian system (ω_h, H_h) is equivalent to the semi-discrete Euler–Lagrange equations (3.2).*

Proof. Since we assumed that L_h is hyperregular, i.e., that the associated Legendre transform is a diffeomorphism $T\Lambda_h^k \to T^*\Lambda_h^k$, we have $\dot{\varphi}^i$ as a function of (φ^j, π_j). To verify the equivalence, we compute the equations (3.9) for our given system. Compute for L evaluated at $(t, \varphi^i v_i, \dot{\varphi}^i v_i)$,

$$\begin{aligned}
M_j^{\ k}\dot{\pi}_k &= -\frac{\partial H_h}{\partial \varphi^j} = -\frac{\partial}{\partial \varphi^j}\Big(M_i^{\ k}\pi_k\dot{\varphi}^i - L\Big) \\
&= -M_i^{\ k}\pi_k\frac{\partial \dot{\varphi}^i}{\partial \varphi^j} + \frac{\partial}{\partial \varphi^j}\int_{\Sigma_t}\mathscr{L}(x^\mu, \varphi^i v_i, \dot{\varphi}^i v_i, \varphi^i dv_i) \\
&= -M_i^{\ k}\pi_k\frac{\partial \dot{\varphi}^i}{\partial \varphi^j} + \int_{\Sigma_t}\Big[\partial_2\mathscr{L}\wedge\star\frac{\partial(\varphi^i v_i)}{\partial \varphi^j} + \partial_3\mathscr{L}\wedge\star\frac{\partial(\dot{\varphi}^i v_i)}{\partial \varphi^j} + \partial_4\mathscr{L}\wedge\star\frac{\partial(\varphi^i dv_i)}{\partial \varphi^j}\Big] \\
&= -M_i^{\ k}\pi_k\frac{\partial \dot{\varphi}^i}{\partial \varphi^j} + \int_{\Sigma_t}\Big[\partial_2\mathscr{L}\wedge\star v_j + \partial_3\mathscr{L}\wedge\star v_i\frac{\partial \dot{\varphi}^i}{\partial \varphi^j} + \partial_4\mathscr{L}\wedge\star dv_j\Big] \\
&= -M_i^{\ k}\pi_k\frac{\partial \dot{\varphi}^i}{\partial \varphi^j} + (\partial_3\mathscr{L}, v_i)\frac{\partial \dot{\varphi}^i}{\partial \varphi^j} + (\partial_2\mathscr{L}, v_j)_{L^2} + (\partial_4\mathscr{L}, dv_j)_{L^2} \\
&= (\partial_2\mathscr{L}, v_j)_{L^2} + (\partial_4\mathscr{L}, dv_j)_{L^2},
\end{aligned}$$

where in the second to last line, the first two terms cancel since $(\partial_3\mathscr{L}, v_i) = \langle \pi, v_i\rangle = \langle \pi_k v^k, v_i\rangle = M_i^{\ k}\pi_k$. Then, note the left hand side is equivalently given by

$$M_j^{\ k}\dot{\pi}_k = M_j^{\ k}\frac{d}{dt}\pi_k = \frac{d}{dt}\big(M_j^{\ k}\pi_k\big) = \frac{d}{dt}\big(\langle v^k, v_j\rangle\pi_k\big) = \frac{d}{dt}\langle \pi, v_j\rangle = \frac{d}{dt}(\partial_3\mathscr{L}, v_j)_{L^2}.$$

Thus,

$$\frac{d}{dt}(\partial_3\mathscr{L}, v_j)_{L^2} = (\partial_2\mathscr{L}, v_j)_{L^2} + (\partial_4\mathscr{L}, dv_j)_{L^2},$$

which holds for each j and hence is equivalent to (3.2). □

Remark 1.3.7. *In the above proposition, we assumed that L_h was hyperregular for the equivalence. If L_h is not hyperregular, corresponding to a degenerate field theory, the dynamics associated to H_h evolve over a primary constraint surface. In this case, the dynamics of H_h on the constraint surface corresponds to a (not necessarily unique) solution of the semi-discrete Euler–Lagrange equation. In this setting, the dynamics are associated to the modified Hamiltonian $\bar{H}(\vec{\varphi}, \vec{\pi}, \lambda) = H(\vec{\varphi}, \vec{\pi}) + \lambda^A\Phi_A(\vec{\varphi}, \vec{\pi})$.*

The above also shows that, in the hyperregular case, the semi-discrete Euler–Lagrange equations correspond to a symplectic flow. The associated symplectic form is the pullback of

ω_h by the Legendre transform $\mathbb{F}L_h : T\Lambda_h^k \to T^*\Lambda_h^k$. In the non-regular case, the semi-discrete Euler–Lagrange equations correspond to a presymplectic flow.

To summarize, in this section, we have pulled back the symplectic structure on $T^*H\Lambda^k$ to $T^*\Lambda_h^k$ and showed that the dynamics of the Hamiltonian system (ω_h, H_h) is equivalent, in the hyperregular case, to the semi-discrete Euler–Lagrange equations of the corresponding Lagrangian system. By applying a numerical integrator for the finite-dimensional Hamiltonian system associated to H_h, we obtain a full discretization of the evolution problem for a field theory.

1.3.3 Energy-Momentum Map

In this section, we examine how symmetries in the canonical formulation are affected by the semi-discretization of the field theory. In the canonical setting, the manifestation of the covariant momentum map is the energy-momentum map. If a vector in the Lie algebra of the symmetry group gives rise to an infinitesimal generator on X which is transverse to the foliation, its pairing with the energy-momentum map equals the instantaneous Hamiltonian defined by that generator (the "energy" component). On the other hand, if the corresponding generator is tangent to the foliation, the pairing is given by the usual momentum map of the instantaneous Hamiltonian theory, corresponding to the canonical form (3.6) (the "momentum" component). We will see that, in the case of an equivariant discretization, the iterated pullback of the energy-momentum map provides the natural energy-momentum structure of the semi-discrete theory.

We start by investigating the momentum map structure of the semi-discrete theory. Let K be a Lie group acting on $H\Lambda^k$, with Lie algebra $\mathfrak{k} := T_eK$. For $\eta \in K$, we denote the group action $\overline{\eta}\varphi := \eta \cdot \varphi$ and the associated cotangent action is given by $\widetilde{\eta} := (\overline{\eta^{-1}})^*$. We use the same notation for these actions restricted to Λ_h^k and $T^*\Lambda_h^k$, where the restriction is well-defined if the projection is group-equivariant.

Proposition 1.3.3. *Assume that K acts by symplectomorphisms on $(T^*H\Lambda^k,\omega)$. Since K acts by cotangent lifts on $T^*H\Lambda^k$, it admits a canonical momentum map $J: T^*H\Lambda^k \to \mathfrak{k}^*$. Furthermore, assume that the projection map π_h is equivariant with respect to the K-action on $H\Lambda^k$ and Λ^k_h, i.e., $\pi_h\bar{\eta}\varphi = \bar{\eta}\pi_h\varphi$. Then, K acts by cotangent-lifted symplectomorphisms on $(T^*\Lambda^k_h,\omega_h)$ and the canonical momentum map for this action J_h is given by $J_h = \pi_h^{**}J = J\circ\pi_h^*$.*

Proof. To see that K preserves ω_h, for any $\eta \in K$, by equivariance, we have that

$$\widetilde{\eta}^*\omega_h = (\overline{\eta^{-1}})^{**}\pi_h^{**}\omega = (\overline{\eta^{-1}}\pi_h)^{**}\omega = (\pi_h\overline{\eta^{-1}})^{**}\omega = \pi_h^{**}(\overline{\eta^{-1}})^{**}\omega = \pi_h^{**}\omega = \omega_h.$$

A similar result holds for θ_h, since K preserves θ by virtue of the fact that it acts by cotangent lifted actions.

The canonical momentum map J is given by $\langle J(\varphi,\pi),\xi\rangle = \xi_{T^*H\Lambda^k}(\varphi,\pi)\lrcorner\,\theta|_{(\varphi,\pi)}$ for $(\varphi,\pi)\in T^*H\Lambda^k$ whereas $\langle J_h(\varphi,\pi),\xi\rangle = \xi_{T^*\Lambda^k_h}(\varphi,\pi)\lrcorner\,\theta_h|_{(\varphi,\pi)}$ for $(\varphi,\pi)\in T^*\Lambda^k_h$. These are both momentum maps for their respective actions since K acts by cotangent lifts. Then,

$$\begin{aligned}
\langle J_h(\varphi,\pi),\xi\rangle &= \xi_{T^*\Lambda^k_h}(\varphi,\pi)\lrcorner\,\theta_h = \xi_{T^*\Lambda^k_h}(\varphi,\pi)\lrcorner\,\pi_h^{**}\theta \\
&= [T\pi_h^*\xi_{T^*\Lambda^k_h}(\varphi,\pi)]\lrcorner\,\theta = \left[T\pi_h^*\frac{d}{dt}\Big|_{t=0}\widetilde{e^{t\xi}}(\varphi,\pi)\right]\lrcorner\,\theta \\
&= \left[\frac{d}{dt}\Big|_{t=0}\pi_h^*(\overline{e^{-t\xi}})^*(\varphi,\pi)\right]\lrcorner\,\theta \\
&= \left[\frac{d}{dt}\Big|_{t=0}(\overline{e^{-t\xi}}\pi_h)^*(\varphi,\pi)\right]\lrcorner\,\theta \\
&= \left[\frac{d}{dt}\Big|_{t=0}(\pi_h\overline{e^{-t\xi}})^*(\varphi,\pi)\right]\lrcorner\,\theta \\
&= \left[\frac{d}{dt}\Big|_{t=0}(\overline{e^{-t\xi}})^*\pi_h^*(\varphi,\pi)\right]\lrcorner\,\theta \\
&= \xi_{T^*H\Lambda^k}(\pi_h^*(\varphi,\pi))\lrcorner\,\theta = \langle (J\circ\pi_h^*)(\varphi,\pi),\xi\rangle.
\end{aligned}$$

where we have implicitly evaluated θ_h at (φ,π) and θ at $\pi_h^*(\varphi,\pi)$. Hence, $J_h = J\circ\pi_h^*$ or, equivalently, $J_h = \pi_h^{**}J$. □

Remark 1.3.8. *As can be seen in the proof, one does not need full K-equivariance of the* *projection, but only infinitesimal equivariance, i.e.,* $\pi_h(e^{t\xi}\varphi) - e^{t\xi}\pi_h\varphi = o(t)$.

Furthermore, one can weaken the notion of equivariance to $\pi_h\bar{\eta} = \overline{\psi_h(\eta)}\pi_h$, *where* $\psi_h : K \to K$ *is a Lie group homomorphism. In this case, if* $\tilde{\psi}_h$ *denotes the induced Lie algebra homomorphism, we can see from the above proof that the semi-discrete momentum map is related to the original momentum map via* $\langle J_h, \xi \rangle = \langle J \circ \pi_h^*, \tilde{\psi}_h(\xi) \rangle$.

As discussed in the covariant case, the weakening of this condition can allow us to construct more general projections.

Corollary 1.3.1. *Assuming as in the proposition, if J is Ad***-equivariant, then so is* J_h.

Proof. This follows immediately from $J_h = J \circ \pi_h^*$, K-equivariance of π_h, and Ad^*-equivariance of J, $J \circ \widetilde{\eta} = \mathrm{Ad}^*_\eta J$ (where $\mathrm{Ad}^*_\eta := (\mathrm{Ad}(\eta^{-1}))^*$),

$$\begin{aligned} J_h \circ \widetilde{\eta} &= J \circ \pi_h^* \circ (\overline{\eta^{-1}})^* = J \circ (\overline{\eta^{-1}})^* \circ \pi_h^* \\ &= J \circ \widetilde{\eta} \circ \pi_h^* = (\mathrm{Ad}^*_\eta J) \circ \pi_h^* = \mathrm{Ad}^*_\eta (J \circ \pi_h^*) = \mathrm{Ad}^*_\eta J_h, \end{aligned}$$

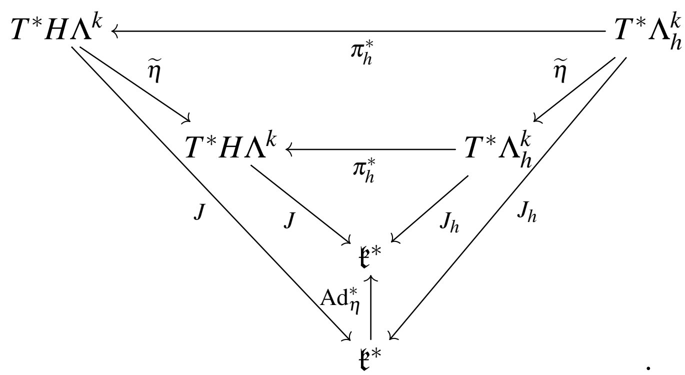
where the equality $(\mathrm{Ad}^*_\eta J) \circ \pi_h^* = \mathrm{Ad}^*_\eta (J \circ \pi_h^*)$ holds since the coadjoint action acts on J after it is evaluated on its input, which is then an element of $\mathfrak{k}^*$. In particular, $(\mathrm{Ad}^*_\eta J)(\varphi, \pi) := \mathrm{Ad}^*_\eta (J(\varphi, \pi))$, so that

$$((\mathrm{Ad}^*_\eta J) \circ \pi_h^*)(\varphi, \pi) = (\mathrm{Ad}^*_\eta J)(\pi_h^*(\varphi, \pi)) = \mathrm{Ad}^*_\eta (J(\pi_h^*(\varphi, \pi))) = \mathrm{Ad}^*_\eta ((J \circ \pi_h^*)(\varphi, \pi))).$$

Stated another way, this follows from associativity of the composition of functions, viewing Ad^*_η as a function $\mathfrak{k}^* \to \mathfrak{k}^*$. □

Remark 1.3.9. *Of course, since K acts by cotangent lifts and hence by canonical symplectomorphisms, J is an Ad***-equivariant momentum map, and the corollary tells us that* J_h *is as well. However, as we remark below, one may consider more general actions which admit momentum maps, and it is not necessarily the case that those momentum maps are Ad***-equivariant. The* *result of the previous corollary still holds in this more general setting.*

The naturality of the momentum map structures from the previous proposition and corollary can be summarized via the following commuting diagram; for any $\eta \in K$,



Remark 1.3.10. *In the above proposition, we only assumed that π_h was equivariant with respect to the K-action on the configuration space, and it follows that π_h^* is equivariant with respect to the lifted action on the cotangent space. However, for more general actions on the cotangent space that do not arise from a cotangent lift, one must instead assume π_h^* is equivariant with respect to this action. In this case, if the K-action on $T^*H\Lambda^k$ admits a momentum map J, then $J_h = \pi_h^{**}J$ is a momentum map for the action on $T^*\Lambda^k_h$. To verify this, let $(\varphi,\pi) \in T^*\Lambda^k_h$. We know that $d\langle J,\xi\rangle = i_{\xi_{T^*H\Lambda^k}}\omega$. Thus,*

$$d\langle J_h,\xi\rangle = \pi_h^{**} d\langle J,\xi\rangle = \pi_h^{**}(i_{\xi_{T^*H\Lambda^k}}\omega).$$

Then, observe that by equivariance, $\xi_{T^*H\Lambda^k}(\varphi,\pi) = T\pi_h^*\xi_{T^*\Lambda^k_h}(\varphi,\pi)$. Then, for any $X \in TT^*_{(\varphi,\pi)}\Lambda^k_h$,

$$d\langle J_h,\xi\rangle(X) = (i_{\xi_{T^*H\Lambda^k}}\omega)(T\pi_h^*X) = \omega(T\pi_h^*\xi_{T^*\Lambda^k_h}, T\pi_h^*X) = (\pi_h^{**}\omega)(\xi_{T^*\Lambda^k_h}, X) = (i_{\xi_{T^*\Lambda^k_h}}\omega_h)(X),$$

where the above is evaluated at (φ,π), which verifies that J_h is a momentum map. For the subsequent discussion, we will assume that K acts by cotangent lifts.

We now define the energy-momentum map (Gotay et al. [45]) and its semi-discrete counterpart. We consider vectors on Σ_t with both tangent components in $T\Sigma_t$ and components transverse to the foliation, which in our adapted coordinates are in the span of $\partial/\partial t$. We extend the canonical form θ to act on vector fields on the extended phase space in the same way that we extended ω_h in our previous discussion of time-dependence. Let $\widetilde{\mathscr{L}}$ denote the Lagrangian density on the full spacetime, which is related to the instantaneous Lagrangian density by $\mathscr{L} = i_t^* \partial_t \lrcorner \tilde{\mathscr{L}}$. Define the map $\mathscr{J}$ from $I \times T^* H\Lambda^k$ to the dual of the space of vector fields on the extended phase space, via

$$\langle \mathfrak{J}(t, \varphi, \pi), V \rangle = (V \lrcorner \theta)(t, \varphi, \pi) - \int_\Sigma i_t^* V_t \lrcorner \widetilde{\mathscr{L}}(x^\mu, \varphi, \dot{\varphi}, d\varphi), \tag{3.10}$$

where we view $\dot{\varphi}$ as a function of (φ, π), and where V_t is the tangent-lift of the bundle projection $I \times T^* H\Lambda^k(\Sigma_t) \to I$ applied to V.

Proposition 1.3.4. $\mathfrak{J}$ *is the energy-momentum map, in the following sense:*

(i) ***(Energy)*** *Let Φ_t^H denote the Hamiltonian flow of H, and X_H be the associated generator on the extended phase space, then,*

$$\langle \mathfrak{J}(t, \varphi, \pi), X_H \rangle = H(t, \varphi, \pi).$$

(ii) ***(Momentum)*** *If V is tangent to the foliation, then,*

$$\langle \mathfrak{J}(t, \varphi, \pi), V \rangle = (V \lrcorner \theta)(t, \varphi, \pi),$$

and in particular, if there is a K-action as in Proposition (1.3.3) on the phase space over Σ_t, its momentum map J is given by

$$\langle J(t, \varphi, \pi), \xi \rangle = \langle \mathfrak{J}(t, \varphi, \pi), \xi_{T^* H\Lambda^k} \rangle,$$

such that, for each fixed t, $d\langle J(t,\varphi,\pi),\xi\rangle = \xi_{T^*H\Lambda^k} \lrcorner\, \omega(t,\varphi,\pi)$.

Proof. For the proof of (i), in local coordinates, we have that

$$X_H = \frac{d}{dt}\Big|_{t=0} \Phi_t^H(t',\varphi,\pi) = \frac{\partial}{\partial t} + \dot{\varphi}^A \frac{\partial}{\partial \varphi^A} + \dot{\pi}_B \frac{\partial}{\partial \pi_B},$$

and $(X_H)_t = \partial/\partial t$. Using expressions (3.6) and (3.10), and the definition of the instantaneous Lagrangian density $\mathscr{L} = i_t^* \partial_t \lrcorner\, \widetilde{\mathscr{L}}$, we have that

$$\begin{aligned}
\langle \mathfrak{J}(t,\varphi,\pi), X_H\rangle &= (X_H \lrcorner\, \theta)(t,\varphi,\pi) - \int_\Sigma i_t^* (X_H)_t \lrcorner\, \widetilde{\mathscr{L}}(x^\mu,\varphi,\dot{\varphi},d\varphi) \\
&= \dot{\varphi}^A \frac{\partial}{\partial \varphi^A} \lrcorner \Big(\int_{\Sigma_t} \pi_A d\varphi^A \otimes d^n x_0 \Big) - \int_\Sigma i_t^* \frac{\partial}{\partial t} \lrcorner\, \widetilde{\mathscr{L}}(x^\mu,\varphi,\dot{\varphi},d\varphi) \\
&= \int_{\Sigma_t} \pi_A \dot{\varphi}^A d^n x_0 - \int_\Sigma \mathscr{L}(t,x^i,\varphi,\dot{\varphi},d\varphi) \\
&= \langle \pi,\dot{\varphi}\rangle - L(t,\varphi,\dot{\varphi}) = H(t,\varphi,\pi).
\end{aligned}$$

For the proof of (ii), note that for V tangent to the foliation, $V_t = 0$, which immediately gives the first equation of (ii). Setting the vector field to an infinitesimal generator of a K-action gives the momentum map

$$\langle \mathfrak{J}(t,\varphi,\pi), \xi_{T^*H\Lambda^k}\rangle = (\xi_{T^*H\Lambda^k} \lrcorner\, \theta)(t,\varphi,\pi).$$

□

We now define the semi-discrete analogue of the energy-momentum map (3.10). Define the semi-discrete energy-momentum map $\mathscr{J}_h$ from $I \times T^*\Lambda_h^k$ to the dual of vector fields on the extended discrete phase space, via

$$\langle \mathfrak{J}_h(t,\varphi,\pi), V\rangle = (V \lrcorner\, \theta_h)(t,\varphi,\pi) - \int_\Sigma i_t^* V_{t,h} \lrcorner\, \widetilde{\mathscr{L}_h}(x^\mu,\varphi,\dot{\varphi},d\varphi), \tag{3.11}$$

where $V_{t,h} = (T\pi_h^* V)_t$ and $\widetilde{\mathscr{L}_h}$ is the restriction of $\widetilde{\mathscr{L}}$ via precomposition with π_h^*. Of course, the analogous statement of the previous proposition holds for the semi-discrete energy-momentum map. Furthermore, $\mathscr{J}_h$ is the restriction of $\mathscr{J}$ in the following sense.

Proposition 1.3.5. *For (t,φ,π) in the extended discrete phase space and V a vector field over this space,*

$$\langle \mathfrak{J}_h(t,\varphi,\pi), V\rangle = \langle \mathfrak{J}(t,\pi_h^*(\varphi,\pi)), T\pi_h^* V\rangle.$$

Proof. This follows directly from the definitions,

$$\begin{aligned}
\langle \mathfrak{J}(t,\pi_h^*(\varphi,\pi)), T\pi_h^* V\rangle &= (T\pi_h^* V \lrcorner\, \theta)(t,\pi_h^*(\varphi,\pi)) - \int_\Sigma i_t^*(T\pi_h^* V)_t \lrcorner\, \widetilde{\mathscr{L}}(t,\pi_h^*[(\varphi,\dot{\varphi},d\varphi)|_{(\varphi,\pi)}]) \\
&= (V \lrcorner\, \pi_h^{**}\theta)(t,\varphi,\pi) - \int_\Sigma i_t^* V_{t,h} \lrcorner\, \widetilde{\mathscr{L}_h}(t,\varphi,\dot{\varphi},d\varphi) \\
&= (V \lrcorner\, \theta_h)(t,\varphi,\pi) - \int_\Sigma i_t^* V_{t,h} \lrcorner\, \widetilde{\mathscr{L}_h}(t,\varphi,\dot{\varphi},d\varphi) = \langle \mathfrak{J}_h(t,\varphi,\pi), V\rangle.
\end{aligned}$$

□

The significance of this definition of the semi-discrete energy-momentum map is that it recovers the properties of Proposition 1.3.4 in the semi-discrete setting.

Proposition 1.3.6.

(i) ***(Semi-discrete Energy)*** *For (t,φ,π) in the extended discrete phase space,*

$$\langle \mathfrak{J}_h(t,\varphi,\pi), X_{H_h}\rangle = H_h(t,\varphi,\pi).$$

(ii) ***(Semi-discrete Momentum)*** *If there is a K-action on the discrete phase space, then the momentum map J_h is given by*

$$\langle J_h(t,\varphi,\pi),\xi\rangle = \langle \mathfrak{J}_h(t,\varphi,\pi), \xi_{T^*\Lambda_h^k}\rangle.$$

Furthermore, if the K-action on the discrete space arises from an action on the full space *such that π_h is K-equivariant, then for any $\xi \in \mathfrak{k}$,*

$$\langle \mathfrak{J}_h(t,\varphi,\pi), \xi_{T^*\Lambda_h^k} \rangle = \langle \mathfrak{J}(t,\pi_h^*(\varphi,\pi)), \xi_{T^*H\Lambda^k} \rangle.$$

Proof. The first two equations follow from analogous computations to the proof of Proposition 1.3.4. The last equation follows from the equivariance of π_h,

$$T\pi_h^* \xi_{T^*\Lambda_h^k}(\varphi,\pi) = \xi_{T^*H\Lambda^k}(\pi_h^*(\varphi,\pi)),$$

and Proposition 1.3.5. □

The significance of a semi-discrete analogue of the energy-momentum map, aside from extending the semi-discrete momentum map structure, that was discussed in Proposition 1.3.3, is in determining semi-discrete analogues of Noether's second theorem, which we will pursue in subsequent work.

1.3.4 Temporal Discretization of the Semi-Discrete Theory

To complete the discussion of the semi-discrete theory, we must of course discretize in time. We obtain a full discretization of the semi-discrete theory by discretizing the semi-discrete Euler–Lagrange equation (3.2) in time via a Galerkin Lagrangian variational integrator applied to the instantaneous semi-discrete Lagrangian (3.3), and show that this is equivalent to the full spacetime DEL (2.8) with tensor product elements. The associated finite element on the full spacetime is a tensor product mesh, obtained by discretizing the space Σ and extending these elements in time by a partition of I. Of course, this is not the most general setup for a spacetime discretization, but often one wishes to discretize in time separately. For example, by choosing the appropriate temporal basis functions, the computation becomes local in time so that one can time march the solution from the initial data, instead of solving the entire DEL on the spacetime grid. Furthermore, there are constructions of cochain projections for tensor product elements

(Arnold [6]) so that with these finite element spaces, the naturality of the variational principle discussed in Section 2 carries over in the tensor product setting.

Assume the same setup as in the discussion of the semi-discrete theory. Furthermore, assume that we have a finite element discretization of $H_0(I)$, the space of square integrable functions in time with square integrable derivative, which vanish on ∂I, with basis functions $\{w_\alpha\}$. Recall the instantaneous semi-discrete Lagrangian (3.3) is a function of the curves $\varphi^i(t), \dot{\varphi}^i(t)$ which are the coefficients of the expansions of $\varphi(t), \dot{\varphi}(t) \in \Lambda^k_h$ relative to the basis $\{v_i\}$ of Λ^k_h. Using the basis $\{w_\alpha\}$, we discretize these curves as

$$\varphi^i(t) = (\varphi^i)^\alpha w_\alpha(t),$$

where $\varphi(t) = (\varphi^i)^\alpha w_\alpha(t) v_i \in \Lambda^k_h$ in this notation. We consider the associated fully discrete action as a function of the coefficients,

$$S[\{(\varphi^i)^\alpha\}] = \int_I dt L_h(t, \varphi^i(t), \dot{\varphi}^i(t)) = \int_I dt L_h(t, (\varphi^i)^\alpha w_\alpha, (\varphi^i)^\alpha \dot{w}_\alpha).$$

Enforcing the discrete variational principle in time gives the weak form of the Euler–Lagrange equations,

$$0 = \frac{\delta S}{\delta(\varphi^i)^\alpha} = \left(\frac{\partial L_h}{\partial \varphi^i}, w_\alpha\right)_{L^2(I)} + \left(\frac{\partial L_h}{\partial \dot{\varphi}^i}, \dot{w}_\alpha\right)_{L^2(I)}.$$

Substituting equations (3.5a) and (3.5b) gives

$$\begin{aligned}
0 &= -((\partial_3 \mathscr{L}, v_i)_{L^2\Lambda^k(\Sigma)}, \dot{w}_\alpha)_{L^2(I)} - ((\partial_2 \mathscr{L}, v_i)_{L^2\Lambda^k(\Sigma)}, w_\alpha)_{L^2(I)} - ((\partial_4 \mathscr{L}, dv_i)_{L^2\Lambda^{k+1}(\Sigma)}, w_\alpha)_{L^2(I)} \\
&= -(\partial_3 \mathscr{L}, v_i \dot{w}_\alpha)_{L^2(I, L^2\Lambda^k(\Sigma))} - (\partial_2 \mathscr{L}, v_i w_\alpha)_{L^2(I, L^2\Lambda^k(\Sigma))} - (\partial_4 \mathscr{L}, (dv_i) w_\alpha)_{L^2(I, L^2\Lambda^{k+1}(\Sigma))} \\
&= -\left(\frac{\partial \mathscr{L}}{\partial \dot{\varphi}}, v_i \dot{w}_\alpha\right)_{L^2(I, L^2\Lambda^k(\Sigma))} - \left(\frac{\partial \mathscr{L}}{\partial \varphi}, v_i w_\alpha\right)_{L^2(I, L^2\Lambda^k(\Sigma))} \\
&\quad - \left(\frac{\partial \mathscr{L}}{\partial (d\varphi)}, (dv_i) w_\alpha\right)_{L^2(I, L^2\Lambda^{k+1}(\Sigma))}.
\end{aligned}$$

Note that these equations can also be obtained directly from the semi-discrete Euler–Lagrange equations (3.2) by applying the Galerkin method in time with respect to the basis $\{w_\alpha\}$. Here, d denotes the spatial exterior derivative on Σ. If d_t denotes the temporal exterior derivative and we identity functions on I with one-forms on I, we have $\dot{w}_\alpha \cong d_t w_\alpha$. If $d_T = d + d_t$ denotes the total exterior derivative on $\Sigma \times I$, then $d_T(v_i w_\alpha) = (dv_i)w_\alpha + v_i d_t w_\alpha$, where, as discussed in Remark 1.3.1, we are considering k-forms of the form $\sum_{J \in I^k_\Sigma} \phi_J(t,x)dx^J$. We now view the time-dependent k-form $\varphi : t \mapsto \varphi(t)$ as a k-form ϕ on spacetime, so the above can be written as

$$
\begin{aligned}
0 = &-\left(\frac{\partial \mathscr{L}}{\partial \phi}, v_i w_\alpha\right)_{L^2\Lambda^k(\Sigma\times I)} \\
&- \left(\frac{\partial \mathscr{L}}{\partial (d\phi)}, (dv_i)w_\alpha\right)_{L^2(I,L^2\Lambda^{k+1}(\Sigma))} - \left(\frac{\partial \mathscr{L}}{\partial (d_t\phi)}, v_i d_t w_\alpha\right)_{L^2\Lambda^1(I,L^2\Lambda^k(\Sigma))} \\
= &-\left(\frac{\partial \mathscr{L}}{\partial \phi}, v_i w_\alpha\right)_{L^2(\Sigma\times I)} - \left(\frac{\partial \mathscr{L}}{\partial (d_T\phi)}, d_T(v_i w_\alpha)\right)_{L^2\Lambda^{k+1}(\Sigma\times I)},
\end{aligned}
$$

which is the DEL (2.8) with tensor product basis $\{v_i w_\alpha\}$.

Note that this result can also be obtained from the semi-discrete Hamiltonian setting, assuming that L_h is hyperregular, using the fact that the semi-discrete Hamiltonian and semi-discrete Lagrangian formulations are equivalent by Proposition 1.3.2, and the fact that Galerkin Lagrangian variational integrators and Galerkin Hamiltonian variational integrators are equivalent in the hyperregular case, as established in Leok and Zhang [76].

1.4 Conclusion and Future Directions

In this paper, we showed how discretizing the variational principle for Lagrangian field theories using finite element cochain projections naturally gives rise to a discrete variational structure which is analogous to the continuum variational structure. Namely, the discrete variational structure is encoded by the discrete Cartan form. Our discrete Cartan form generalizes the discrete Cartan form introduced by Marsden et al. [85] to more general finite element spaces within the finite element exterior calculus framework. Using the discrete Cartan form, we expressed a discrete multisymplectic form formula and a discrete Noether theorem in direct analogy to their continuum counterparts. Furthermore, we studied semi-discretization of Lagrangian PDEs by spatial cochain projections, showing that such semi-discretization gives rise to semi-discrete symplectic, Hamiltonian, and energy-momentum map structures. Finally, we related the methods obtained by covariant discretization and canonical semi-discretization in the case of tensor product finite elements.

In the paper, we outlined several possible research directions, including studying particular field theories and showing rigorous convergence of the discrete Cartan form, constructing group-equivariant cochain projections, and establishing a discrete Noether's second theorem utilizing the semi-discrete energy-momentum map. Another natural research direction would be to extend the discrete variational structures presented here to the discontinuous Galerkin setting and compare them with the results obtained in the multisymplectic Hamiltonian setting by McLachlan and Stern [90]. In particular, we expect that in this setting, the discrete Cartan form would only involve integration over ∂U, since boundary variations can be localized to codimension-one simplices, unlike for conforming finite element spaces. Furthermore, we aim to investigate how the discrete variational structures presented in this paper in the conforming setting, and extended to the discontinuous Galerkin setting, can be used to provide a geometric variational framework for studying lattice field theories, building on the discrete variational framework for lattice field theories initiated in Arjang and Zapata [5].

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Chapter 2

Multisymplectic Hamiltonian Variational Integrators

2.1 Introduction

Variational integrators have become an important class of geometric numerical integrators for the simulation of mechanical systems, and provides a systematic method of constructing symplectic integrators. The variational approach has numerous benefits, the first of which is that the resulting numerical integrators are automatically symplectic, and if they are group-invariant, then they satisfy a discrete Noether's theorem and preserve a discrete momentum map. In addition, it can be shown that the order of accuracy is related to the best approximation properties of the finite-dimensional function spaces and the order of the quadrature rule used to construct the variational integrator [52].

However, the variational integrator approach has traditionally been applied to Lagrangian formulations of mechanical systems, as summarized in Marsden and West [84], and the development of Hamiltonian variational integrators has been less extensive. The notion of Hamiltonian variational integrators was first introduced in Lall and West [65] as the dual formulation of a discrete constrained variational principle, but it did not provide an explicit characterization of the discrete Hamiltonian in terms of the continuous Hamiltonian and the corresponding discrete Noether's theorem, which was introduced in Leok and Zhang [76]. This involves constructing the exact Type II/Type III generating functions for the Hamiltonian flow of a mechanical system, which can be viewed as the analogue of Jacobi's solution of the Hamilton–Jacobi equation. The variational error analysis result for Hamiltonian variational integrators was established in Schmitt and Leok [107], and methods based on Taylor expansions were developed in Schmitt et al. [108].

Hamiltonian variational integrators also find application in discrete optimal control and discrete Hamilton–Jacobi theory, and it was shown in Ohsawa et al. [95] that the Bellman equations of discrete optimal control are the lowest order approximation of a continuous optimal control problem arising from a particular choice of Hamiltonian variational integrator. The Poincaré transformed Hamiltonian was used independently by Hairer [50] and Reich [97] as a means of constructing time-adaptive symplectic integrators, and an adaptive approach based on Hamiltonian variational integrators was developed in Duruisseaux et al. [37]. The Hamiltonian approach is necessary in this case as many monitor functions result in Poincaré transformed Hamiltonians that are degenerate, for which no Lagrangian analogue exists.

In the setting of Lagrangian and Hamiltonian partial differential equations, multisymplectic integrators that can be viewed as generalizations of symplectic integrators for mechanical systems to field theories were introduced from a Lagrangian perspective in Marsden et al. [85], and from the Hamiltonian, but non-variational perspective, in Bridges and Reich [20]. Our approach to constructing a variational description of multisymplectic integrators for Hamiltonian partial differential equations is based on the notion of generating functionals for multisymplectic relations that was introduced in Vankerschaver et al. [116].

The advantage of the discrete variational principle approach is that it automatically yields multisymplectic integrators, and exhibit a discrete analogue of Noether's theorem. Furthermore, they naturally lend themselves to Galerkin discretizations that allow for the systematic construction of multisymplectic integrators by choosing a finite-dimensional approximation space for sections of the configuration bundle, and a numerical quadrature rule. In addition, group-invariant discretizations that exhibit a discrete Noether's theorem can be constructed from finite-dimensional approximation spaces that are equivariant with respect to the Lie symmetry group that generates the relevant momentum map.

2.1.1 Lagrangian and Hamiltonian Variational Integrators

Geometric numerical integration aims to preserve geometric conservation laws under discretization, and this field is surveyed in the monograph by Hairer et al. [51]. Discrete variational mechanics [75; 84] provides a systematic method of constructing symplectic integrators. It is typically approached from a Lagrangian perspective by introducing the *discrete Lagrangian*, $L_d : Q \times Q \to \mathbb{R}$, which is a Type I generating function of a symplectic map and approximates the *exact discrete Lagrangian*, which is constructed from the Lagrangian $L : TQ \to \mathbb{R}$ as

$$L_d^E(q_0, q_1; h) = \operatorname{ext}_{\substack{q \in C^2([0,h],Q) \\ q(0)=q_0, q(h)=q_1}} \int_0^h L(q(t), \dot{q}(t))dt, \tag{1.1}$$

which is equivalent to Jacobi's solution of the Hamilton–Jacobi equation. The exact discrete Lagrangian generates the exact discrete-time flow map of a Lagrangian system, but, in general, it cannot be computed explicitly. Instead, this can be approximated by replacing the integral with a quadrature formula, and replacing the space of C^2 curves with a finite-dimensional function space.

Given a finite-dimensional function space $\mathbb{M}^n([0,h]) \subset C^2([0,h],Q)$ and a quadrature formula $\mathcal{G} : C^2([0,h],Q) \to \mathbb{R}$, $\mathcal{G}(f) = h\sum_{j=1}^m b_j f(c_j h) \approx \int_0^h f(t)dt$, the *Galerkin discrete Lagrangian* is

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

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

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

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

$$q_k^1 = q_{k+1}^0, \qquad p_{k+1} = D_2 L_d(q_k^0, q_k^1), \qquad p_k = -D_1 L_d(q_k^0, q_k^1), \tag{1.2}$$

where D_i denotes the partial derivative with respect to the i-th argument. Making the identification $q_k = q_k^0 = q_{k-1}^1$, we obtain the *discrete Lagrangian map* and *discrete Hamiltonian map* which are $F_{L_d} : (q_{k-1}, q_k) \mapsto (q_k, q_{k+1})$ and $\tilde{F}_{L_d} : (q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$, respectively. The last two equations of (4.1.2) define the *discrete fiber derivatives*, $\mathbb{F}L_d^{\pm} : Q \times Q \to T^*Q$,

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

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

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

Theorem 2.1.1 (Discrete Noether's theorem (Theorem 1.3.3 of [84]))**.** *If a discrete Lagrangian L_d is invariant under the diagonal action of G on $Q \times Q$, then the single unique discrete momentum map, $\mathbf{J}_{L_d} = (\mathbb{F}L_d^{\pm})^* \mathbf{J}$, is invariant under the discrete Lagrangian map F_{L_d}, i.e., $F_{L_d}^* \mathbf{J}_{L_d} = \mathbf{J}_{L_d}$.*

Theorem 2.1.2 (Variational error analysis (Theorem 2.3.1 of [84]))**.** *If a discrete Lagrangian L_d approximates the exact discrete Lagrangian L_d^E to order p, i.e., $L_d(q_0, q_1; h) = L_d^E(q_0, q_1; h) +$*

$\mathscr{O}(h^{p+1})$, *then the discrete Hamiltonian map* $\tilde{F}_{L_d}$ *is an order p accurate one-step method.*

The bounded energy error of variational integrators can be understood by performing backward error analysis, which then shows that the discrete flow map is approximated with exponential accuracy by the exact flow map of the Hamiltonian vector field of a modified Hamiltonian [11; 111].

Given a degenerate Hamiltonian, where the Legendre transform $\mathbb{F}H : T^*Q \to TQ$, $(q,p) \mapsto (q, \frac{\partial H}{\partial p})$, is noninvertible, there is no equivalent Lagrangian formulation. Thus, a characterization of variational integrators directly in terms of the continuous Hamiltonian is desirable. This is achieved by considering the Type II analogue of Jacobi's solution, given by

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

A computable Galerkin discrete Hamiltonian H_d^+ is obtained by choosing a finite-dimensional function space and a quadrature formula,

$$H_d^+(q_0, p_1) = \operatorname{ext}_{\substack{q\in\mathbb{M}^n([0,h]) \\ q(0)=q_0 \\ (q(c_jh),p(c_jh))\in T^*Q}} \left[p_1 q(t_1) - h\sum\nolimits_{j=1}^m b_j [p(c_jh)\dot{q}(c_jh) - H(q(c_jh), p(c_jh))] \right].$$

Interestingly, the Galerkin discrete Hamiltonian does not require a choice of a finite-dimensional function space for the curves in the momentum, as the quadrature approximation of the action integral only depend on the momentum values $p(c_jh)$ at the quadrature points, which are determined by the extremization principle. In essence, this is because the action integral does not depend on the time derivative of the momentum $\dot{p}$. As such, both the Galerkin discrete Lagrangian and the Galerkin discrete Hamiltonian depend only on the choice of a finite-dimensional function space for curves in the position, and a quadrature rule. It was shown in Proposition 4.1 of [76] that when the Hamiltonian is hyperregular, and for the same choice of function space and quadrature rule, they induce equivalent numerical methods.

The *Type II discrete Hamilton's phase space variational principle* states that

$$\delta\left\{p_N q_N - \sum_{k=0}^{N-1}\left[p_{k+1}q_{k+1} - H_d^+(q_k, p_{k+1})\right]\right\} = 0,$$

for discrete curves in T^*Q with fixed (q_0, p_N) boundary conditions. This yields the *discrete Hamilton's equations*, which are given by

$$q_{k+1} = D_2 H_d^+(q_k, p_{k+1}), \qquad p_k = D_1 H_d^+(q_k, p_{k+1}). \tag{1.3}$$

Given a discrete Hamiltonian H_d^+, we introduce the *discrete fiber derivatives* (or discrete Legendre transforms), $\mathbb{F}^+ H_d^+$,

$$\begin{aligned}\mathbb{F}^+ H_d^+ &: (q_0, p_1) \mapsto (D_2 H_d^+(q_0, p_1), p_1),\\ \mathbb{F}^- H_d^+ &: (q_0, p_1) \mapsto (q_0, D_1 H_d^+(q_0, p_1)).\end{aligned}$$

The discrete Hamiltonian map can be expressed in terms of the discrete fiber derivatives,

$$\tilde{F}_{H_d^+}(q_0, p_0) = \mathbb{F}^+ H_d^+ \circ (\mathbb{F}^- H_d^+)^{-1}(q_0, p_0) = (q_1, p_1),$$

Similar to the Lagrangian case, we have a discrete Noether's theorem and variational error analysis result for Hamiltonian variational integrators.

Theorem 2.1.3 (Discrete Noether's theorem (Theorem 5.3 of [76]))**.** *Let Φ^{T^*Q} be the cotangent lift action of the action Φ on the configuration manifold Q. If the generalized discrete Lagrangian $R_d(q_0, q_1, p_1) = p_1 q_1 - H_d^+(q_0, p_1)$ is invariant under the cotangent lifted action Φ^{T^*Q}, then the discrete Hamiltonian map $\tilde{F}_{H_d^+}$ preserves the momentum map, i.e., $\tilde{F}_{H_d^+}^* \mathbf{J} = \mathbf{J}$.*

Theorem 2.1.4 (Variational error analysis (Theorem 2.2 of [107]))**.** *If a discrete Hamiltonian H_d^+ approximates the exact discrete Hamiltonian $H_d^{+,E}$ to order p, i.e., $H_d^+(q_0, p_1; h) =$*

$H_d^{+,E}(q_0, p_1; h) + \mathscr{O}(h^{p+1})$, *then the discrete Hamiltonian map* $\tilde{F}_{H_d^+}$ *is an order* p *accurate one-step method.*

It should be noted that there is an analogous theory of discrete Hamiltonian variational integrators based on Type III generating functions $H_d^-(p_0, q_1)$.

Remark 2.1.1. *It should be noted that the current construction of Hamiltonian variational integrators is only valid on vector spaces and local coordinate charts as it involves Type II/Type III generating functions* $H_d^+(q_k.p_{k+1})$, $H_d^-(p_k, q_{k+1})$, *which depend on the position at one boundary point, and the momentum at the other boundary point. However, this does not make intrinsic sense on a manifold, since one needs the base point in order to specify the corresponding cotangent space. One possible approach to constructing an intrinsic formulation of Hamiltonian variational integrators is to start with discrete Dirac mechanics [75], and consider a generating function* $E_d^+(q_k, q_{k+1}, p_{k+1})$, $E_d^-(q_k, p_k, q_{k+1})$, *that depends on the position at both boundary points and the momentum at one of the boundary points. This approach can be viewed as a discretization of the generalized energy* $E(q,v,p) = \langle p,v\rangle - L(q,v)$, *in contrast to the Hamiltonian* $H(q,p) = \text{ext}_v\langle p,v\rangle - L(q,v) = \langle p,v\rangle - L(q,v)|_{p=\frac{\partial L}{\partial v}}$.

2.1.2 Multisymplectic Hamiltonian Field Theory

While classical field theories can be viewed as an infinite-dimensional Hamiltonian system with time as the independent variable (see, for example, Abraham and Marsden [1]), we will adopt the multisymplectic formulation with spacetime as the independent variables, which has been extensively studied in, for example, Gotay et al. [44, 45], Marsden and Shkoller [83], Marsden et al. [87]. The description of multisymplectic classical field theories in the literature is traditionally formulated in the Lagrangian setting or in the Hamiltonian setting via the covariant Legendre transform to pass between the two settings. However, as we are interested in constructing variational integrators purely within the Hamiltonian setting, we will outline the necessary ingredients of multisymplectic Hamiltonian field theory in this section, without the use of the Lagrangian framework or the covariant Legendre transform.

Consider a trivial vector bundle $E = X \times Q \to X$ over an oriented spacetime X (although we will refer to X as spacetime with evolutionary Hamiltonian PDEs in mind, X could be either Riemannian or Lorentzian), with volume form denoted $d^{n+1}x$. Let Θ be the Cartan form on the dual jet bundle J^1E^*, which has coordinates $(x^\mu, \phi^A, p, p^A_\mu)$, where x^μ are the coordinates on spacetime, ϕ^A are the coordinates on Q, and p and p^A_μ are the coordinates of the affine map on the jet bundle, $v^A_\mu \mapsto (p + p^\mu_A v^A_\mu) d^{n+1}x$. Define the restricted dual jet bundle $\widetilde{J^1E^*}$ as the quotient of J^1E^* by horizontal one-forms; this space is coordinatized by (x^μ, ϕ^A, p^A_μ) and is the relevant configuration bundle for a Hamiltonian field theory; we interpret ϕ^A as the value of the field and p^μ_A as the associated momenta in the direction x^μ. The dual jet bundle can be viewed as a bundle over the restricted bundle, $\mu : J^1E^* \to \widetilde{J^1E^*}$ (see León et al. [77]). Let $H \in C^\infty(\widetilde{J^1E^*})$ be the Hamiltonian of our theory. This defines a section of μ, in coordinates $\tilde{H}(x^\mu, \phi^A, p^\mu_A) = (x^\mu, \phi^A, -H, p^\mu_A)$ or using the projections $\pi^{j,k}$ from the bundle of $(j+k)$-forms on E to the subbundle of j-horizontal, k-vertical forms, this can be defined as the set of $z \in J^1E^*$ such that $\pi^{n+1,0}(z) = -H(\pi^{n,1}(z)) d^{n+1}x$. Using this section, one can pullback the Cartan form to a form on the restricted bundle,

$$\Theta_H = \tilde{H}^*\Theta = p^\mu_A d\phi^A \wedge d^n x_\mu - H d^{n+1}x.$$

We then define the action S^U (relative to an arbitrary region $U \subset X$) as a functional on the sections of $\widetilde{J^1E^*}$ (viewed as a bundle over spacetime),

$$S^U[\phi, p] = \int_U (\phi, p)^* \Theta_H. \tag{1.4}$$

Hamilton's principle states that this action is stationary for compactly supported vertical variations, i.e.,

$$0 = dS^U[\phi, p] \cdot V = \int_U (\phi, p)^* i_V d\Theta_H + \underbrace{\int_{\partial U} (\phi, p)^* i_V \Theta_H}_{=0,\ V \Subset U}.$$

Since U is arbitrary, for a sufficiently smooth solution, this gives the strong form of Hamilton's equations, $(\phi,p)^* i_V \Omega_H = 0$, where we defined the multisymplectic form $\Omega_H = -d\Theta_H$. In coordinates, for $V = \delta\phi^A \partial/\partial\phi^A + \delta p^\mu_A \partial/\partial p^\mu_A$, these equations read

$$\delta\phi^A(\partial_\mu p^\mu_A + \frac{\partial H}{\partial \phi^A})d^{n+1}x + \delta p^\mu_A(-\partial_\mu \phi^A + \frac{\partial H}{\partial p^\mu_A})d^{n+1}x = 0.$$

Since this must hold for $\delta\phi^A, \delta p^\mu_A$ independent, this gives the De Donder–Weyl equations

$$\partial_\mu p^\mu_A = -\frac{\partial H}{\partial \phi^A}, \tag{1.5a}$$

$$\partial_\mu \phi^A = \frac{\partial H}{\partial p^\mu_A}. \tag{1.5b}$$

To write these equations as a multi-Hamiltonian system, define $z^A = (\phi^A, p^0_A, \dots, p^n_A)^T$; it is clear that the De Donder–Weyl equations can be written as

$$\underbrace{\begin{pmatrix} 0 & -1 & 0 & \dots & 0 \\ 1 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}}_{\equiv K^0} \partial_0 z^A + \dots + \underbrace{\begin{pmatrix} 0 & 0 & \dots & 0 & -1 \\ 0 & \ddots & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ddots & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}}_{\equiv K^n} \partial_n z^A = \nabla_{z^A} H,$$

or $K^0\partial_0 z^A + \dots + K^n \partial_n z^A = \nabla_{z^A} H$, where the matrices K^μ are $(n+2)\times(n+2)$ skew-symmetric matrices which have value -1 in the $(0,\mu+1)$ entry and 1 in the $(\mu+1,0)$ entry (we are indexing the matrices from 0 to $n+1$), and 0 everywhere else. This form of the equations was studied in Bridges [18]. We can associate to each of these matrices a degenerate two-form on the restricted dual jet bundle,

$$\omega^\mu \equiv \sum_A d(z^A)^T \otimes K^\mu dz^A = (-dp^\mu_A \otimes d\phi^A + d\phi^A \otimes dp^\mu_A) = d\phi^A \wedge dp^\mu_A.$$

For simplicity of notation, we will implicitly suppress the duality pairing between $(\phi^A)_A$ (valued in Q) and $(p^\mu_A)_A$ (valued in Q^*) and write this as $\omega^\mu = d\phi \wedge dp^\mu$ (throughout, we will suppress this duality pairing, e.g. $p^\mu \phi \equiv p^\mu_A \phi^A$). Hamilton's equations $(\phi, p)^* i_V \Omega_H = 0$ can then be written as $\omega^\mu(\partial_\mu z, V) = 0$ (sum over μ), which relates the multisymplectic structure Ω_H to $(n+1)$-pre-symplectic structures $\{\omega^\mu\}$.

Remark 2.1.2. *The multisymplectic structure is more fundamental, since the ω^μ were constructed via a particular coordinate representation. In fact, as discussed in Marsden and Shkoller [83], the ω^μ are a particular coordinate decomposition of the multisymplectic form; in general, the ω^μ are not intrinsic unless the dual jet bundle is trivial, although their combination as the multisymplectic form is intrinsic. Since we will utilize Cartesian coordinates on a rectangular mesh for discretization and we will assume trivial bundles for the discrete theory, these coordinate representatives will be simpler to deal with and correspond to the current literature on multisymplectic Hamiltonian integrators. It would be interesting to investigate variational discretizations of field theories where the dual jet bundle is not trivial; in this setting, utilizing the multisymplectic structure is more fundamental.*

Multisymplecticity and the Boundary Hamiltonian. The above Hamiltonian system admits a notion of conserving multisymplecticity, which generalizes the usual notion of symplecticity. In particular, let V, W be two first variations, i.e., vector fields whose flows map solutions of Hamilton's equations again to solutions; then, for any region $U \subset X$, one has the multisymplectic form formula:

$$\int_{\partial U} (\phi, p)^* (i_V i_W \Omega_H) = 0, \tag{1.6}$$

which follows from $d^2 S^U[\phi, p] \cdot (V, W) = 0$ for a solution (ϕ, p) of Hamilton's equations. In coordinates where $V = \delta\phi^A \partial/\partial\phi^A + \delta p^\mu_A \partial/\partial p^\mu_A$ and $V = \delta y^A \partial/\partial\phi^A + \delta\pi^\mu_A \partial/\partial p^\mu_A$, this reads

$$0 = \int_{\partial U} (\phi, p)^*(i_V i_W \Omega_H) = \int_{\partial U} (\delta\phi^A \delta\pi^\mu_A - \delta y^A \delta p^\mu_A)|_{(\phi,p)} d^n x_\mu = \int_{\partial U} \omega^\mu|_{(\phi,p)}(V,W) d^n x_\mu.$$

Applying Stokes' theorem and noting that U is arbitrary, the strong form of the multisymplectic form formula can be expressed $\partial_\mu \omega^\mu = 0$, which holds when evaluated on two first variations at a solution of Hamilton's equations (ϕ, p). In terms of our coordinate representation of Hamilton's equations, by taking the exterior derivative of Hamilton's equations, a first variation is a vector field V which satisfies

$$K^0 dz_0(V) + \cdots + K^n dz_n(V) = (D_{zz}H) dz(V),$$

where $z_\mu \equiv \partial_\mu z$. One of the aims of this paper is to construct variational integrators for multi-Hamiltonian PDEs which admit a discrete analog of the multisymplectic conservation law for a suitably defined discrete notion of first variations.

Analogous to how the Type II generating functions are utilized in the construction of Galerkin Hamiltonian variational integrators (see Leok and Zhang [76]), we will utilize the boundary Hamiltonian introduced in Vankerschaver et al. [116], which will act as a generalized Type II generating functional. Consider a domain $U \subset X$ and partition the boundary $\partial U = A \cup B$; we supply fixed field boundary values φ_A on A and fixed normal momenta π_B on B. The boundary Hamiltonian is defined as a functional on these boundary values

$$\begin{aligned} H_{\partial U}(\varphi_A, \pi_B) &= \text{ext}\Big[\int_B p^\mu \phi d^n x_\mu - \int_U (\phi, p)^* \Theta_H\Big] \\ &= \text{ext}\Big[\int_B p^\mu \phi d^n x_\mu - \int_U (p^\mu \partial_\mu \phi - H(\phi, p)) d^{n+1}x\Big], \end{aligned} \tag{1.7}$$

where one extremizes over all fields (ϕ, p) satisfying the fixed boundary conditions along A and B.

An extremizer of the above expression restricted to the aforementioned boundary conditions satisfies the De Donder–Weyl equations, which follows from

$$\begin{aligned}
&\delta\Big[\int_B p^\mu \phi d^n x_\mu - \int_U (p^\mu \partial_\mu \phi - H(\phi,p)) d^{n+1}x\Big] \\
&\quad = \int_B \cancel{\delta p^\mu} \phi d^n x_\mu + \int_B p^\mu \delta\phi d^n x_\mu \\
&\qquad - \int_U (\delta p^\mu \partial_\mu \phi + p^\mu \partial_\mu \delta\phi - \frac{\partial H(\phi,p)}{\partial p^\mu}\delta p^\mu - \frac{\partial H(\phi,p)}{\partial \phi}\delta\phi) d^{n+1}x \\
&\quad = \int_B p^\mu \delta\phi d^n x_\mu - \int_{\partial U = A\cup B} p^\mu \delta\phi d^n x_\mu \\
&\qquad - \int_U (\delta p^\mu \partial_\mu \phi - \partial_\mu p^\mu \delta\phi - \frac{\partial H(\phi,p)}{\partial p^\mu}\delta p^\mu - \frac{\partial H(\phi,p)}{\partial \phi}\delta\phi) d^{n+1}x \\
&\quad = -\int_{\partial U = A} p^\mu \cancel{\delta\phi} d^n x_\mu - \int_U \Big[(\partial_\mu \phi - \frac{\partial H(\phi,p)}{\partial p^\mu})\delta p^\mu - (\partial_\mu p^\mu + \frac{\partial H(\phi,p)}{\partial \phi})\delta\phi\Big] d^{n+1}x,
\end{aligned}$$

where we used $\delta p^\mu|_B = 0 = \delta\phi|_A$.

This is a Type II generating functional in the sense that it generates the boundary values for the field along B (denoted $\phi|_B$) and the normal momenta along A (denoted $p^n|_A$),

$$\frac{\delta H_{\partial U}}{\delta \varphi_A} = -p^n|_A, \quad \frac{\delta H_{\partial U}}{\delta \pi_B} = \phi|_B. \tag{1.8}$$

To obtain (1.8), perform an analogous computation as the one above (take the variation, integrate by parts, and use that the internal field satisfies the De Donder–Weyl equations), which gives

$$dH_{\partial U}(\varphi_A, \pi_B)\cdot(\delta\varphi_A, \delta\pi_B) = \int_B \delta\pi_B \cdot \phi|_B - \int_A \pi|_A \cdot \delta\varphi_A;$$

i.e., (1.8). Note that the generating relation (1.8) only determines the normal component of the momentum along A; this is consistent with the De Donder–Weyl equation (1.5a), since it only specifies $\partial_\mu p^\mu$.

Since an extremizer of $H_{\partial U}(\varphi_A, \pi_B)$ satisfies the De Donder–Weyl equations, it satisfies the multisymplectic form formula. Since the multisymplectic form formula is expressed as an integral over ∂U and the generating functional gives us the field values on ∂U, $(\varphi,\pi) = (\varphi_A,\varphi_B,\pi_A,\pi_B)$, the above generating map (1.8) is multisymplectic in the sense

$$\int_{\partial U} \omega^\mu|_{(\varphi,\pi)}(V,W)d^n x_\mu = 0,$$

for first variations V and W.

We will utilize a discrete approximation of the boundary Hamiltonian and its property as a generating functional to construct variational integrators which are naturally multisymplectic.

Noether's Theorem. Another important conservative property of Hamiltonian systems arises from symmetries. Suppose there is a smooth group action of G on the restricted dual jet bundle which leaves the action S^U invariant. Let $\tilde{\xi}$ denote the infinitesimal generator vector field for $\xi \in \mathfrak{g}$ associated to this action. For a solution (ϕ, p) of Hamilton's equations, one has

$$0 = \pounds_{\tilde{\xi}} S^U[\phi,p] = dS^U[\phi,p]\cdot\tilde{\xi} = \int_U (\phi,p)^* i_{\tilde{\xi}} d\Theta_H + \int_{\partial U}(\phi,p)^* i_{\tilde{\xi}}\Theta_H.$$

Note that the term involving the integral over U vanishes, even though $\tilde{\xi}$ is not necessarily compactly supported in U, since Hamilton's equations hold pointwise (U is arbitrary). Hence, Noether's theorem in this setting is the statement

$$\int_{\partial U}(\phi,p)^* i_{\tilde{\xi}}\Theta_H = 0. \tag{1.9}$$

In the discrete setting, we will be particularly concerned with vertical variations (where the group action on the base space X is the identity). In this case, we can write the above in coordinates as

$$\int_{\partial U} p^\mu (i_{\tilde{\xi}} d\phi) d^n x_\mu = 0. \tag{1.10}$$

We will see that if there is a group action on the discrete analog of the restricted dual jet bundle which leaves the discrete action (the generalized discrete Lagrangian) invariant, then there is a discrete analog of Noether's theorem, equation (1.10).

2.1.3 Multisymplectic Integrators for Hamiltonian PDEs

Consider the class of Hamiltonian PDEs,

$$K^0 z_0 + \cdots + K^n z_n = \nabla_z H(z), \tag{1.11}$$

with independent variable $x = (x^0, \ldots, x^n) \in \mathbb{R}^{n+1}$, dependent variable $z : \mathbb{R}^n \to \mathbb{R}^m$, each K^μ is an $m \times m$ skew-symmetric matrix, and the Hamiltonian $H : \mathbb{R}^m \to \mathbb{R}$ is sufficiently smooth.

Defining a two-form for each K^μ, $\omega^\mu(U,V) = \langle K^\mu U, V \rangle$ (with respect to an inner product $\langle \cdot, \cdot \rangle$ on $\mathbb{R}^m$), the equation (1.11) admits the multisymplectic conservation law

$$\partial_\mu \omega^\mu(U,V) = 0, \tag{1.12}$$

for any pair of first variations U,V satisfying the variational equation

$$K^0 dz_0 + \cdots + K^n dz_n = D_{zz} H(z).$$

As we saw, the De Donder–Weyl equations, which arose from the variational principle applied to the Hamiltonian action (1.4), are an example of a Hamiltonian PDE in the form (1.11). From our variational perspective, the action and variational principle are more fundamental, as opposed to the field equations (1.11). However, as shown by Chen [29], the Hamiltonian system (1.11) arises from the variational principle, so there is no loss of generality working with the formulation based on the Hamiltonian action (1.4).

For the Hamiltonian system (1.11), a multisymplectic integrator is defined in Bridges and Reich [20] to be a method

$$K^0\partial_0^{i_0\dots i_n} z_{i_0\dots i_n} + \cdots + K^n \partial_n^{i_0\dots i_n} z_{i_0\dots i_n} = (\nabla_z S(z_{i_0\dots i_n}))_{i_0\dots i_n},$$

where $\partial_\mu^{i_0\dots i_n}$ is a discretization of ∂_μ, such that a discrete analog of equation (1.12) holds,

$$\partial_\mu^{i_0\dots i_n} \omega^\mu (U_{i_0\dots i_n}, V_{i_0\dots i_n}) = 0,$$

when evaluated on discrete first variations $U_{i_0\dots i_n}, V_{i_0\dots i_n}$ satisfying the discrete variational equations

$$K^0\partial_0^{i_0\dots i_n} dz_{i_0\dots i_n} + \cdots + K^n \partial_n^{i_0\dots i_n} dz_{i_0\dots i_n} = d\Big((\nabla_z S(z_{i_0\dots i_n}))_{i_0\dots i_n}\Big).$$

We will see that the variational integrators that we construct will automatically satisfy a discrete multisymplectic conservation law, as a consequence of the Type II variational principle. Furthermore, we will show in Section 2.2.4 that this discrete multisymplectic conservation law reproduces the Bridges and Reich notion of multisymplecticity.

Example 2.1.1. *An example of a multisymplectic integrator in* $1+1$ *spacetime dimensions is the centered Preissman scheme,*

$$K^0 \frac{z^1_{1/2} - z^0_{1/2}}{\Delta t} + K^1 \frac{z^{1/2}_1 - z^{1/2}_0}{\Delta x} = \nabla_z H\Big(z^{1/2}_{1/2}\Big),$$

where $z^0_{1/2} = \frac{1}{2}(z^0_0 + z^0_1)$*, etc. and* $z^{1/2}_{1/2} = \frac{1}{4}(z^1_1 + z^0_1 + z^1_0 + z^0_0)$*. As noted in Reich [99], this can be obtained from a cell-vertex finite volume discretization on a rectangular grid, or alternatively, as observed in Reich [98], it is an example of a multisymplectic Gauss–Legendre collocation method, in the case of one collocation point. Furthermore, the multisymplectic Gauss–Legendre collocation methods are members of a larger class of multisymplectic integrators, the multisymplectic partitioned Runge–Kutta methods (see, for example, Hong et al. [55], Ryland et al. [104]). In Section 2.2.3, we will derive the class of multisymplectic partitioned Runge–Kutta* *methods within our variational framework.*

2.1.4 Main Contributions

In this paper, we introduce a variational construction of multisymplectic Hamiltonian integrators utilizing a discrete approximation of the boundary Hamiltonian and the corresponding Type II variational principle. Although variational integrators have been extensively studied in the setting of Lagrangian PDEs, where they have been used to construct robust and flexible numerical methods for nonlinear elasticity [78], collision and impact dynamics for continuum mechanics [36], and geometrically exact beam dynamics [72], the variational perspective has not been studied in the setting of integrators for Hamiltonian PDEs.

This paper serves as a stepping stone in constructing variational integrators in the Hamiltonian PDE setting. Our hope is that, by introducing a variational perspective in the setting of integrators for Hamiltonian PDEs, the well-developed techniques and machinery of variational integrators for Lagrangian PDEs can be analogously developed on the Hamiltonian side. It should be noted that the theory in this paper relies on a trivial configuration bundle, since the notion of a boundary Hamiltonian is only intrinsic in the case that the bundle is trivial. Analogous to an intrinsic approach to variational integrators for Hamiltonian mechanics, outlined in Remark 4.1.1, one possible approach for constructing an intrinsic formulation of multisymplectic integrators is to start with a discrete notion of a multi-Dirac structure (for details on multi-Dirac structures in classical field theories, see Vankerschaver et al. [115]) and discretize the variational principle utilizing the generalized energy as a generating functional; we will investigate this in future work.

In Section 2.2.1, we begin by developing a discrete notion of Hamiltonian field theory, the discrete boundary Hamiltonian, and the corresponding Type II variational principle. Subsequently, we specialize to the case of a spacetime tensor product rectangular mesh which allows us to give an explicit characterization of the equations resulting from the Type II variational principle. We prove discrete analogues of multisymplecticity and Noether's theorem for these equations. In Section 2.2.2, we utilize a Galerkin approximation of the action to complete the discretization of the boundary Hamiltonian. Subsequently, in Section 2.2.3, we utilize a particular choice of Galerkin approximation to derive the class of multisymplectic partitioned Runge–Kutta methods. In Section 2.2.4, we reinterpret the discrete multisymplectic conservation law as one that is naturally associated to the difference equations which approximate the De Donder–Weyl equations. Finally, in Section 2.3, we provide a numerical example which allows us to visualize multisymplecticity as symplecticity in the spatial and temporal directions for the class of sine–Gordon soliton solutions.

2.2 Multisymplectic Hamiltonian Variational Integrators

2.2.1 Discrete Hamiltonian Field Theory

We will discuss our construction of a discrete boundary Hamiltonian for the general case of an arbitrary mesh and subsequently study the particular case of a rectangular mesh where the variational equations can be written explicitly. Let $X \subset \mathbb{R}^{n+1}$ be a polygonal domain and $\mathscr{T}(X)$ an associated mesh. In general, a discrete configuration bundle consists of a choice of finite element space taking values in the fiber Q that is subordinate to the mesh $\mathscr{T}(X)$. To be more concrete, for every mesh element $\triangle \in \mathscr{T}(X)$, we introduce nodes $x_i \in \triangle, i \in I$, and parametrize the finite element space by the fiber value at each node. A multisymplectic variational integrator based on finite elements was developed from the Lagrangian perspective in Chen [30].

The discrete analog of the configuration bundle, on an element by element level, is the base space $\{x_i\}_{i\in I}$ with fiber Q over each node; the total space is $\{x_i\}_{i\in I} \times Q$ and a section is a map from each node to Q, denoted $\phi_i \in Q$. Analogously, the discrete analog of the restricted dual jet bundle is $\{x_i\}_{i\in I} \times Q \times (Q^*)^{n+1}$, where a section is specified by $\phi_i \in Q, p_i^\mu \in Q^*$. Let $S_d^\triangle[\phi_i, p_i^\mu]$ be some discrete approximation of the action $S^\triangle[\phi, p]$. As in the discussion of the boundary Hamiltonian (1.7), partition the boundary of the element $\partial\triangle = A \cup B$ and let $\sum\!\!\!\!\int_B \pi_B \varphi_B$ be some discrete approximation to the boundary integral $\int_B p^\mu \phi d^n x_\mu$, depending only on the field and normal momenta boundary values on the nodes $x_i \in B$, which we denoted φ_B and π_B respectively. Define the discrete boundary Hamiltonian

$$H_d^{\partial\triangle}(\varphi_A,\pi_B) = \operatorname{ext}_{\substack{\phi_i\in Q, p_i^\mu \in Q^* \\ \phi|_A=\varphi_A, p^n|_B=\pi_B}} \left[\sum\!\!\!\!\!\!\int \pi_B\varphi_B - S_d^{\triangle}[\phi_i, p_i^\mu] \right],$$

where $p^n|_B$ denotes the normal component of the momenta along B. Repeat the above construction for each $\triangle \in \mathscr{T}(X)$; partitioning the boundaries $\partial\triangle = A(\triangle)\cup B(\triangle)$ and the boundary of the full region $\partial X = A(X)\cup B(X)$ (where $A(X) = \cup_{\Delta\in\mathscr{T}(X)}(A(\Delta)\cap\partial X)$ and $B(X) = \cup_{\Delta\in\mathscr{T}(X)}(B(\Delta)\cap\partial X)$). Define the discrete action sum

$$S_d[\{\varphi_{A(\triangle)},\pi_{B(\triangle)}\}_{\triangle\in\mathscr{T}(X)}] = \sum\!\!\!\!\!\!\int_{B(X)} \pi_{B(X)}\varphi_{B(X)} - \sum_{\triangle\in\mathscr{T}(X)} \Big[\sum\!\!\!\!\!\!\int_{B(\triangle)} \pi_{B(\triangle)}\varphi_{B(\triangle)} - H_d^{\partial\triangle}(\varphi_A,\pi_B) \Big].$$

The Type II variational principle $\delta S_d = 0$ (subject to variations of φ vanishing along $A(X)$ and variations of π vanishing along $B(X)$) gives a set of (generally coupled) maps $(\varphi_{A(\triangle)},\pi_{B(\triangle)}) \mapsto (\varphi_{B(\triangle)},\pi_{A(\triangle)})$ in analogy with the generating functional relation, equation (1.8). In the case of finite element spaces which are not parametrized by the nodal values, we evaluate the discrete boundary Hamiltonian on the discrete space of boundary data induced by the choice of mesh and discrete configuration bundle, and extremize the expressions above over the finite elements that satisfy the prescribed boundary conditions. This is the most general form of our multisymplectic Hamiltonian variational integrator.

Spacetime Tensor Product Rectangular Mesh. Now, consider the particular case of a rectangular domain X and an associated rectangular mesh $\mathscr{T}(X)$. For simplicity and clarity in the notation, we will focus on the case of $1+1$ spacetime dimensions, although higher dimensions can be treated similarly (we treat the case of higher dimensions in Appendix 2.6.1).

Consider a rectangle $[t,t+\Delta t]\times[x,x+\Delta x] = \square \in \mathscr{T}(X)$. Introduce nodes on the intervals $\{t_1 = t, t_2,\dots,t_{s-1},t_s = t+\Delta t\}$ and $\{x_1 = x, x_2,\dots,x_{\sigma-1},x_\sigma = x+\Delta x\}$ (as we will introduce in the next section for Galerkin Hamiltonian variational integrators, these nodes correspond to quadrature points along the time and space intervals). The discrete base space is $X_d = \{(t_i, x_j) \mid i = 1, \ldots, s,\ j = 1, \ldots, \sigma\}$, the discrete configuration bundle is $X_d \times Q$, where a section is map from each node (t_i, x_j) to (t_i, x_j, ϕ_{ij}), where $\phi_{ij} \in Q$. Analogously, the discrete restricted dual jet bundle is $X_d \times Q \times (Q^*)^2$, where a section is specified by $\phi_{ij} \in Q, p^\mu_{ij} \in Q^*$. Let $S^\square_d[\phi_{ij}, p^\mu_{ij}]$ be some discrete approximation to $S^\square[\phi, p]$ (we will explicitly construct such a discrete approximation in the next section using Galerkin techniques and quadrature). Partitioning the boundary $\partial\square = A(\square) \cup B(\square)$, the discrete boundary Hamiltonian is given by

$$H^{\partial\square}_d(\varphi_{A(\square)}, \pi_{B(\square)}) = \underset{\substack{\phi_{ij}\in Q, p^\mu_{ij}\in Q^* \\ \phi|_{A(\square)}=\varphi_{A(\square)}, p^n|_{B(\square)}=\pi_{B(\square)}}}{\text{ext}} \left[\oint_{B(\square)} \pi_{B(\square)}\varphi_{B(\square)} - S^\square_d[\phi_{ij}, p^\mu_{ij}] \right], \tag{2.1}$$

where $\varphi_{A(\square)}$ denotes the boundary values on $A(\square)$, i.e., at nodes $(t_i, x_j) \in A$ (and similarly for π). The discrete action sum is

$$S_d\left[\{\varphi_{A(\square)}, \pi_{B(\square)}\}_{\square\in\mathscr{T}(X)}\right] = \oint_{B(X)} \pi_{B(X)}\varphi_{B(X)} - \sum_{\square\in\mathscr{T}(X)} \left[\oint_{B(\square)} \pi_{B(\square)}\varphi_{B(\square)} - H^{\partial\square}_d(\varphi_{A(\square)}, \pi_{B(\square)}) \right].$$

Recall the Type II variational principle $\delta S_d = 0$ gives a set of maps $(\varphi_{A(\square)}, \pi_{B(\square)}) \mapsto (\varphi_{B(\square)}, \pi_{A(\square)})$. To give a more explicit characterization of these maps, let us introduce a quadrature approximation of the boundary integral over B. First, consider the simple case of one quadrature point along each edge of $\square_{ab} = [t_0 + a\Delta t, t_0 + (a+1)\Delta t] \times [x_0 + b\Delta x, x_0 + (b+1)\Delta x]$, where $\mathscr{T}(X) = \{\square_{ab}\}_{a,b}$. Let $\varphi_{[a]b}$ denote the field boundary value at the quadrature point along the bottom edge $(t_a, t_a + \Delta t) \times \{x_b\}$ (where we orient our axes such that time is horizontal and space is vertical) and $\varphi_{a[b]}$ denote its value at the quadrature point along the left edge $\{t_a\} \times (x_b, x_b + \Delta x)$ (and similarly $\varphi_{[a]b+1}$ for the top edge, $\varphi_{a+1[b]}$ for the right edge). We take A to be the bottom and left edges, and B to the top and right edges. The normal momenta through the top edge is the momenta associated to the x direction (at the quadrature point), which we denote $\pi^1_{[a]b+1}$, and the normal momenta through the right edge is the momenta associated to the t direction, which we denote $\pi^0_{a+1[b]}$. Since we only have one quadrature point along each edge, the quadrature weight for the temporal edge is Δt and similarly for the spatial edge is Δx. See Figure 2.1.

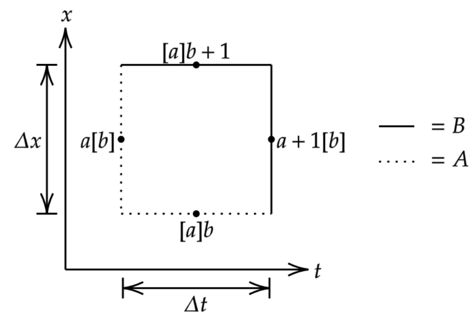

Figure 2.1. Schematic for one quadrature point along each edge of $\Box_{ab} \in \mathscr{T}(X)$.

Then, the boundary integral can be approximated

$$\begin{aligned}\int_B p^\mu \phi d^n x_\mu &= \int_{t_a}^{t_{a+1}} (p^1\phi)|_{x=x_{b+1}} dt + \int_{x_b}^{x_{b+1}} (p^0\phi)_{t=t_{a+1}} dx \\ &\approx \pi^1_{[a]b+1}\varphi_{[a]b+1}\Delta t + \pi^0_{a+1[b]}\varphi_{a+1[b]}\Delta x \equiv \sum\!\!\!\!\!\!\int_B \pi_B \varphi_B.\end{aligned}$$

The associated discrete boundary Hamiltonian is

$$H_d^+(\varphi_{[a]b}, \varphi_{a[b]}, \pi^1_{[a]b+1}, \pi^0_{a+1[b]}) = \operatorname{ext}\left(\pi^1_{[a]b+1}\varphi_{[a]b+1}\Delta t + \pi^0_{a+1[b]}\varphi_{a+1[b]}\Delta x - S_d^{\Box_{ab}}[\phi, p]\right),$$

where the $+$ specifies that we chose B to be in the forward direction (in the direction of increasing temporal and spatial values), analogous to the notion of discrete right Hamiltonian in discrete mechanics. Again, we extremize over ϕ, p satisfying the boundary conditions (note we have not given an explicit construction for such a $S_d^{\Box_{ab}}$ yet; see Section 2.2.2).

Proposition 2.2.1. *The Type II variational principle $\delta S_d = 0$, subject to variations of φ vanishing* *along $A(X)$ and variations of π vanishing along $B(X)$, yields the following,*

$$\pi^1_{[a]b} = \frac{1}{\Delta t} D_1 H_d^+(\varphi_{[a]b}, \varphi_{a[b]}, \pi^1_{[a]b+1}, \pi^0_{a+1[b]}), \tag{2.2a}$$

$$\pi^0_{a[b]} = \frac{1}{\Delta x} D_2 H_d^+(\varphi_{[a]b}, \varphi_{a[b]}, \pi^1_{[a]b+1}, \pi^0_{a+1[b]}), \tag{2.2b}$$

$$\varphi_{[a]b+1} = \frac{1}{\Delta t} D_3 H_d^+(\varphi_{[a]b}, \varphi_{a[b]}, \pi^1_{[a]b+1}, \pi^0_{a+1[b]}), \tag{2.2c}$$

$$\varphi_{a+1[b]} = \frac{1}{\Delta x} D_4 H_d^+(\varphi_{[a]b}, \varphi_{a[b]}, \pi^1_{[a]b+1}, \pi^0_{a+1[b]}), \tag{2.2d}$$

where D_i denotes differentiation with respect to the i^{th} argument. We refer to these equations as the discrete forward Hamilton's equations (in the case of one quadrature point). Note that these equations define a map $(\varphi_A, \pi_B) = (\varphi_{[a]b}, \varphi_{a[b]}, \pi^1_{[a]b+1}, \pi^0_{a+1[b]}) \mapsto (\varphi_B, \pi_A) = (\varphi_{[a]b+1}, \varphi_{a+1[b]}, \pi^1_{[a]b}, \pi^0_{a[b]})$.

Proof. Recall the full mesh $\mathscr{T}(X) = \{\square_{ab}\}_{a,b}$; say $a = 0, \ldots, N-1$, and $b = 0, \ldots, M-1$ (so that $X = [t_0, t_0 + N\Delta t] \times [x_0, x_0 + M\Delta x]$). $B(X)$ consists of the forward edges of X, i.e.,

$$B(X) = \Big([t_0, t_0 + N\Delta t] \times \{x_0 + M\Delta x\}\Big) \cup \Big(\{t_0 + N\Delta t\} \times [x_0, x_0 + M\Delta x]\Big).$$

Consider the discrete action sum

$$
\begin{aligned}
&S_d[\{\varphi_{A(\square)}, \pi_{B(\square)}\}] \\
&\quad = \oint\!\!\!\!\!\!\sum_{B(X)} \pi_{B(X)} \varphi_{B(X)} - \sum_{\square \in \mathscr{T}(X)} \Big[\oint\!\!\!\!\!\!\sum_{B(\square)} \pi_{B(\square)} \varphi_{B(\square)} - H_d^+(\varphi_{A(\square)}, \pi_{B(\square)}) \Big] \\
&\quad = \sum_{a=0}^{N-1} \pi^1_{[a]M} \varphi_{[a]M} \Delta t + \sum_{b=0}^{M-1} \pi^0_{N[b]} \varphi_{N[b]} \Delta x \\
&\qquad - \sum_{a,b=0}^{N-1,M-1} \Big[\pi^1_{[a]b+1} \varphi_{[a]b+1} \Delta t + \pi^0_{a+1[b]} \varphi_{a+1[b]} \Delta x - H_d^+(\varphi_{[a]b}, \varphi_{a[b]}, \pi^1_{[a]b+1}, \pi^0_{a+1[b]}) \Big] \\
&\quad = \underbrace{- \sum_{a,b=0}^{N-1,M-2} \pi^1_{[a]b+1} \varphi_{[a]b+1} \Delta t}_{\equiv (a)} \underbrace{- \sum_{a,b=0}^{N-2,M-1} \pi^0_{a+1[b]} \varphi_{a+1[b]} \Delta x}_{\equiv (b)} \\
&\qquad \underbrace{+ \sum_{a,b=0}^{N-1,M-1} H_d^+(\varphi_{[a]b}, \varphi_{a[b]}, \pi^1_{[a]b+1}, \pi^0_{a+1[b]})}_{\equiv (c)}.
\end{aligned}
$$

The Type II variational principle states $0 = \delta S_d = \delta(a) + \delta(b) + \delta(c)$, subject to variations of φ vanishing along $A(X)$ (i.e., $\delta\varphi_{[a]0} = 0 = \delta\varphi_{0[b]}$) and variations of π vanishing along $B(X)$ (i.e., $\delta\pi^0_{N[b]} = 0 = \delta\pi^1_{[a]M}$). Compute the variations of $(a), (b), (c)$ keeping only the independent variations $\delta\varphi_{[a]b}$, $\delta\varphi_{a[b]}$, $\delta\pi^0_{a[b]}$, $\delta\pi^1_{[a]b}$ not required to vanish by the boundary conditions (note such vanishing variations will only appear in (c)).

$$
\begin{aligned}
\delta(a) &= -\Delta t \sum_{a=0}^{N-1} \sum_{b=0}^{M-2} \Big(\varphi_{[a]b+1} \delta\pi^1_{[a]b+1} + \pi^1_{[a]b+1} \delta\varphi_{[a]b+1} \Big) \\
&= -\Delta t \sum_{a=0}^{N-1} \sum_{b=0}^{M-2} \varphi_{[a]b+1} \delta\pi^1_{[a]b+1} - \Delta t \sum_{a=0}^{N-1} \sum_{b=1}^{M-1} \pi^1_{[a]b} \delta\varphi_{[a]b}, \\
\delta(b) &= -\Delta x \sum_{a=0}^{N-2} \sum_{b=0}^{M-1} \Big(\varphi_{a+1[b]} \delta\pi^0_{a+1[b]} + \pi^0_{a+1[b]} \delta\varphi_{a+1[b]} \Big) \\
&= -\Delta x \sum_{a=0}^{N-2} \sum_{b=0}^{M-1} \varphi_{a+1[b]} \delta\pi^0_{a+1[b]} - \Delta x \sum_{a=1}^{N-1} \sum_{b=0}^{M-1} \pi^0_{a[b]} \delta\varphi_{a[b]}.
\end{aligned}
$$

For brevity, denote $H_d^+[a,b] \equiv H_d^+(\varphi_{[a]b}, \varphi_{a[b]}, \pi^1_{[a]b+1}, \pi^0_{a+1[b]})$. Compute

$$\begin{aligned}
\delta(c) &= \sum_{a,b=0}^{N-1,M-1} \Big(D_1 H_d^+[a,b]\delta\varphi_{[a]b} + D_2 H_d^+[a,b]\delta\varphi_{a[b]} \\
&\qquad\qquad + D_3 H_d^+[a,b]\delta\pi^1_{[a]b+1} + D_4 H_d^+[a,b]\delta\pi^0_{a+1[b]} \Big) \\
&= \sum_{a=0}^{N-1}\sum_{b=0}^{M-1} D_1 H_d^+[a,b]\delta\varphi_{[a]b} + \sum_{a=0}^{N-1}\sum_{b=0}^{M-1} D_2 H_d^+[a,b]\delta\varphi_{a[b]} \\
&\quad + \sum_{a=0}^{N-1}\sum_{b=0}^{M-1} D_3 H_d^+[a,b]\delta\pi^1_{[a]b+1} + \sum_{a=0}^{N-1}\sum_{b=0}^{M-1} D_4 H_d^+[a,b]\delta\pi^0_{a+1[b]}.
\end{aligned}$$

Note in the first double sum above, $\delta\varphi_{[a]0} = 0$ so we remove the $b = 0$ terms. In the second double sum, $\delta\varphi_{0[b]} = 0$ so we remove the $a = 0$ terms. In the third double sum above, $\delta\pi^1_{[a]M} = 0$ so we remove the $b = M-1$ terms. In the fourth double sum above, $\delta\pi^0_{N[b]} = 0$ so we remove the $a = N-1$ terms. This gives,

$$\begin{aligned}
\delta(c) &= \sum_{a=0}^{N-1}\sum_{b=1}^{M-1} D_1 H_d^+[a,b]\delta\varphi_{[a]b} + \sum_{a=1}^{N-1}\sum_{b=0}^{M-1} D_2 H_d^+[a,b]\delta\varphi_{a[b]} \\
&\quad + \sum_{a=0}^{N-1}\sum_{b=0}^{M-2} D_3 H_d^+[a,b]\delta\pi^1_{[a]b+1} + \sum_{a=0}^{N-2}\sum_{b=0}^{M-1} D_4 H_d^+[a,b]\delta\pi^0_{a+1[b]}.
\end{aligned}$$

Putting everything together, we have

$$\begin{aligned}
0 &= \delta S_d = \delta(a) + \delta(b) + \delta(c) \\
&= \sum_{a=0}^{N-1}\sum_{b=1}^{M-1} (-\Delta t\ \pi^1_{[a]b} + D_1 H_d^+[a,b])\delta\varphi_{[a]b} + \sum_{a=1}^{N-1}\sum_{b=0}^{M-1} (-\Delta x\ \pi^0_{a[b]} + D_2 H_d^+[a,b])\delta\varphi_{a[b]} \\
&\quad + \sum_{a=0}^{N-1}\sum_{b=0}^{M-2} (-\Delta t\ \varphi_{[a]b+1} + D_3 H_d^+[a,b])\delta\pi^1_{[a]b+1} \\
&\quad + \sum_{a=0}^{N-2}\sum_{b=0}^{M-1} (-\Delta x\ \varphi_{a+1[b]} + D_4 H_d^+[a,b])\delta\pi^0_{a+1[b]}.
\end{aligned}$$

The variations in the above expression are all independent, so this gives (2.2a)-(2.2d). □

Discrete Multisymplecticity. Analogous to the continuum case, we define a discrete first variation as a vector field such that the above equations (2.2a)-(2.2d) still hold when evaluated at the level of the exterior derivative, e.g. for equation (2.2a),

$$d\pi^1_{[a]b} = \frac{1}{\Delta t} d\Big(D_1 H_d^+(\varphi_{[a]b}, \varphi_{a[b]}, \pi^1_{[a]b+1}, \pi^0_{a+1[b]})\Big).$$

and similarly for the others. As we saw in the continuum theory, the map generated by the boundary Hamiltonian implies the multisymplectic form formula, since the multisymplectic form formula can be expressed over the boundary ∂U. Since we constructed a discrete approximation to the boundary Hamiltonian before enforcing the variational principle, we would naturally expect a discrete notion of multisymplecticity to arise as well. Furthermore, in the continuum theory, multisymplecticity follows from $d^2 = 0$ applied to the boundary Hamiltonian, evaluated on first variations. As we will see, our discrete multisymplectic form formula follows from computing $d^2 = 0$ applied to the discrete boundary Hamiltonian, in analogy with the continuum theory.

Proposition 2.2.2. *The discrete forward Hamilton's equations (2.2a)-(2.2d) are multisymplectic, in the sense that for a solution of the discrete forward Hamilton's equations,*

$$\Delta t\ d\varphi_{[a]b+1} \wedge d\pi^1_{[a]b+1} - \Delta t\ d\varphi_{[a]b} \wedge d\pi^1_{[a]b} + \Delta x\ d\varphi_{a+1[b]} \wedge d\pi^0_{a+1[b]} - \Delta x\ d\varphi_{a[b]} \wedge d\pi^0_{a[b]} = 0,$$

evaluated on discrete first variations.

Proof. In what follows, H_d^+ will be evaluated at $(\varphi_{[a]b}, \varphi_{a[b]}, \pi^1_{[a]b+1}, \pi^0_{a+1[b]})$. Compute

$$\begin{aligned} 0 = d^2 H_d^+ &= d\Big(D_1 H_d^+ d\varphi_{[a]b} + D_2 H_d^+ d\varphi_{a[b]} + D_3 H_d^+ d\pi^1_{[a]b+1} + D_4 H_d^+ d\pi^0_{a+1[b]}\Big) \\ &= d(D_1 H_d^+) \wedge d\varphi_{[a]b} + d(D_2 H_d^+) \wedge d\varphi_{a[b]} + d(D_3 H_d^+) \wedge d\pi^1_{[a]b+1} + d(D_4 H_d^+) \wedge d\pi^0_{a+1[b]}. \end{aligned}$$

Then, by our definition of discrete first variations, we have

$$\begin{aligned} d(D_1 H_d^+) &= \Delta t \; d\pi^1_{[a]b}, \\ d(D_2 H_d^+) &= \Delta x \; d\pi^0_{a[b]}, \\ d(D_3 H_d^+) &= \Delta t \; d\varphi_{[a]b+1}, \\ d(D_4 H_d^+) &= \Delta x \; d\varphi_{a+1[b]}. \end{aligned}$$

Substituting these expressions into the equation for $d^2 H_d^+$ yields

$$\begin{aligned} 0 &= d(D_1 H_d^+) \wedge d\varphi_{[a]b} + d(D_2 H_d^+) \wedge d\varphi_{a[b]} + d(D_3 H_d^+) \wedge d\pi^1_{[a]b+1} + d(D_4 H_d^+) \wedge d\pi^0_{a+1[b]} \\ &= \Delta t \; d\pi^1_{[a]b} \wedge d\varphi_{[a]b} + \Delta x \; d\pi^0_{a[b]} \wedge d\varphi_{a[b]} + \Delta t \; d\varphi_{[a]b+1} \wedge d\pi^1_{[a]b+1} + \Delta x \; d\varphi_{a+1[b]} \wedge d\pi^0_{a+1[b]} \\ &= -\Delta t \; d\varphi_{[a]b} \wedge d\pi^1_{[a]b} - \Delta x \; d\varphi_{a[b]} \wedge d\pi^0_{a[b]} + \Delta t \; d\varphi_{[a]b+1} \wedge d\pi^1_{[a]b+1} + \Delta x \; d\varphi_{a+1[b]} \wedge d\pi^0_{a+1[b]} \\ &= \Delta t \; d\varphi_{[a]b+1} \wedge d\pi^1_{[a]b+1} - \Delta t \; d\varphi_{[a]b} \wedge d\pi^1_{[a]b} + \Delta x \; d\varphi_{a+1[b]} \wedge d\pi^0_{a+1[b]} - \Delta x \; d\varphi_{a[b]} \wedge d\pi^0_{a[b]}. \end{aligned}$$

$\square$

Remark 2.2.1. *Recall that $\omega^\mu = d\varphi \wedge d\pi^\mu$. Observe that if we divide the above discrete multisymplectic form formula by $\Delta t \Delta x$, it is just a first-order finite difference approximation of $\partial_\mu \omega^\mu = 0$.*

Furthermore, it is clear that the above equation is precisely quadrature applied to the multisymplectic form formula $\int_{\partial\square} \omega^\mu|_{(\varphi,\pi)}(\cdot,\cdot) d^n x_\mu = 0$.

Finally, we note that a discrete notion of multisymplecticity holds in the more general setting described at the beginning of Section 2.2.1. In the more general setting, discrete multisymplecticity is interpreted as $d^2 H_d^{\partial\Delta} = 0$ (when evaluated on first variations), which reduces to the "usual" notion of multisymplecticity in the spacetime tensor product case.

General Quadrature Approximation. From here, the generalization to multiple quadrature points is straight-forward. For simplicity, we take the bottom-left vertex of $\square \in \mathscr{T}(X)$ to be $(0,0)$. Then, $\square = [0,\Delta t] \times [0,\Delta x]$. In the temporal direction, introduce quadrature points $c_i \in [0,1]$, $i = 1,\ldots,s$, and associated quadrature weights b_i; we normalize these such that $\sum_i b_i = 1$ (for both c_i and b_i, we'll have to explicitly include a factor of Δt later) and without loss of generality, we assume each $b_i \neq 0$. Similarly, for the spatial direction, introduce quadrature points $\tilde{c}_\alpha$, $\alpha = 1,\ldots,\sigma$ and the associated non-zero weights $\tilde{b}_\alpha$ (normalized as before). Let $\varphi_{[i]0} = \varphi(c_i\Delta t, 0)$, $\varphi_{0[\alpha]} = (0, \tilde{c}_\alpha \Delta x)$, $\varphi_{[i]1} = \varphi(c_i\Delta t, \Delta x)$, $\varphi_{1[\alpha]} = (\Delta t, \tilde{c}_\alpha \Delta x)$. Similarly define $\pi^0_{0[\alpha]}$, $\pi^1_{[i]0}$, $\pi^0_{1[\alpha]}$, $\pi^1_{[i]1}$. As before, we take B to be the part of the boundary in the forward direction. See Figure 2.2.

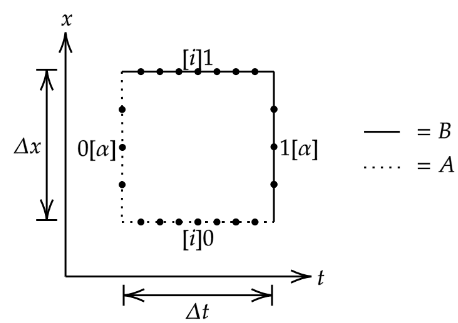

Figure 2.2. Schematic for multiple quadrature points along each edge of $\square \in \mathscr{T}(X)$.

Then, use quadrature to approximate the boundary integral:

$$\begin{aligned}\int_B p^\mu \phi d^n x_\mu &= \int_0^{\Delta t} (p^1\phi)|_{x=\Delta x} dt + \int_0^{\Delta x} (p^0\phi)_{t=\Delta t} dx \\ &\approx \sum_{i=1}^{s} \Delta t\; b_i \pi^1_{[i]1} \varphi_{[i]1} + \sum_{\alpha=1}^{\sigma} \Delta x \tilde{b}_\alpha p^0_{1[\alpha]} \varphi_{1[\alpha]} \equiv \sum\!\!\!\!\!\!\int_B \pi_B \varphi_B .\end{aligned}$$

The associated discrete boundary Hamiltonian is

$$H_d^+(\{\varphi_{[i]0}, \varphi_{0[\alpha]}, \pi^1_{[i]1}, \pi^0_{1[\alpha]}\}_{i,\alpha}) = \text{ext}\Big(\sum_{i=1}^{s} \Delta t\; b_i \pi^1_{[i]1} \varphi_{[i]1} + \sum_{\alpha=1}^{\sigma} \Delta x \tilde{b}_\alpha \pi^0_{1[\alpha]} \varphi_{1[\alpha]} - S_d^{\square^{ab}}[\phi, p] \Big).$$

Proposition 2.2.3. *The discrete forward Hamilton's equations arising from the Type II variational* *principle are*

$$\pi^1_{[i]0} = \frac{1}{b_i \Delta t} D_{1,i} H_d^+(\{\varphi_{[j]0}, \varphi_{0[\beta]}, \pi^1_{[j]1}, \pi^0_{1[\beta]}\}_{j,\beta}), \qquad i = 1, \ldots, s, \tag{2.3a}$$

$$\pi^0_{0[\alpha]} = \frac{1}{\tilde{b}_\alpha \Delta x} D_{2,\alpha} H_d^+(\{\varphi_{[j]0}, \varphi_{0[\beta]}, \pi^1_{[j]1}, \pi^0_{1[\beta]}\}_{j,\beta}), \qquad \alpha = 1, \ldots, \sigma, \tag{2.3b}$$

$$\varphi_{[i]1} = \frac{1}{b_i \Delta t} D_{3,i} H_d^+(\{\varphi_{[j]0}, \varphi_{0[\beta]}, \pi^1_{[j]1}, \pi^0_{1[\beta]}\}_{j,\beta}), \qquad i = 1, \ldots, s, \tag{2.3c}$$

$$\varphi_{1[\alpha]} = \frac{1}{\tilde{b}_\alpha \Delta x} D_{4,\alpha} H_d^+(\{\varphi_{[j]0}, \varphi_{0[\beta]}, \pi^1_{[j]1}, \pi^0_{1[\beta]}\}_{j,\beta}), \qquad \alpha = 1, \ldots, \sigma, \tag{2.3d}$$

where $D_{1,i} \equiv \partial/\partial\varphi_{[i]0}$, $D_{2,\alpha} \equiv \partial/\partial\varphi_{0[\alpha]}$, $D_{3,i} \equiv \partial/\partial\pi^1_{[i]1}$, $D_{4,\alpha} \equiv \partial/\partial\pi^0_{1[\alpha]}$. *Furthermore, a solution of the discrete forward Hamilton's equations (2.3a)-(2.3d) satisfies the discrete multisymplectic conservation law,*

$$\sum_{i=1}^{s} \Delta t\, b_i \Big(d\varphi_{[i]1} \wedge d\pi^1_{[i]1} - d\varphi_{[i]0} \wedge d\pi^1_{[i]0} \Big) + \sum_{\alpha=1}^{\sigma} \Delta x\, \tilde{b}_\alpha \Big(d\varphi_{1[\alpha]} \wedge d\pi^0_{1[\alpha]} - d\varphi_{0[\alpha]} \wedge d\pi^0_{0[\alpha]} \Big) = 0, \tag{2.4}$$

evaluated on discrete first variations.

Proof. The proof follows similarly to the case of one quadrature point, Proposition 2.2.1. Namely, the discrete forward Hamilton's equations follow from the Type II variational principle $\delta S_d = 0$ subject to variations of φ vanishing along $A(X)$ and variations of π vanishing along $B(X)$. The discrete multisymplectic conservation law follows from

$$d^2 H_d^+(\{\varphi_{[j]0}, \varphi_{0[\beta]}, \pi^1_{[j]1}, \pi^0_{1[\beta]}\}_{j,\beta}) = 0.$$

□

As in the case of one quadrature point, the discrete multisymplectic conservation law is the given quadrature rule applied to $\int_{\partial\square} \omega^\mu|_{(\varphi,\pi)}(\cdot,\cdot) d^n x_\mu = 0$.

Remark 2.2.2. *The above discrete forward Hamilton's equations were defined on* $\square = [0,\Delta t] \times [0,\Delta x]$. *For* $\square_{ab} = [t_a, t_a + \Delta t] \times [x_b, x_b + \Delta x]$, *shift the indices* $0,1$ *appropriately to* $a, a+1$ *and*

$b, b+1$, i.e., $\varphi_{[i]0} \to \varphi_{[i]b}$, $\varphi_{[i]1} \to \varphi_{[i]b+1}$, $\varphi_{0[\alpha]} \to \varphi_{a[\alpha]}$, $\varphi_{1[\alpha]} \to \varphi_{a+1[\alpha]}$ and similarly for the momenta.

Boundary Conditions and Solution Method. Recall that the discrete forward Hamilton's equations produce a map $(\varphi_{A(\Box)}, \pi_{B(\Box)}) \mapsto (\varphi_{B(\Box}, \pi_{A(\Box)})$ for each $\Box \in \mathscr{T}(X)$. However, depending on the boundary conditions that we supply on ∂X, the actual realization of these maps may be different (in that the boundary conditions determine the variables in $(\varphi_{A(\Box)}, \pi_{B(\Box)}) \mapsto (\varphi_{B(\Box}, \pi_{A(\Box)})$ that we implicitly solve for). The key point is that we must specify the field value or the normal momenta along four edges (and the edges may repeat, such as supplying field values and normal momenta on the same edge; see the discussion of evolutionary systems below). This will depend on whether the Hamiltonian PDE we are considering is stationary or evolutionary.

Consider a stationary system (e.g., an elliptic system). Then, along ∂X, we can specify either Dirichlet boundary conditions, given by the field value φ, or Neumann boundary conditions, given by the normal momenta value π. If we supply such boundary conditions, then each $\Box \in \mathscr{T}(X)$ either has two edges with supplied boundary conditions (those on the corners of X), has one edge with supplied boundary conditions (those on the edges of X), or no supplied boundary conditions (those on the interior). However, the field values and normal momenta values have to be the same along interior edges, which makes up the other required degrees of freedom (recall, we need to specify the field value or normal momenta along four edges). This couples all of the implicit maps $(\varphi_{A(\Box)}, \pi_{B(\Box)}) \mapsto (\varphi_{B(\Box}, \pi_{A(\Box)})$ together, so that the solution must be solved simultaneously for every $\Box \in \mathscr{T}(X)$. See Figure 2.3.

For an evolutionary system (e.g., a hyperbolic system), we specify the initial conditions at $t = 0$, which consist of both the field and normal momenta value (π^0). On the spatial boundaries, we can either supply Dirichlet or Neumann conditions as above. The continuity of field and normal momenta on the interior edges couples the maps $(\varphi_{A(\Box)}, \pi_{B(\Box)}) \mapsto (\varphi_{B(\Box}, \pi_{A(\Box)})$ together for each $\Box$ in the same time slice and produces the remaining required degrees of freedom.

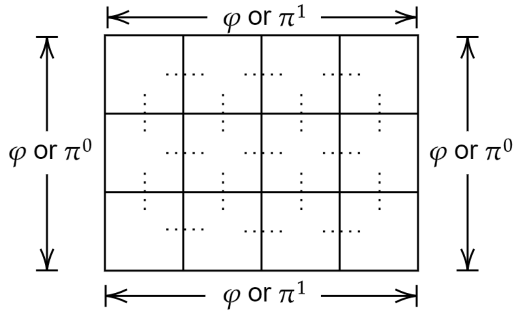

Figure 2.3. Coupling of all of the discrete forward Hamilton's equations for stationary Hamiltonian PDEs; dashed lines along interior edges denote field and normal momenta continuity.

Hence, one solves these coupled equations on the first time slice which supplies new initial conditions for the subsequent timeslice; one then continues this process recursively for each time step, thereby allowing the discrete solution to be computed in a time marching fashion. See Figure 2.4.

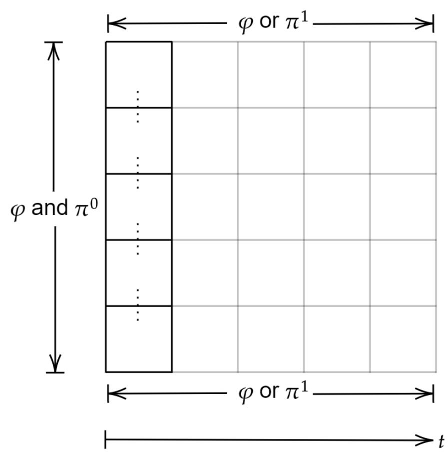

Figure 2.4. Coupling of the discrete forward Hamilton's equations in the same time slice for evolutionary Hamiltonian PDEs; dashed lines along interior edges denote field and normal momenta continuity.

Remark 2.2.3. ***Solvability.*** *It should be noted that the map* $(\varphi_A, \pi_B) \mapsto (\varphi_B, \pi_A)$ *defined by the discrete forward Hamilton's equations are always well-defined, as can be seen explicitly from the equations (2.3a)-(2.3d). This is a property of the (discrete) generating functional and is agnostic* *to the specific Hamiltonian in question. However, as discussed above, with regard to constructing a numerical method, the implementation of the method in general involves implicitly inverting the relation* $(\varphi_A, \pi_B) \mapsto (\varphi_B, \pi_A)$ *for the desired variables. For example, if one specifies Neumann boundary conditions on all of* ∂X *for a stationary system, then the numerical method is given by solving for the map* $(\pi_A, \pi_B) \mapsto (\varphi_A, \varphi_B)$ *implicitly from the map* $(\varphi_A, \pi_B) \mapsto (\varphi_B, \pi_A)$*. As another example, for an evolutionary problem, if one specifies Neumann spatial boundary conditions and specifies initial conditions (with both* φ *and* π^0*), then the numerical method is given by solving for the map* $(\varphi_A, \pi_A) \mapsto (\varphi_B, \pi_B)$ *implicitly from the map* $(\varphi_A, \pi_B) \mapsto (\varphi_B, \pi_A)$*. As these two examples indicate, in general, the form of the map necessary to implement the method is highly dependent on the type of Hamiltonian, as well as the supplied boundary conditions. As such, a discussion of the well-definedness of the implemented map is beyond the scope of this paper, since such a discussion would be highly dependent on the type of problem and boundary conditions, and the functional analytic tools needed in each case would differ drastically.*

We will outline the general argument, although the specifics are left to future work. Note that equations (2.3a)-(2.3d) can be written formally as

$$\pi_A = \hat{D}_{\varphi_A} H_d^+(\varphi_A, \pi_B), \tag{2.5a}$$

$$\varphi_B = \hat{D}_{\pi_B} H_d^+(\varphi_A, \pi_B), \tag{2.5b}$$

where $\hat{D}$ *denotes the differentiation operators in (2.3a)-(2.3d) (and appropriately scaled by the quadrature weights). Showing that one can invert the relations (2.5a)-(2.5b) for the implemented map would then rest on an implicit function theorem type argument, for a sufficiently small* $\square \subset X$*. The derivatives of the equations (2.5a)-(2.5b) would then involve second derivatives of* H_d^+*, so hyperregularity would prove crucial in such a proof. For degenerate Hamiltonians, some form of constraint or gauge-fixing would be necessary to complete the proof. We aim to explore issues dealing with solvability in future work, as well as related issues such as error analysis, which is again highly dependent on the specific class of Hamiltonians and boundary conditions* *considered.*

Discrete Noether's Theorem. In the continuum theory, we saw that for a vertical group action on the restricted dual jet bundle which leaves the action invariant, there is an associated Noether conservation law (1.10) for solutions of Hamilton's equations.

In the discrete setting, suppose there is a differentiable and vertical G action on the discrete restricted dual jet bundle $\{t_i, x_j\} \times Q \times (Q^*)^2$ (relative to $\square \in \mathscr{T}(X)$) which leaves invariant the generalized discrete Lagrangian

$$\begin{aligned} R_d^{\square}(\varphi_{A(\square)}, \varphi_{B(\square)}, \pi_{B(\square)}) &= \oint_{B(\square)} \pi_{B(\square)} \varphi_{B(\square)} - H_d^+(\varphi_{A(\square)}, \pi_{B(\square)}) \\ &= \sum_{i=1}^{s} \Delta t \; b_i \pi_{[i]1}^1 \varphi_{[i]1} + \sum_{\alpha=1}^{\sigma} \Delta x \tilde{b}_\alpha p_{1[\alpha]}^0 \varphi_{1[\alpha]} - H_d^+(\{\varphi_{[i]0}, \varphi_{0[\alpha]}, \pi_{[i]1}^1, \pi_{1[\alpha]}^0\}_{i,\alpha}). \end{aligned}$$

Proposition 2.2.4. *If the generalized discrete Lagrangian is invariant under a differentiable and vertical G action on the discrete restricted dual jet bundle, then a solution of the discrete forward Hamilton's equations (2.3a)-(2.3d) admits a discrete analog of Noether's theorem:*

$$\begin{aligned} &\sum_i \Delta t \; b_i \pi_{[i]1}^1 i_{\tilde{\xi}} d\varphi_{[i]1} + \sum_\alpha \Delta x \; \tilde{b}_\alpha \pi_{1[\alpha]}^0 i_{\tilde{\xi}} d\varphi_{1[\alpha]} \\ &\qquad - \sum_i \Delta t \; b_i \pi_{[i]0}^1 i_{\tilde{\xi}} d\varphi_{[i]0} - \sum_\alpha \Delta x \; \tilde{b}_\alpha \pi_{0[\alpha]}^0 i_{\tilde{\xi}} d\varphi_{0[\alpha]} = 0, \end{aligned} \tag{2.6}$$

where $\tilde{\xi}$ is the infinitesimal generator associated with $\xi \in \mathfrak{g}$.

Proof. For brevity, we will omit the arguments of $R_d^{\square}$ and H_d^+ (refer to the definition of $R_d^{\square}$ above). Since the generalized discrete Lagrangian is invariant under the G action, that means that the directional derivative in the direction of the infinitesimal generator vanishes,

$$
\begin{aligned}
0 &= dR_d^{\Box} \cdot \tilde{\xi} \\
&= \sum_i \Delta t\ b_i i_{\tilde{\xi}} d(\pi^1_{[i]1} \varphi_{[i]1}) + \sum_\alpha \Delta x\ \tilde{b}_\alpha i_{\tilde{\xi}} d(\pi^0_{1[\alpha]} \varphi_{1[\alpha]}) \\
&\quad - \sum_i \left(D_{1,i} H_d^+ i_{\tilde{\xi}} d\varphi_{[i]0} + D_{3,i} H_d^+ i_{\tilde{\xi}} d\pi^1_{[i]1} \right) - \sum_\alpha \left(D_{2,\alpha} H_d^+ i_{\tilde{\xi}} d\varphi_{0[\alpha]} + D_{4,\alpha} H_d^+ i_{\tilde{\xi}} d\pi^0_{1[\alpha]} \right) \\
&= \sum_i \Delta t\ b_i \big(\cancelto{(1)}{i_{\tilde{\xi}} d\pi^1_{[i]1} \varphi_{[i]1}} + \pi^1_{[i]1} i_{\tilde{\xi}} d\varphi_{[i]1} \big) + \sum_\alpha \Delta x\ \tilde{b}_\alpha \big(\cancelto{(2)}{i_{\tilde{\xi}} d\pi^0_{1[\alpha]} \varphi_{1[\alpha]}} + \pi^0_{1[\alpha]} i_{\tilde{\xi}} d\varphi_{1[\alpha]} \big) \\
&\quad - \sum_i \Delta t\ b_i \left(\pi^1_{[i]0} i_{\tilde{\xi}} d\varphi_{[i]0} + \cancelto{(1)}{\varphi_{[i]1} i_{\tilde{\xi}} d\pi^1_{[i]1}} \right) - \sum_\alpha \Delta x\ \tilde{b}_\alpha \left(\pi^0_{0[\alpha]} i_{\tilde{\xi}} d\varphi_{0[\alpha]} + \cancelto{(2)}{\varphi_{1[\alpha]} i_{\tilde{\xi}} d\pi^0_{1[\alpha]}} \right).
\end{aligned}
$$

□

Remark 2.2.4. *Note that the above looks like quadrature applied to the continuous Noether's theorem,*

$$\int_{\partial \Box} p^\mu (i_{\tilde{\xi}} d\phi) d^n x_\mu = 0$$

(with the caveat that, in the continuum case, G acts on the restricted dual jet bundle, whereas in the discrete case, G acts on the discrete restricted dual jet bundle). One can obtain such a G-invariant R_d via G-equivariant interpolation (see Leok and Zhang [76] and Leok [74]), in which case, the discrete Noether theorem is precisely quadrature applied to Noether's theorem.

Also, note that a discrete Noether's theorem holds in the more general setting described at the beginning of Section 2.2.1. In the more general setting, the discrete Noether's theorem is interpreted as $dR_d^{\Delta} \cdot \tilde{\xi} = 0$ (for a G-invariant generalized discrete Lagrangian), which reduces to the "usual" coordinate notion of the discrete Noether's theorem, equation (2.6), in the spacetime tensor product case.

Remark 2.2.5. *Another way to interpret this discrete Noether's theorem is to view the map determined by the discrete forward Hamilton's equations, $(\varphi_{A(\Box)}, \pi_{B(\Box)}) \mapsto (\varphi_{B(\Box)}, \pi_{A(\Box)})$, as implicitly defining a forward map $F_{H_d^+} : (\varphi_{A(\Box)}, \pi_{A(\Box)}) \mapsto (\varphi_{B(\Box)}, \pi_{B(\Box)})$. For some subset S* *of $\partial\Box$, define the discrete (Hamiltonian) Cartan form (at a solution of the discrete forward Hamilton's equations)*

$$\Theta_d^S = \sum_{(t_k,x_l)\in S} \beta_{kl}\pi_{kl}^n d\varphi_{kl}, \tag{2.7}$$

where π^n denotes the normal component of the momenta and β^{kl} denotes the quadrature weight at $(t_k,x_l) \in S$ (which equals $\Delta t\ b_i$ for the i^{th} node of S along fixed x and equals $\Delta x\ \tilde{b}_\alpha$ for the α^{th} node of S along fixed t). Such a discrete Cartan form involving summing over nodes corresponding to boundary variations was introduced by Marsden et al. [85] in the Lagrangian framework; in the discrete Hamiltonian setting which we constructed, (2.7) is the appropriate definition since $\Theta_d^{\partial\Box}$ precisely encodes such discrete boundary variations.

Then, the discrete Noether theorem (2.6) can be expressed as

$$F^*_{H_d^+}(\Theta_d^{B(\Box)})\cdot\tilde{\xi} = \Theta_d^{A(\Box)}\cdot\tilde{\xi}.$$

Note also that the discrete multisymplectic form formula (2.4) can be expressed as

$$d\Theta_d^{\partial\Box}(\cdot,\cdot) = 0,$$

when evaluated on discrete first variations.

2.2.2 Galerkin Hamiltonian Variational Integrators

The missing ingredient in our construction of a variational integrator is the discrete approximation of the action over $\Box \in \mathscr{T}(X)$, $S_d^{\Box}[\phi,p]$. We will extend the construction of Galerkin Hamiltonian variational integrators, introduced in Leok and Zhang [76] for Hamiltonian ODEs, to the case of Hamiltonian PDEs.

Remark 2.2.6. *To be definitive, we will assume that the space(time) X has the Euclidean metric. The discussion below is equally valid for the Minkowski metric, except one has to include the appropriate minus signs throughout.*

Consider for simplicity $[0,\Delta t]\times[0,\Delta x] = \square \in \mathscr{T}(X)$. Fix quadrature rules in the temporal direction (weights b_i and nodes c_i, $i = 1,\dots,s$) and spatial direction (weights $\tilde{b}_\alpha$ and nodes $\tilde{c}_\alpha$, $\alpha = 1,\dots,\sigma$) as before. Note the action $S[\phi,p] = \int (p^\mu \partial_\mu \phi - H(\phi,p^0,p^1))d^2x$ involves the fields ϕ, their derivatives $\partial_\mu \phi$, and the multimomenta p^μ ($\mu = 0,1$). For the field and their derivatives, we could either approximate the field using a finite-dimensional subspace and subsequently take derivatives; or conversely, approximate the derivatives and subsequently integrate to obtain the values of the field. We will take the latter approach (we will extremize over the internal stages at the end, so the two approaches are equivalent). Introduce basis functions $\{\chi_i(\tau)\}_{i=1}^s$, $\tau \in [0,1]$, for an s-dimensional function space and similarly $\{\tilde{\chi}_\alpha(\tau)\}_{\alpha=1}^\sigma$ for a σ-dimensional function space. We will use the tensor product basis $\{\chi_i(\tau\Delta t)\tilde{\chi}_\alpha(\rho\Delta x)\}_{i,\alpha}$ to discretize the derivatives of the field. Approximate the derivatives as

$$\partial_t \phi_d(\tau\Delta t,\rho\Delta x) = \sum_{i,\alpha} V^{i\alpha}\chi_i(\tau)\tilde{\chi}_\alpha(\rho), \tag{2.8a}$$

$$\partial_x \phi_d(\tau\Delta t,\rho\Delta x) = \sum_{i,\alpha} W^{i\alpha}\chi_i(\tau)\tilde{\chi}_\alpha(\rho). \tag{2.8b}$$

We can integrate in time or space to determine the field values. In particular, the internal stages are given by the field values at the nodes $(c_i\Delta t, \tilde{c}_\alpha \Delta x)$:

$$\Phi_{i\alpha} \equiv \phi(c_i\Delta t,\tilde{c}_\alpha\Delta x) = \phi(0,\tilde{c}_\alpha\Delta x) + \Delta t \sum_{j,\beta} V^{j\beta}\int_0^{c_i}\chi_j(s)ds\ \tilde{\chi}_\beta(\tilde{c}_\alpha) = \varphi_{0[\alpha]} + \Delta t\sum_{j,\beta} A_{i\alpha,j\beta}V^{j\beta},$$
$$\Phi_{i\alpha} \equiv \phi(c_i\Delta t,\tilde{c}_\alpha\Delta x) = \phi(c_i\Delta t,0) + \Delta x \sum_{j,\beta} W^{j\beta}\chi_j(c_i)\int_0^{c_\alpha}\tilde{\chi}_\beta(s)ds = \varphi_{[i]0} + \Delta x\sum_{j,\beta} \tilde{A}_{i\alpha,j\beta}W^{j\beta},$$

where $A_{i\alpha,j\beta} = \int_0^{c_i}\chi_j(s)ds\ \tilde{\chi}_\beta(\tilde{c}_\alpha)$ and $\tilde{A}_{i\alpha,j\beta} = \chi_j(c_i)\int_0^{c_\alpha}\tilde{\chi}_\beta(s)ds$. Note that $\Phi_{i\alpha}$ must of course be single-valued, so we have a relation between the two above equations:

$$\phi_{0[\alpha]} + \Delta t A_{i\alpha,j\beta}V^{j\beta} = \Phi_{i\alpha} = \phi_{[i]0} + \Delta x \tilde{A}_{i\alpha,j\beta}W^{j\beta}. \tag{2.9}$$

We expect such a relation since extremizing over $\Phi_{i\alpha}$ is equivalent to extremizing over $V_{i\alpha}$ or $W_{i\alpha}$ (but not both; however, we will relax this assumption in the subsequent discussion).

Integrating to 1 gives the unknown field boundary values,

$$\varphi_{1[\alpha]} \equiv \phi(\Delta t, \tilde{c}_\alpha \Delta x) = \phi(0, \tilde{c}_\alpha \Delta x) + \Delta t \sum_{j,\beta} V^{j\beta} \int_0^1 \chi_j(s) ds \, \tilde{\chi}_\beta(\tilde{c}_\alpha) = \varphi_{0[\alpha]} + \Delta t \sum_{j,\beta} B_{\alpha,j\beta} V^{j\beta},$$
$$\varphi_{[i]1} \equiv \phi(c_i \Delta t, \Delta x) = \phi(c_i \Delta t, 0) + \Delta x \sum_{j,\beta} W^{j\beta} \chi_j(c_i) \int_0^1 \tilde{\chi}_\beta(s) ds = \varphi_{[i]0} + \Delta x \sum_{j,\beta} \tilde{B}_{i,j\beta} W^{j\beta},$$

where $B_{\alpha,j\beta} = \int_0^1 \chi_j(s) ds \, \tilde{\chi}_\beta(\tilde{c}_\alpha)$ and $\tilde{B}_{i,j\beta} = \chi_j(c_i) \int_0^1 \tilde{\chi}_\beta(s) ds$.

We define the internal stages for the momenta $P^0_{i\alpha} = p^0(c_i \Delta t, \tilde{c}_\alpha \Delta x), P^1_{i\alpha} = p^1(c_i \Delta t, \tilde{c}_\alpha \Delta x)$. Unlike the field internal stage expansions, one does not need to introduce an approximating function space for the momenta internal stages, since the action only involves derivatives of the field and not the momenta. At this point, we could work directly with these internal stages; however, we will expand the momenta similarly to the fields,

$$P^0_{i\alpha} = \pi^0_{1[\alpha]} - \Delta t \sum_{j,\beta} A'_{i\alpha,j\beta} X^{j\beta},$$
$$P^1_{i\alpha} = \pi^1_{[i]1} - \Delta x \sum_{j,\beta} \tilde{A}'_{i\alpha,j\beta} Y^{j\beta},$$

where $A'_{i\alpha,j\beta}$ and $\tilde{A}'_{i\alpha,j\beta}$ are arbitrary expansion coefficients and $X^{j\beta}, Y^{j\beta}$ are internal variables representing $\partial_0 p^0$ and $\partial_1 p^1$ respectively. The unknown momenta boundary values are similarly defined as

$$\pi^0_{0[\alpha]} = \pi^0_{1[\alpha]} - \Delta t \sum_{j,\beta} B'_{\alpha,j\beta} X^{j\beta},$$
$$\pi^1_{[i]0} = \pi^1_{[i]1} - \Delta x \sum_{j,\beta} \tilde{B}'_{i,j\beta} Y^{j\beta},$$

where $B'_{\alpha,j\beta}$ and $\tilde{B}'_{i,j\beta}$ are again arbitrary expansion coefficients. We will see later that the expansion coefficients will have to satisfy symplecticity conditions in order for the method to be well-defined.

We then approximate the action integral $S[\phi,p]=\int(p^\mu\partial_\mu\phi - H(\phi,p^0,p^1))d^2x$ using quadrature and the above internal stages

$$S_d^{\square}[\Phi_{i\alpha},P_{i\alpha}] = \Delta t\Delta x \sum_{i,\alpha} b_i\tilde{b}_\alpha\Big(P^0_{i\alpha}\partial_t\phi_d(c_i\Delta t,\tilde{c}_\alpha\Delta x)+P^1_{i\alpha}\partial_x\phi_d(c_i\Delta t,\tilde{c}_\alpha\Delta x)-H(\Phi_{i\alpha},P^0_{i\alpha},P^1_{i\alpha})\Big).$$

The discrete boundary Hamiltonian is obtained by extremizing over the internal stages Φ, P^0, P^1, which are defined in terms of V,X,Y. Since we have already enforced the boundary conditions in the above field and momenta expansions, we can construct the discrete boundary Hamiltonian by extremizing over $V^{i\alpha}$, $X^{i\alpha}$, $Y^{i\alpha}$ (for every $i=1,\dots,s$ and $\alpha=1,\dots,\sigma$),

$$\begin{aligned}&H_d^+(\{\varphi_{[i]0},\varphi_{0[\alpha]},\pi^1_{[i]1},\pi^0_{1[\alpha]}\}_{i,\alpha})\\ &\qquad = \operatorname*{ext}_{V^{i\alpha},X^{i\alpha},Y^{i\alpha}}\Bigg(\underbrace{\sum_{i=1}^{s}\Delta t\; b_i\pi^1_{[i]1}\varphi_{[i]1}+\sum_{\alpha=1}^{\sigma}\Delta x\;\tilde{b}_\alpha\pi^0_{1[\alpha]}\varphi_{1[\alpha]}-S_d^{\square}[\Phi_{i\alpha},P_{i\alpha}]}_{\equiv K(\{\varphi_A,\pi_B,V^{i\alpha},X^{i\alpha},Y^{i\alpha}\})}\Bigg).\end{aligned}$$

H_d^+ is then given by extremizing $K(\{\varphi_A,\pi_B,V^{i\alpha},X^{i\alpha},Y^{i\alpha}\})$ with respect to $V^{i\alpha}, X^{i\alpha}$, and $Y^{i\alpha}$ (where again we denote $\varphi_A=\{\varphi_{[i]0},\varphi_{0[\alpha]}\}$ and $\pi_B=\{\pi^1_{[i]1},\pi^0_{1[\alpha]}\}$). Expanding K, we have

$$\begin{aligned}&K(\{\varphi_A,\pi_B,V^{i\alpha},X^{i\alpha},Y^{i\alpha}\})\\ &\quad=\Delta t\sum_i b_i\pi^1_{[i]1}(\varphi_{[i]0}+\Delta x\sum_{j,\beta}\tilde{B}_{i,j\beta}W^{j\beta})+\Delta x\sum_\alpha\tilde{b}_\alpha\pi^0_{1[\alpha]}(\varphi_{0[\alpha]}+\Delta t\sum_{j,\beta}B_{\alpha,j\beta}V^{j\beta})\\ &\qquad-\Delta t\Delta x\sum_{i,\alpha}b_i\tilde{b}_\alpha\Big(\pi^0_{1[\alpha]}-\Delta t\sum_{k,\gamma}A'_{i\alpha,k\gamma}X^{k\gamma}\Big)\sum_{j,\beta}V^{j\beta}\chi_j(c_i)\tilde{\chi}_\alpha(\tilde{c}_\alpha)\\ &\qquad-\Delta t\Delta x\sum_{i,\alpha}b_i\tilde{b}_\alpha\Big(\pi^1_{[i]1}-\Delta x\sum_{k,\gamma}\tilde{A}'_{i\alpha,k\gamma}Y^{k\gamma}\Big)\sum_{j,\beta}W^{j\beta}\chi_j(c_i)\tilde{\chi}_\alpha(\tilde{c}_\alpha)\\ &\qquad+\Delta t\Delta x\sum_{i,\alpha}b_i\tilde{b}_\alpha H(\Phi_{i\alpha},P^0_{i\alpha},P^1_{i\alpha}).\end{aligned}$$

The stationarity conditions $\partial K/\partial V^{i\alpha} = 0$, $\partial K/\partial X^{i\alpha} = 0$, $\partial K/\partial Y^{i\alpha} = 0$, combined with the discrete forward Hamilton's equations (2.3a)-(2.3d) define our multisymplectic variational integrator.

Supposing that one solves the stationarity conditions for $V^{i\alpha}$, $X^{i\alpha}$, $Y^{i\alpha}$ in terms of φ_A and π_B, this gives $H_d^+(\{\varphi_A, \pi_B\}) = K(\{\varphi_A, \pi_B, V^{i\alpha}(\varphi_A, \pi_B), X^{i\alpha}(\varphi_A, \pi_B), Y^{i\alpha}(\varphi_A, \pi_B)\})$. The right hand side of the discrete forward Hamilton's equations, (2.3a)-(2.3d), can then be computed in terms of K via

$$\begin{aligned}
\frac{\partial}{\partial \varphi_{[i]0}} H_d^+(\{\varphi_A, \pi_B\}) &= \frac{\partial}{\partial \varphi_{[i]0}} K(\{\varphi_A, \pi_B, V^{i\alpha}(\varphi_A, \pi_B), X^{i\alpha}(\varphi_A, \pi_B), Y^{i\alpha}(\varphi_A, \pi_B)\}) \\
&= \frac{\partial}{\partial \varphi_{[i]0}} K + \sum_{j,\alpha} \Big(\cancel{\frac{\partial K}{\partial V^{j\alpha}}} \frac{\partial V^{j\alpha}}{\partial \varphi_{[i]0}} + \cancel{\frac{\partial K}{\partial X^{j\alpha}}} \frac{\partial X^{j\alpha}}{\partial \varphi_{[i]0}} + \cancel{\frac{\partial K}{\partial Y^{j\alpha}}} \frac{\partial Y^{j\alpha}}{\partial \varphi_{[i]0}} \Big) \\
&= \frac{\partial}{\partial \varphi_{[i]0}} K,
\end{aligned}$$

and similarly for the other specified boundary values. Hence, the derivatives of H_d^+ with respect to φ_A, π_B can be computed using only the explicit dependence of K on φ_A, π_B.

2.2.3 Multisymplectic Partitioned Runge–Kutta Method

Let us suppose that instead of the basis $\{\chi_i\}, \{\tilde{\chi}_\alpha\}$, we choose basis functions $\{\psi_i\}$, $\{\tilde{\psi}_\alpha\}$ that have the interpolating property $\psi_i(c_j) = \delta_{ij}$, $\tilde{\psi}_\alpha(\tilde{c}_\beta) = \delta_{\alpha\beta}$. Note that one can always transform the previous set of basis functions to a set of basis functions with this property, assuming that the original choice of basis functions $\chi_i, \tilde{\chi}_\alpha$ have the property that the matrices with entries $M_{ij} = \chi_i(c_j)$, $\tilde{M}_{\alpha\beta} = \tilde{\chi}_\alpha(\tilde{c}_\beta)$ are invertible. If they are not, then the expansion of the derivatives, equations (2.8a)-(2.8b), does not depend independently on all of the $V^{i\alpha}$, $W^{i\alpha}$ and hence one needs to reduce the number of independent variables; to avoid this, ensure that the matrices with entries $\chi_i(c_j)$ and $\tilde{\chi}_\alpha(\tilde{c}_\beta)$ are invertible. Letting $\chi(\cdot) = (\chi_1(\cdot), \ldots, \chi_s(\cdot))^T$ and $\tilde{\chi}(\cdot) = (\tilde{\chi}_1(\cdot), \ldots, \tilde{\chi}_\sigma(\cdot))^T$ (and similarly define ψ, $\tilde{\psi}$), a set of basis functions with the interpolating property can be constructed by $\psi = M^{-1}\chi$, $\tilde{\psi} = \tilde{M}^{-1}\tilde{\chi}$. In particular, the $\{\psi_i\}$,

$\{\tilde{\psi}_\alpha\}$ span the same function spaces as the $\{\chi_i\}$, $\{\tilde{\chi}_\alpha\}$ respectively, so there is no loss of generality.

With this assumption, we approximate the derivatives of the fields as

$$\partial_t \phi_d(c_i \Delta t, \tilde{c}_\alpha \Delta x) = \sum_{j,\beta} V^{j\beta} \psi_j(c_i) \tilde{\psi}_\beta(\tilde{c}_\alpha) = V^{i\alpha},$$
$$\partial_x \phi_d(c_i \Delta t, \tilde{c}_\alpha \Delta x) = \sum_{j,\beta} W^{j\beta} \psi_j(c_i) \tilde{\psi}_\beta(\tilde{c}_\alpha) = W^{i\alpha}.$$

Integrating gives the internal stages and the unknown boundary values,

$$\Phi_{i\alpha} = \varphi_{0[\alpha]} + \Delta t \sum_j a_{ij} V^{j\alpha},$$
$$\Phi_{i\alpha} = \varphi_{[i]0} + \Delta x \sum_\beta \tilde{a}_{\alpha\beta} W^{i\beta}$$
$$\varphi_{1[\alpha]} = \varphi_{0[\alpha]} + \Delta t \sum_j b_j V^{j\alpha},$$
$$\varphi_{[i]1} = \varphi_{[i]0} + \Delta x \sum_\beta \tilde{b}_\beta W^{i\beta},$$

where $a_{ij} = \int_0^{c_i} \psi_j(s) ds$, $\tilde{a}_{\alpha\beta} = \int_0^{\tilde{c}_\alpha} \tilde{\psi}_\beta(s) ds$ and the quadrature weights $b_i = \int_0^1 \psi_i(s) ds$, $\tilde{b}_\alpha = \int_0^1 \tilde{\psi}_\alpha(s) ds$ are chosen so that quadrature is exact on the span of the basis functions. As before, expand the momenta using a different set of coefficients.

$$
\begin{aligned}
X^{i\alpha} &= \partial_t p_d^0(c_i\Delta t, \tilde{c}_\alpha \Delta x), \\
Y^{i\alpha} &= \partial_x p_d^1(c_i\Delta t, \tilde{c}_\alpha \Delta x), \\
P^0_{i\alpha} &= \pi^0_{1[\alpha]} - \Delta t \sum_j a'_{ij} X^{j\alpha}, \\
P^1_{i\alpha} &= \pi^1_{[i]1} - \Delta x \sum_\beta \tilde{a}'_{\alpha\beta} Y^{i\beta}, \\
\pi^0_{0[\alpha]} &= \pi^0_{1[\alpha]} - \Delta t \sum_j b'_j X^{j\alpha}, \\
\pi^1_{[i]0} &= \pi^1_{[i]1} - \Delta x \sum_\beta \tilde{b}'_\beta Y^{i\beta}.
\end{aligned}
$$

We impose that $b'_j > 0$, $\tilde{b}'_\beta > 0$ and that $\sum_j b'_j = 1$, $\sum_\beta \tilde{b}'_\beta = 1$ for the approximation to be consistent. We will later derive a condition on the coefficients a'_{ij}, $\tilde{a}'_{\alpha\beta}$, b'_i, $\tilde{b}'_\alpha$ in order for the method to be well-defined. For now, we proceed formally.

With these, K can be expressed as

$$
\begin{aligned}
&K(\{\varphi_A, \pi_B, V^{i\alpha}, X^{i\alpha}, Y^{i\alpha}\}) \\
&\quad = \Delta x \sum_\alpha \tilde{b}_\alpha \pi^0_{1[\alpha]}(\varphi_{0[\alpha]} + \Delta t \sum_j b_j V^{j\alpha}) + \Delta t \sum_i b_i \pi^1_{[i]1}(\varphi_{[i]0} + \Delta x \sum_\beta \tilde{b}_\beta W^{i\beta}) \\
&\quad\quad - \Delta t \Delta x \sum_{i,\alpha} b_i \tilde{b}_\alpha \Big(\pi^0_{1[\alpha]} - \Delta t \sum_j a'_{ij} X^{j\alpha}\Big) V^{i\alpha} \\
&\quad\quad - \Delta t \Delta x \sum_{i,\alpha} b_i \tilde{b}_\alpha \Big(\pi^1_{[i]1} - \Delta x \sum_\beta \tilde{a}'_{\alpha\beta} Y^{i\beta}\Big) W^{i\alpha} \\
&\quad\quad + \Delta t \Delta x \sum_{i,\alpha} b_i \tilde{b}_\alpha H(\Phi_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}).
\end{aligned}
$$

Now, we compute the stationarity conditions. First, note that V and W are not independent, since they are related by

$$\varphi_{0[\alpha]} + \Delta t \sum_j a_{ij} V^{j\alpha} = \Phi_{i\alpha} = \varphi_{[i]0} + \Delta x \sum_\beta \tilde{a}_{\alpha\beta} W^{i\beta};$$

then, taking the derivative with respect to $V^{j\beta}$,

$$\Delta t a_{ij} \delta_{\alpha\beta} = \Delta x \sum_\gamma \tilde{a}_{\alpha\gamma} \frac{\partial W^{i\gamma}}{\partial V^{j\beta}}.$$

Let us assume that the Runge–Kutta matrices (a_{ij}) and $(\tilde{a}_{\alpha\gamma})$ are invertible (however, in the subsequent section, we will show how to derive the stationarity conditions without this assumption using independent internal stages). Then, the above relation can be inverted to give

$$\frac{\partial W^{i\sigma}}{\partial V^{j\beta}} = \frac{\Delta t}{\Delta x} a_{ij} (\tilde{a}^{-1})_{\sigma\beta}.$$

Extremizing K with respect to $X^{j\alpha}$,

$$0 = \frac{\partial K}{\partial X^{j\alpha}} = \Delta t^2 \Delta x \sum_i b_i \tilde{b}_\alpha a'_{ij} V^{i\alpha} - \Delta t^2 \Delta x \sum_i b_i \tilde{b}_\alpha a'_{ij} \frac{\partial H}{\partial p^0}(\Phi_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}).$$

Dividing by $\Delta t^2 \Delta x \tilde{b}_\alpha$ gives

$$\sum_i b_i a'_{ij} \left(V^{i\alpha} - \frac{\partial H}{\partial p^0}(\Phi_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}) \right) = 0.$$

Similarly, extremizing K with respect to $Y^{j\alpha}$ gives

$$\sum_\beta \tilde{b}_\beta \tilde{a}'_{\beta\alpha} \left(W^{j\beta} - \frac{\partial H}{\partial p^1}(\Phi_{j\beta}, P^0_{j\beta}, P^1_{j\beta}) \right) = 0.$$

These are respectively the internal stage approximations to the De Donder–Weyl equations $\partial_t \phi = \partial H / \partial p^0$ and $\partial_x \phi = \partial H / \partial p^1$.

Extremizing K with respect to $V^{j\beta}$,

$$0 = \frac{\partial K}{\partial V^{j\beta}} = \Delta t \Delta x b_j \tilde{b}_\beta \pi^0_{1[\beta]} + \Delta t \Delta x \sum_{i,\sigma} b_i \tilde{b}_\sigma \pi^1_{[i]1} \frac{\Delta t}{\Delta x} a_{ij} (\tilde{a}^{-1})_{\sigma\beta} - \Delta t \Delta x b_j \tilde{b}_\beta P^0_{j\beta}$$
$$- \Delta t \Delta x \sum_{i,\sigma} b_i \tilde{b}_\sigma P^1_{i\sigma} \frac{\Delta t}{\Delta x} a_{ij} (\tilde{a}^{-1})_{\sigma\beta} + \Delta t \Delta x \sum_i b_i \tilde{b}_\beta \Delta t a_{ij} \frac{\partial H}{\partial \phi}(\Phi_{i\beta}, P^0_{i\beta}, P^1_{i\beta}).$$

Dividing by $\Delta t^2 \Delta x$ and grouping gives

$$b_j \tilde{b}_\beta \frac{\pi^0_{1[\beta]} - P^0_{j\beta}}{\Delta t} + \sum_{i,\sigma} b_i \tilde{b}_\sigma a_{ij} (\tilde{a}^{-1})_{\sigma\beta} \frac{\pi^1_{[i]1} - P^1_{i\sigma}}{\Delta x} = - \sum_i b_i \tilde{b}_\beta a_{ij} \frac{\partial H}{\partial \phi}(\Phi_{i\beta}, P^0_{i\beta}, P^1_{i\beta}).$$

Substitute $\frac{\pi^0_{1[\beta]} - P^0_{j\beta}}{\Delta t} = \sum_k a'_{jk} X^{k\beta}$ and $\frac{\pi^1_{[i]1} - P^1_{i\sigma}}{\Delta x} = \sum_\gamma \tilde{a}'_{\sigma\gamma} Y^{i\gamma}$,

$$\sum_k b_j \tilde{b}_\beta a'_{jk} X^{k\beta} + \sum_{i,\sigma,\gamma} b_i \tilde{b}_\sigma a_{ij} (\tilde{a}^{-1})_{\sigma\beta} \tilde{a}'_{\sigma\gamma} Y^{i\gamma} = - \sum_i b_i \tilde{b}_\beta a_{ij} \frac{\partial H}{\partial \phi}(\Phi_{i\beta}, P^0_{i\beta}, P^1_{i\beta}).$$

To symmetrize the above equations, multiply by $\tilde{a}_{\beta\delta}$ and sum over β, which yields

$$\sum_{k,\beta} b_j \tilde{b}_\beta a'_{jk} \tilde{a}_{\beta\delta} X^{k\beta} + \sum_{i,\gamma} b_i \tilde{b}_\delta a_{ij} \tilde{a}'_{\delta\gamma} Y^{i\gamma} = - \sum_{i,\beta} b_i \tilde{b}_\beta a_{ij} \tilde{a}_{\beta\delta} \frac{\partial H}{\partial \phi}(\Phi_{i\beta}, P^0_{i\beta}, P^1_{i\beta}).$$

This is the internal stage approximation to the remaining De Donder–Weyl equation $\partial_t p^0 + \partial_x p^1 = -\partial H / \partial \phi$. Note that the above form of the stationarity condition does not involve a^{-1} or $\tilde{a}^{-1}$, so it is plausible that one can derive these equations without assuming the invertibility of the Runge–Kutta matrices; later, we will show that this is the case using independent internal stages.

Now, we compute the discrete forward Hamilton's equations. We have

$$
\begin{aligned}
\varphi_{1[\alpha]} &= \frac{1}{\tilde{b}_\alpha \Delta x} \frac{\partial H_d^+}{\partial \pi^0_{1[\alpha]}} \\
&= \frac{1}{\tilde{b}_\alpha \Delta x} \frac{\partial K}{\partial \pi^0_{1[\alpha]}} \\
&= \varphi_{0[\alpha]} + \Delta t \sum_j b_j V^{j\alpha} - \Delta t \sum_j b_j V^{j\alpha} + \Delta t \sum_j b_j \frac{\partial H}{\partial p^0}(\Phi_{j\alpha}, P^0_{j\alpha}, P^1_{j\alpha}) \\
&= \varphi_{0[\alpha]} + \Delta t \sum_j b_j \frac{\partial H}{\partial p^0}(\Phi_{j\alpha}, P^0_{j\alpha}, P^1_{j\alpha}).
\end{aligned}
$$

Similarly,

$$
\varphi_{[i]1} = \varphi_{[i]0} + \Delta x \sum_\beta \tilde{b}_\beta \frac{\partial H}{\partial p^1}(\Phi_{i\beta}, P^0_{i\beta}, P^1_{i\beta}).
$$

Computing the discrete forward Hamilton's equations for the momenta gives

$$
\begin{aligned}
\pi^0_{0[\alpha]} &= \pi^0_{1[\alpha]} + \frac{\Delta t}{\tilde{b}_\alpha} \sum_{i,\beta} b_i \tilde{b}_\beta \frac{\partial H}{\partial \phi}(\Phi_{i\beta}, P^0_{i\beta}, P^1_{i\beta}) \frac{\partial \Phi_{i\beta}}{\partial \varphi_{0[\alpha]}}, \\
\pi^1_{[i]0} &= \pi^1_{[i]1} + \frac{\Delta x}{b_i} \sum_{j,\alpha} b_j \tilde{b}_\alpha \frac{\partial H}{\partial \phi}(\Phi_{j\alpha}, P^0_{j\alpha}, P^1_{j\alpha}) \frac{\partial \Phi_{j\alpha}}{\partial \varphi_{[i]0}}.
\end{aligned}
$$

We will postpone the discussion of the discrete forward Hamilton's equations until after discussing independent internal stages, which will give a more explicit characterization of these equations.

To summarize, our method is given by

$$\Phi_{i\alpha} = \varphi_{0[\alpha]} + \Delta t \sum_j a_{ij} V^{j\alpha}, \tag{2.10a}$$

$$P^0_{i\alpha} = \pi^0_{1[\alpha]} - \Delta t \sum_j a'_{ij} X^{j\alpha}, \tag{2.10b}$$

$$\varphi_{1[\alpha]} = \varphi_{0[\alpha]} + \Delta t \sum_j b_j V^{j\alpha}, \tag{2.10c}$$

$$\pi^0_{0[\alpha]} = \pi^0_{1[\alpha]} - \Delta t \sum_j b'_j X^{j\alpha}, \tag{2.10d}$$

$$\Phi_{i\alpha} = \varphi_{[i]0} + \Delta x \sum_\beta \tilde{a}_{\alpha\beta} W^{i\beta} \tag{2.10e}$$

$$P^1_{i\alpha} = \pi^1_{[i]1} - \Delta x \sum_\beta \tilde{a}'_{\alpha\beta} Y^{i\beta}, \tag{2.10f}$$

$$\varphi_{[i]1} = \varphi_{[i]0} + \Delta x \sum_\beta \tilde{b}_\beta W^{i\beta}, \tag{2.10g}$$

$$\pi^1_{[i]0} = \pi^1_{[i]1} - \Delta x \sum_\beta \tilde{b}'_\beta Y^{i\beta}. \tag{2.10h}$$

$$\sum_i b_i a'_{ij} \Big(V^{i\alpha} - \frac{\partial H}{\partial p^0} (\Phi_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}) \Big) = 0, \tag{2.10i}$$

$$\sum_\beta \tilde{b}_\beta \tilde{a}'_{\beta\alpha} \Big(W^{j\beta} - \frac{\partial H}{\partial p^1} (\Phi_{j\beta}, P^0_{j\beta}, P^1_{j\beta}) \Big) = 0, \tag{2.10j}$$

$$\sum_{k,\beta} b_j \tilde{b}_\beta a'_{jk} \tilde{a}_{\beta\delta} X^{k\beta} + \sum_{i,\gamma} b_i \tilde{b}_\delta a_{ij} \tilde{a}'_{\delta\gamma} Y^{i\gamma} = - \sum_{i,\beta} b_i \tilde{b}_\beta a_{ij} \tilde{a}_{\beta\delta} \frac{\partial H}{\partial \phi} (\Phi_{i\beta}, P^0_{i\beta}, P^1_{i\beta}). \tag{2.10k}$$

Independent Internal Stages. We now reformulate the above construction using independent internal stages and derive explicit conditions on the coefficients for the momenta expansion for the method to be well-defined. Recall that in the above construction, we enforced the condition that the internal stages $\Phi_{i\alpha}$ produced by both $V^{i\alpha}$ and $W^{i\alpha}$ had to be the same; we now relax this assumption and let the internal stages be independent, but subsequently enforce that they are the same by using Lagrange multipliers. Compared to the previous formulation, the use of independent internal stages has the advantage that the discrete forward Hamilton's equations can be written explicitly. Furthermore, the generalization to higher spacetime dimensions is straight-forward as opposed to the previous formulation, which would involve inverting the condition that the internal stages obtained from the various spacetime derivative approximations, $\partial_\mu \phi_d$, are consistent.

Hence, we define independent internal stages corresponding to integration in each spacetime direction,

$$\Phi_{i\alpha} \equiv \phi(c_i\Delta t, \tilde{c}_\alpha \Delta x) = \phi(0, \tilde{c}_\alpha \Delta x) + \Delta t \sum_{j,\beta} V^{j\beta} \int_0^{c_i} \psi_j(s) ds \; \tilde{\psi}_\beta(\tilde{c}_\alpha) = \varphi_{0[\alpha]} + \Delta t \sum_j a_{ij} V^{j\alpha},$$

$$\tilde{\Phi}_{i\alpha} \equiv \phi(c_i\Delta t, \tilde{c}_\alpha \Delta x) = \phi(c_i \Delta t, 0) + \Delta x \sum_{j,\beta} W^{j\beta} \psi_j(c_i) \int_0^{c_\alpha} \tilde{\psi}_\beta(s) ds = \varphi_{[i]0} + \Delta x \sum_\beta \tilde{a}_{\alpha\beta} W^{i\beta}.$$

The expansion of the other quantities are the same as the previous discussion.

We will evaluate the Hamiltonian at the weighted combination $\Phi^\theta_{i\alpha} \equiv \theta \Phi_{i\alpha} + (1-\theta)\tilde{\Phi}_{i\alpha}$ for some arbitrary parameter $\theta \in \mathbb{R}$ and subsequently enforce that the two sets of internal stages are the same through a Lagrange multiplier term $\sum_{i,\alpha} \lambda_{i\alpha}(\Phi_{i\alpha} - \tilde{\Phi}_{i\alpha})$. Thus, after enforcing the stationarity conditions, $\Phi^\theta_{i\alpha} = \Phi_{i\alpha} = \tilde{\Phi}_{i\alpha}$. In this formulation, K is

$$\begin{aligned}
K(\{\varphi_A, \pi_B, V^{i\alpha}, W^{i\alpha}, X^{i\alpha}, Y^{i\alpha}, \lambda_{i\alpha}\}) = {}& \Delta x \sum_\alpha \tilde{b}_\alpha \pi^0_{1[\alpha]}(\varphi_{0[\alpha]} + \Delta t \sum_j b_j V^{j\alpha}) \\
& + \Delta t \sum_i b_i \pi^1_{[i]1}(\varphi_{[i]0} + \Delta x \sum_\beta \tilde{b}_\beta W^{i\beta}) \\
& - \Delta t \Delta x \sum_{i,\alpha} b_i \tilde{b}_\alpha \left(\pi^0_{1[\alpha]} - \Delta t \sum_j a'_{ij} X^{j\alpha}\right) V^{i\alpha} \\
& - \Delta t \Delta x \sum_{i,\alpha} b_i \tilde{b}_\alpha \left(\pi^1_{[i]1} - \Delta x \sum_\beta \tilde{a}'_{\alpha\beta} Y^{i\beta}\right) W^{i\alpha} \\
& + \Delta t \Delta x \sum_{i,\alpha} b_i \tilde{b}_\alpha H(\Phi^\theta_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}) + \sum_{i,\alpha} \lambda_{i\alpha}(\Phi_{i\alpha} - \tilde{\Phi}_{i\alpha});
\end{aligned}$$

where now both $\{V^{i\alpha}\}$ and $\{W^{i\alpha}\}$ are independent. The discrete boundary Hamiltonian H_d^+ is given by extremizing K with respect to all of the internal variables, $\{V^{i\alpha}, W^{i\alpha}, X^{i\alpha}, Y^{i\alpha}, \lambda_{i\alpha}\}$.

Extremizing K with respect to $X^{j\alpha}$ and $Y^{j\alpha}$ gives the same stationarity conditions as the previous case of equal internal stages, since the momenta expansions were unchanged, except with H evaluated at $\Phi^\theta_{i\alpha}$. Namely,

$$\sum_i b_i a'_{ij}\Big(V^{i\alpha} - \frac{\partial H}{\partial p^0}(\Phi^\theta_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha})\Big) = 0, \tag{2.11a}$$

$$\sum_\beta \tilde{b}_\beta \tilde{a}'_{\beta\alpha}\Big(W^{j\beta} - \frac{\partial H}{\partial p^1}(\Phi^\theta_{j\beta}, P^0_{j\beta}, P^1_{j\beta})\Big) = 0. \tag{2.11b}$$

Extremizing K with respect to $V^{j\beta}$,

$$\begin{aligned}
0 &= \frac{\partial K}{\partial V^{j\beta}} \\
&= \Delta t \Delta x b_j \tilde{b}_\beta \pi^0_{1[\beta]} - \Delta t \Delta x b_j \tilde{b}_\beta P^0_{j\beta} + \Delta t^2 \Delta x \sum_i b_i \tilde{b}_\beta a_{ij} \theta \frac{\partial H}{\partial \phi}(\Phi^\theta_{i\beta}, P^0_{i\beta}, P^1_{i\beta}) + \Delta t \sum_i \lambda_{i\beta} a_{ij} \\
&= \Delta t^2 \Delta x b_j \tilde{b}_\beta \sum_k a'_{jk} X^{k\beta} + \Delta t^2 \Delta x \sum_i b_i \tilde{b}_\beta a_{ij} \theta \frac{\partial H}{\partial \phi}(\Phi^\theta_{i\beta}, P^0_{i\beta}, P^1_{i\beta}) + \Delta t \sum_i \lambda_{i\beta} a_{ij}.
\end{aligned}$$

Dividing by $\Delta t^2 \Delta x$,

$$\sum_k b_j \tilde{b}_\beta a'_{jk} X^{k\beta} + \sum_i b_i \tilde{b}_\beta a_{ij} \theta \frac{\partial H}{\partial \phi}(\Phi^\theta_{i\beta}, P^0_{i\beta}, P^1_{i\beta}) + \frac{1}{\Delta t \Delta x} \sum_i \lambda_{i\beta} a_{ij} = 0. \tag{2.12}$$

Similarly, extremizing K with respect to $W^{j\beta}$ (and dividing by $\Delta t \Delta x^2$) gives

$$\sum_\alpha b_j \tilde{b}_\beta \tilde{a}'_{\beta\alpha} Y^{j\alpha} + \sum_\alpha b_j \tilde{b}_\alpha \tilde{a}_{\alpha\beta}(1-\theta) \frac{\partial H}{\partial \phi}(\Phi^\theta_{j\alpha}, P^0_{j\alpha}, P^1_{j\alpha}) - \frac{1}{\Delta t \Delta x} \sum_\alpha \lambda_{j\alpha} \tilde{a}_{\alpha\beta} = 0. \tag{2.13}$$

Let us combine these two stationarity conditions to eliminate θ and the Lagrange multiplier terms. Multiply equation (2.12) by $\tilde{a}_{\beta\delta}$ and sum over β; multiply equation (2.13) by a_{ji} and sum over j. Subsequently, add the two resulting equations. This gives

$$\sum_{k,\beta} b_j \tilde{b}_\beta a'_{jk} \tilde{a}_{\beta\delta} X^{k\beta} + \sum_{i,\gamma} b_i \tilde{b}_\delta a_{ij} \tilde{a}'_{\delta\gamma} Y^{i\gamma} = -\sum_{i,\beta} b_i \tilde{b}_\beta a_{ij} \tilde{a}_{\beta\delta} \frac{\partial H}{\partial \phi}(\Phi^\theta_{i\beta}, P^0_{i\beta}, P^1_{i\beta}). \tag{2.14}$$

Finally, extremizing K with respect to $\lambda_{i\alpha}$ enforces that the independent internal stages are the same, $0 = \partial K/\partial \lambda_{i\alpha} = \Phi_{i\alpha} - \tilde{\Phi}_{i\alpha}$, and hence $\Phi^\theta_{i\alpha} = \Phi_{i\alpha} = \tilde{\Phi}_{i\alpha}$. We have rederived the stationarity conditions that we saw in the case of equal internal stages, without the assumption of invertibility of the Runge–Kutta matrices, (a_{ij}), $(\tilde{a}_{\alpha\beta})$.

Now, we aim to provide a more explicit characterization of the discrete forward Hamilton's equations. We will assume again that the Runge–Kutta matrices (a_{ij}), $(\tilde{a}_{\alpha\beta})$ are invertible. Computing the discrete forward Hamilton's equations for the field boundary values,

$$\varphi_{1[\alpha]} = \frac{1}{\tilde{b}_\alpha \Delta x} \frac{\partial H^+_d}{\partial \pi^0_{1[\alpha]}} = \frac{1}{\tilde{b}_\alpha \Delta x} \frac{\partial K}{\partial \pi^0_{1[\alpha]}} = \varphi_{0[\alpha]} + \Delta t \sum_j b_j \frac{\partial H}{\partial p^0}(\Phi^\theta_{j\alpha}, P^0_{j\alpha}, P^0_{j\alpha}),$$
$$\varphi_{[i]1} = \frac{1}{b_i \Delta t} \frac{\partial H^+_d}{\partial \pi^1_{[i]1}} = \frac{1}{b_i \Delta t} \frac{\partial K}{\partial \pi^1_{[i]1}} = \varphi_{[i]0} + \Delta x \sum_\beta \tilde{b}_\beta \frac{\partial H}{\partial p^1}(\Phi^\theta_{i\beta}, P^0_{i\beta}, P^1_{i\beta}).$$

Recall that we also have the expansion for the field boundary values

$$\varphi_{1[\alpha]} = \varphi_{0[\alpha]} + \Delta t \sum_j b_j V^{j\alpha},$$
$$\varphi_{[i]1} = \varphi_{[i]0} + \Delta x \sum_\beta \tilde{b}_\beta W^{i\beta}.$$

We will see shortly that, with a particular condition on the coefficients of the momenta expansion, the discrete forward Hamilton's equations for the field values are consistent with the field expansions, i.e., that $V^{j\alpha} = \frac{\partial H}{\partial p^0}(\Phi^\theta_{j\alpha}, P^0_{j\alpha}, P^0_{j\alpha})$ and similarly $W^{i\beta} = \frac{\partial H}{\partial p^1}(\Phi^\theta_{i\beta}, P^0_{i\beta}, P^1_{i\beta})$.

First, we compute the discrete forward Hamilton's equations for the momenta boundary values,

$$\pi^0_{0[\alpha]} = \frac{1}{\tilde{b}_\alpha \Delta x} \frac{\partial H_d^+}{\partial \varphi_{0[\alpha]}} = \frac{1}{\tilde{b}_\alpha \Delta x} \frac{\partial K}{\partial \varphi_{0[\alpha]}} = \pi^0_{1[\alpha]} + \Delta t \sum_i b_i \theta \frac{\partial H}{\partial \phi}(\Phi^\theta_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}) + \frac{1}{\tilde{b}_\alpha \Delta x} \sum_i \lambda_{i\alpha},$$
$$\pi^1_{[i]0} = \frac{1}{b_i \Delta t} \frac{\partial H_d^+}{\partial \varphi_{[i]0}} = \frac{1}{b_i \Delta t} \frac{\partial K}{\partial \varphi_{[i]0}} = \pi^1_{[i]1} + \Delta x \sum_\alpha \tilde{b}_\alpha (1-\theta) \frac{\partial H}{\partial \theta}(\Phi^\theta_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}) - \frac{1}{b_i \Delta t} \sum_\alpha \lambda_{i\alpha}.$$

For our method to be well-defined, these are required to be consistent with the momenta expansions,

$$\pi^0_{0[\alpha]} = \pi^0_{1[\alpha]} - \Delta t \sum_j b'_j X^{j\alpha},$$
$$\pi^1_{[i]0} = \pi^1_{[i]1} - \Delta x \sum_\beta \tilde{b}'_\beta Y^{i\beta}.$$

To do this, we solve the stationarity conditions (2.12) and (2.13) for the Lagrange multipliers. Multiply equation (2.12) by $(a^{-1})_{jl}$ and sum over j; multiply equation (2.13) by $(\tilde{a}^{-1})_{\beta\gamma}$ and sum over β. This gives

$$\lambda_{l\beta} = -\Delta t \Delta x b_l \tilde{b}_\beta \theta \frac{\partial H}{\partial \phi}(\Phi^\theta_{l\beta}, P^0_{l\beta}, P^1_{l\beta}) - \Delta t \Delta x \sum_{j,k} b_j \tilde{b}_\beta a'_{jk} (a^{-1})_{jl} X^{k\beta},$$
$$\lambda_{j\gamma} = \Delta t \Delta x b_j \tilde{b}_\gamma (1-\theta) \frac{\partial H}{\partial \phi}(\Phi^\theta_{j\gamma}, P^0_{j\gamma}, P^1_{j\gamma}) + \Delta t \Delta x \sum_{\alpha,\beta} b_j \tilde{b}_\beta \tilde{a}'_{\beta\alpha} (\tilde{a}^{-1})_{\beta\gamma} Y^{j\alpha}.$$

Plugging these into the respective discrete forward Hamilton's equations for the momenta boundary values, we have

$$\pi^0_{0[\alpha]} = \pi^0_{1[\alpha]} - \Delta t \sum_{j,k,l} b_j a'_{jk} (a^{-1})_{jl} X^{k\beta} \stackrel{!}{=} \pi^0_{1[\alpha]} - \Delta t \sum_k b'_k X^{k\alpha},$$
$$\pi^1_{[i]0} = \pi^1_{[i]1} - \Delta x \sum_{\alpha,\beta,\gamma} \tilde{b}_\beta \tilde{a}'_{\beta\alpha} (\tilde{a}^{-1})_{\beta\gamma} Y^{i\alpha} \stackrel{!}{=} \pi^1_{[i]1} - \Delta x \sum_\alpha \tilde{b}'_\alpha Y^{i\alpha}.$$

Proposition 2.2.5. *The method arising from approximating the internal stages with the partitioned Runge–Kutta expansion is well-defined if and only if the partitioned Runge–Kutta method* *is symplectic in both space and time, i.e.*

$$\sum_{j,l} b_j a'_{jk}(a^{-1})_{jl} = b'_k,$$

$$\sum_{\beta,\gamma} \tilde{b}_\beta \tilde{a}'_{\beta\alpha}(\tilde{a}^{-1})_{\beta\gamma} = \tilde{b}'_\alpha.$$

A sufficient condition is the usual choice of symplectic partitioned Runge–Kutta coefficients,

$$a'_{jk} = \frac{b'_k a_{kj}}{b_j},$$

$$\tilde{a}'_{\beta\alpha} = \frac{\tilde{b}'_\alpha \tilde{a}_{\alpha\beta}}{\tilde{b}_\beta}.$$

(We will see after expressing the momenta internal stages in terms of π_A instead of π_B that these are the usual choice of symplectic partitioned Runge–Kutta coefficients).

Proof. By comparing the momenta expansions to the discrete forward Hamilton's equations for the momenta, we must have

$$\sum_{j,k,l} b_j a'_{jk}(a^{-1})_{jl} X^{k\beta} = \sum_k b'_k X^{k\alpha}, \tag{2.15a}$$

$$\sum_{\alpha,\beta,\gamma} \tilde{b}_\beta \tilde{a}'_{\beta\alpha}(\tilde{a}^{-1})_{\beta\gamma} Y^{i\alpha} = \sum_\alpha \tilde{b}'_\alpha Y^{i\alpha}. \tag{2.15b}$$

Since the internal variables $\{X^{i\alpha}, Y^{i\alpha}\}$ are generally arbitrary (depending on the choice of Hamiltonian and the supplied boundary data), the above must hold for arbitrary choices of $\{X^{i\alpha}\}$ and $\{Y^{i\alpha}\}$; hence, we have the necessary and sufficient conditions

$$\sum_{j,l} b_j a'_{jk}(a^{-1})_{jl} = b'_k,$$

$$\sum_{\beta,\gamma} \tilde{b}_\beta \tilde{a}'_{\beta\alpha}(\tilde{a}^{-1})_{\beta\gamma} = \tilde{b}'_\alpha.$$

Plugging in the choice (2.15a) and (2.15b) to the left hand sides of the above conditions,

$$\sum_{j,l} b_j a'_{jk} (a^{-1})_{jl} = \sum_{j,l} b'_k a_{kj} (a^{-1})_{jl} = \sum_l b'_k \delta_{kl} = b'_k,$$

$$\sum_{\beta,\gamma} \tilde{b}_\beta \tilde{a}'_{\beta\alpha} (\tilde{a}^{-1})_{\beta\gamma} = \sum_{\beta,\gamma} \tilde{b}'_\alpha \tilde{a}_{\alpha\beta} (\tilde{a}^{-1})_{\beta\gamma} = \sum_\gamma \tilde{b}'_\alpha \delta_{\alpha\gamma} = \tilde{b}'_\alpha;$$

so this choice is sufficient for the method to be well-defined. □

Now, consider the stationarity conditions (2.11a) and (2.11b). Plugging in the choice of coefficients (2.15a) and (2.15b), we have

$$\sum_i b'_j a_{ji} \Big(V^{i\alpha} - \frac{\partial H}{\partial p^0} (\Phi^\theta_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}) \Big) = 0,$$

$$\sum_\beta \tilde{b}'_\alpha \tilde{a}_{\alpha\beta} \Big(W^{j\beta} - \frac{\partial H}{\partial p^1} (\Phi^\theta_{j\beta}, P^0_{j\beta}, P^1_{j\beta}) \Big) = 0.$$

Since (a_{ji}) and $(\tilde{a}_{\alpha\beta})$ are invertible, we have

$$V^{j\alpha} = \frac{\partial H}{\partial p^0} (\Phi^\theta_{j\alpha}, P^0_{j\alpha}, P^0_{j\alpha}) \text{ and } W^{i\beta} = \frac{\partial H}{\partial p^1} (\Phi^\theta_{i\beta}, P^0_{i\beta}, P^1_{i\beta}),$$

so that the discrete forward Hamilton's equations for the field boundary values are also consistent with their expansions. Similarly, plugging this choice of coefficients into the stationarity condition (2.14) gives

$$\sum_{k,\beta} b'_k \tilde{b}_\beta a_{kj} \tilde{a}_{\beta\delta} X^{k\beta} + \sum_{i,\gamma} b_i \tilde{b}'_\gamma a_{ij} \tilde{a}_{\gamma\delta} Y^{i\gamma} = -\sum_{i,\beta} b_i \tilde{b}_\beta a_{ij} \tilde{a}_{\beta\delta} \frac{\partial H}{\partial \phi} (\Phi^\theta_{i\beta}, P^0_{i\beta}, P^1_{i\beta}).$$

To invert this relation, we impose $b'_k = b_k, \tilde{b}'_\gamma = \tilde{b}_\gamma$. Note that the matrix with jk entry $b_k a_{kj}$ is invertible since (a_{jk}) is (its transpose is obtained by multiplying the i^{th} row of (a_{ij}) by $b_i \neq 0$, so the rows are still linearly independent) and similarly for the matrix with $\delta\gamma$ entry $\tilde{b}_\gamma \tilde{a}_{\gamma\delta}$. Hence, this stationarity condition can be inverted to give

$$X^{i\alpha} + Y^{i\alpha} = -\frac{\partial H}{\partial \phi}(\Phi^{\theta}_{i\beta}, P^0_{i\beta}, P^1_{i\beta}).$$

Finally, to write our method in the traditional form of a partitioned Runge–Kutta method, we express the internal stages $P^0_{i\alpha}$ and $P^1_{i\alpha}$ in terms of π_A instead of π_B, by plugging equations (2.10d) and (2.10h) into equations (2.10b) and (2.10f) respectively,

$$P^0_{i\alpha} = \pi^0_{0[\alpha]} + \Delta t \sum_j (b_j - a'_{ij}) X^{j\alpha} = \pi^0_{0[\alpha]} + \Delta t \sum_j \underbrace{\frac{b_j b_i - b_j a_{ji}}{b_i}}_{\equiv a^{(2)}_{ij}} X^{j\alpha},$$

$$P^1_{i\alpha} = \pi^1_{[i]0} + \Delta x \sum_\beta (\tilde{b}_\beta - \tilde{a}'_{\alpha\beta}) Y^{i\beta} = \pi^1_{[i]0} + \Delta x \sum_\beta \underbrace{\frac{\tilde{b}_\beta \tilde{b}_\alpha - \tilde{b}_\beta \tilde{a}_{\beta\alpha}}{\tilde{b}_\alpha}}_{\equiv \tilde{a}^{(2)}_{\alpha\beta}} Y^{i\beta}.$$

To summarize, our method is

$$\Phi_{i\alpha} = \varphi_{0[\alpha]} + \Delta t \sum_j a_{ij} V^{j\alpha}, \tag{2.16a}$$

$$P^0_{i\alpha} = \pi^0_{0[\alpha]} + \Delta t \sum_j a^{(2)}_{ij} X^{j\alpha}, \tag{2.16b}$$

$$\varphi_{1[\alpha]} = \varphi_{0[\alpha]} + \Delta t \sum_j b_j V^{j\alpha}, \tag{2.16c}$$

$$\pi^0_{1[\alpha]} = \pi^0_{0[\alpha]} + \Delta t \sum_j b_j X^{j\alpha}, \tag{2.16d}$$

$$\Phi_{i\alpha} = \tilde{\Phi}_{i\alpha} = \varphi_{[i]0} + \Delta x \sum_\beta \tilde{a}_{\alpha\beta} W^{i\beta} \tag{2.16e}$$

$$P^1_{i\alpha} = \pi^1_{[i]0} + \Delta x \sum_\beta \tilde{a}^{(2)}_{\alpha\beta} Y^{i\beta}, \tag{2.16f}$$

$$\varphi_{[i]1} = \varphi_{[i]0} + \Delta x \sum_\beta \tilde{b}_\beta W^{i\beta}, \tag{2.16g}$$

$$\pi^1_{[i]1} = \pi^1_{[i]0} + \Delta x \sum_\beta \tilde{b}_\beta Y^{i\beta}. \tag{2.16h}$$

$$V^{i\alpha} = \frac{\partial H}{\partial p^0}(\Phi_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}), \tag{2.16i}$$

$$W^{i\alpha} = \frac{\partial H}{\partial p^1}(\Phi_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}), \tag{2.16j}$$

$$X^{i\alpha} + Y^{i\alpha} = -\frac{\partial H}{\partial \phi}(\Phi_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}), \tag{2.16k}$$

where $a^{(2)}_{ij} = \frac{b_j b_i - b_j a_{ji}}{b_i}$ and $\tilde{a}^{(2)}_{\alpha\beta} = \frac{\tilde{b}_\beta \tilde{b}_\alpha - \tilde{b}_\beta \tilde{a}_{\beta\alpha}}{\tilde{b}_\alpha}$. This is the usual form of a multisymplectic partitioned Runge–Kutta method. Note that our choice of $a^{(2)}_{ij}$ and $\tilde{a}^{(2)}_{\alpha\beta}$ (or equivalently our choice of $a'_{ij}, \tilde{a}'_{\alpha\beta}$) is the usual choice for the coefficients in the momenta expansion for a partitioned Runge–Kutta method to be multisymplectic (see, for example, Hong et al. [55], Reich [98], Ryland et al. [104]). Interestingly, however, from our perspective, our method based on the discrete boundary Hamiltonian is guaranteed to be multisymplectic so we had to impose no such conditions on the coefficients to ensure multisymplecticity; rather, the conditions for the coefficients arose from the necessity of the method to be well-defined, i.e., that the expansions of the field and momenta boundary values agreed with the discrete forward Hamilton's equations.

Remark 2.2.7. *In the above construction, we saw that the Runge–Kutta matrices (a_{ij}) and $(\tilde{a}_{\alpha\beta})$ were required to be invertible. We can see this directly from the internal stage expansions*

$$\Phi_{i\alpha} = \varphi_{0[\alpha]} + \Delta t \sum_j a_{ij} V^{j\alpha},$$

$$\tilde{\Phi}_{i\alpha} = \varphi_{[i]0} + \Delta x \sum_\beta \tilde{a}_{\alpha\beta} W^{i\beta},$$

since only when (a_{ij}) and $(\tilde{a}_{\alpha\beta})$ are invertible is extremizing K over $V^{i\alpha}$ and $W^{i\alpha}$ equivalent to extremizing K over $\Phi_{i\alpha}$ and $\tilde{\Phi}_{i\alpha}$, respectively. In the case of non-invertible Runge–Kutta matrices, the internal stages $\Phi_{i\alpha}$ and $\tilde{\Phi}_{i\alpha}$ do not depend independently on all of the $V^{i\alpha}$, $W^{i\alpha}$. For collocation Runge–Kutta methods, non-invertibility arises from the choice of the first quadrature point $c_1 = 0$. In our construction, if we choose $c_1 = 0$, then we are specifying an internal stage at a quadrature point where the field boundary value φ_A is already specified; thus, the internal stage at this point is not free to extremize over. Hence, in the non-invertible case, one has to use the specified boundary values to eliminate the degeneracy in the internal variables $V^{i\alpha}$ and $W^{i\alpha}$, reducing the number of internal variables to an independent subcollection of internal variables. Subsequently, one extremizes only over this independent subcollection of internal variables.

Remark 2.2.8. *It should also be remarked that while certain types of Galerkin multisymplectic Hamiltonian variational integrators recover multisymplectic partitioned Runge–Kutta methods, it remains to see whether there is a more general correspondence between Galerkin multisymplectic Hamiltonian variational integrators with a class of modified multisymplectic partitioned Runge–Kutta methods for the case of spacetime tensor product (hyper)rectangular meshes. This would generalize the connection between Galerkin variational integrators and modified symplectic Runge–Kutta methods in the ODE setting that was observed in [94].*

Momenta Internal Stages. In the above construction, we saw that we had to enforce consistency conditions on the momenta expansion coefficients in order for the method (2.16a)-(2.16k) to be well-defined. The issue is that we over-constrained the form of the momenta internal stages via our particular choice of expansion, since ultimately our goal was to derive the class of multisymplectic partitioned Runge–Kutta methods within our variational framework. One can avoid this problem altogether by working directly with the momenta internal stages $P^0_{i\alpha}$ and $P^1_{i\alpha}$ instead of the internal variables $X^{i\alpha}$ and $Y^{i\alpha}$, although the method will not ultimately be in the form of a multisymplectic partitioned Runge–Kutta method. This is possible for the momenta internal stages since the action does not depend on the derivatives of the momenta, unlike the field variable. We outline this procedure.

Assume the same expansions of $\Phi_{i\alpha}, \tilde{\Phi}_{i\alpha}, \varphi_{1[\alpha]}, \varphi_{[i]1}$ in terms of $\{V^{i\alpha}\}$ and $\{W^{i\alpha}\}$. For the momenta, we work directly with the internal stages $P^0_{i\alpha}$, $P^1_{i\alpha}$ instead of using an expansion. In this case, K is

$$\begin{aligned} K(\{\varphi_A, \pi_B, V^{i\alpha}, W^{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}, \lambda_{i\alpha}\}) = \Delta x \sum_\alpha \tilde{b}_\alpha \pi^0_{1[\alpha]}(\varphi_{0[\alpha]} + \Delta t \sum_j b_j V^{j\alpha}) \\ + \Delta t \sum_i b_i \pi^1_{[i]1}(\varphi_{[i]0} + \Delta x \sum_\beta \tilde{b}_\beta W^{i\beta}) \\ - \Delta t \Delta x \sum_{i,\alpha} b_i \tilde{b}_\alpha P^0_{i\alpha} V^{i\alpha} - \Delta t \Delta x \sum_{i,\alpha} b_i \tilde{b}_\alpha P^1_{i\alpha} W^{i\alpha} \\ + \Delta t \Delta x \sum_{i,\alpha} b_i \tilde{b}_\alpha H(\Phi^\theta_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}) + \sum_{i,\alpha} \lambda_{i\alpha}(\Phi_{i\alpha} - \tilde{\Phi}_{i\alpha}). \end{aligned}$$

H^+_d is obtained by extremizing K over the internal variables, $\{V^{i\alpha}, W^{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}, \lambda_{i\alpha}\}$.

The stationarity condition $\partial K/\partial P^0_{i\alpha} = 0$ (divided by $\Delta t \Delta x b_i \tilde{b}_\alpha$) gives

$$V^{i\alpha} = \frac{\partial H}{\partial p^0}(\Phi^\theta_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}).$$

Similarly, the stationarity condition $\partial K/\partial P^1_{i\alpha} = 0$ (divided by $\Delta t \Delta x b_i \tilde{b}_\alpha$) gives

$$W^{i\alpha} = \frac{\partial H}{\partial p^1}(\Phi^\theta_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}).$$

The stationarity condition $\partial K/\partial \lambda_{i\alpha} = 0$ gives $\Phi_{i\alpha} = \tilde{\Phi}_{i\alpha}$. The stationarity conditions $\partial K/\partial V^{j\beta} = 0$ and $\partial K/\partial W^{j\beta} = 0$ give respectively

$$\Delta t \Delta x b_j \tilde{b}_\beta (\pi^0_{1[\beta]} - P^0_{j\beta}) + \Delta t^2 \Delta x \sum_i b_i \tilde{b}_\beta a_{ij} \theta \frac{\partial H}{\partial \phi}(\Phi^\theta_{i\beta}, P^0_{i\beta}, P^1_{i\beta}) + \Delta t \sum_i \lambda_{i\beta} a_{ij} = 0,$$
$$\Delta t \Delta x b_j \tilde{b}_\beta (\pi^1_{[j]1} - P^1_{j\beta}) + \Delta x^2 \Delta t \sum_\alpha b_j \tilde{b}_\alpha \tilde{a}_{\alpha\beta} (1-\theta) \frac{\partial H}{\partial \phi}(\tilde{\Phi}_{j\alpha}, P^0_{j\alpha}, P^1_{j\alpha}) - \Delta x \sum_\alpha \lambda_{j\alpha} \tilde{a}_{\alpha\beta} = 0.$$

Performing the same procedure we used to combine equations (2.12) and (2.13) to eliminate θ and the Lagrange multipliers, these two stationarity conditions can be combined to give

$$\sum_\beta b_j \tilde{b}_\beta \tilde{a}_{\beta\delta} \frac{(\pi^0_{1[\beta]} - P^0_{j\beta})}{\Delta x} + \sum_i b_i \tilde{b}_\delta a_{ij} \frac{(\pi^1_{[i]1} - P^1_{i\delta})}{\Delta t} = -\sum_{i,\beta} b_i \tilde{b}_\beta a_{ij} \tilde{a}_{\beta\delta} \frac{\partial H}{\partial \phi}(\Phi^\theta_{i\beta}, P^0_{i\beta}, P^1_{i\beta}).$$

This combined condition, together with the other stationarity conditions

$$V^{i\alpha} = \partial H/\partial p^0(\Phi^\theta_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}),\ W^{i\alpha} = \partial H/\partial p^1(\Phi^\theta_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}),\ \Phi_{i\alpha} = \tilde{\Phi}_{i\alpha},$$

(ranging over all free indices) can be used to solve for the collection of internal variables $\{V^{i\alpha}, W^{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}\}_{i,\alpha}$ in terms of the supplied boundary data.

To conclude, we compute the discrete forward Hamilton's equations. For the field boundary values,

$$\varphi_{1[\alpha]} = \frac{1}{\tilde{b}_\alpha \Delta x} \frac{\partial K}{\partial \pi^0_{1[\alpha]}} = \varphi_{0[\alpha]} + \Delta t \sum_j b_j V^{j\alpha},$$
$$\varphi_{[i]1} = \frac{1}{b_i \Delta t} \frac{\partial K}{\partial \pi^1_{[i]1}} = \varphi_{[i]0} + \Delta x \sum_\beta b_\beta W^{i\beta}.$$

Note that these equations already agree with the field expansion. For the momenta boundary values,

$$\pi^0_{0[\alpha]} = \frac{1}{\tilde{b}_\alpha \Delta x}\frac{\partial K}{\partial \varphi_{0[\alpha]}} = \pi^0_{1[\alpha]} + \Delta t \sum_i b_i \theta \frac{\partial H}{\partial \phi}(\Phi^\theta_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}) + \frac{1}{\tilde{b}_\alpha \Delta x}\sum_i \lambda_{i\alpha},$$
$$\pi^1_{[i]0} = \frac{1}{b_i \Delta t}\frac{\partial K}{\partial \varphi_{[i]0}} = \pi^1_{[i]1} + \Delta x \sum_\alpha \tilde{b}_\alpha (1-\theta)\frac{\partial H}{\partial \phi}(\Phi^\theta_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}) - \frac{1}{b_i \Delta t}\sum_\alpha \lambda_{i\alpha}.$$

As we did before for the partitioned Runge–Kutta method, we can act on the stationarity conditions $\partial K/\partial V^{j\beta} = 0 = \partial K/\partial W^{j\beta}$ by the inverses of the Runge–Kutta matrices to solve for the Lagrange multipliers and substitute them into the discrete forward Hamilton's equations for the momenta, ultimately eliminating θ and the Lagrange multipliers. The discrete forward Hamilton's equations for the momenta are then

$$\pi^0_{0[\alpha]} = \pi^0_{1[\alpha]} - \Delta t \sum_{j,l} b_j (a^{-1})_{jl} \frac{\pi^0_{1[\alpha]} - P^0_{j\alpha}}{\Delta x},$$
$$\pi^1_{[i]0} = \pi^1_{[i]1} - \Delta x \sum_{\alpha,\beta} \tilde{b}_\alpha (\tilde{a}^{-1})_{\alpha\beta} \frac{\pi^1_{[i]1} - P^1_{i\alpha}}{\Delta t}.$$

Hence, by working with the internal stages for the momenta directly, as opposed to utilizing an expansion, we see that the method we derived is already well-defined (and also automatically multisymplectic), although it is not directly in the form of a multisymplectic partitioned Runge–Kutta method.

These various approaches demonstrate the versatility of our variational framework; once one chooses an approximation for the fields, its derivatives, and the momenta (as well as some approximation for the various integrals involved), one can construct the discrete boundary Hamiltonian and subsequently the variational framework produces a multisymplectic integrator. If one over-constrains the form of the momenta expansion, as opposed to using the internal stages directly, one must also check whether the method is well-defined. Another approach that is possible within this framework is to discretize at the level of the field using some (possibly non-tensor product) function space and subsequently take derivatives of the basis functions to obtain an approximation of the derivatives of the fields. For example, we expect that utilizing spectral element bases to discretize at the level of the field within our framework will produce multisymplectic spectral discretizations like those obtained in Bridges and Reich [21], Islas and Schober [60, 61]. Another interesting application of our construction would be to construct multisymplectic discretizations of the total exterior algebra bundle (see Bridges and Reich [22]) using Galerkin discretizations arising from the Finite Element Exterior Calculus framework (Arnold et al. [7, 8], Hiptmair [54]), allowing one to discretize Hamiltonian PDEs with more general configuration bundles.

2.2.4 Multisymplecticity Revisited

Now, we discuss in what sense the discrete multisymplectic form formula (2.4) corresponds to our discretization of the field equations. Consider the integral form of the De Donder–Weyl equations over $\square = [0, \Delta t] \times [0, \Delta x]$,

$$\int_{\square} \Big(\partial_\mu p^\mu + \frac{\partial H}{\partial \phi}(\phi, p^0, p^1) \Big) d^2x = 0, \tag{2.17a}$$

$$\int_{\square} \Big(\partial_0 \phi - \frac{\partial H}{\partial p^0}(\phi, p^0, p^1) \Big) d^2x = 0., \tag{2.17b}$$

$$\int_{\square} \Big(\partial_1 \phi - \frac{\partial H}{\partial p^1}(\phi, p^0, p^1) \Big) d^2x = 0. \tag{2.17c}$$

Applying our quadrature approximation to equation (2.17a),

$$\begin{aligned}
0 &= \int_0^{\Delta t} \int_0^{\Delta x} \Big(\partial_0 p^0 + \partial_1 p^1 + \frac{\partial H}{\partial \phi}(\phi, p^0, p^1) \Big) dx dt \\
&= \int_0^{\Delta x} (p^0|_{t=\Delta t} - p^0|_{t=0}) dx + \int_0^{\Delta t} (p^1|_{x=\Delta x} - p^0|_{x=0}) dt + \int_0^{\Delta t} \int_0^{\Delta x} \frac{\partial H}{\partial \phi}(\phi, p^0, p^1) dx dt \\
&\approx \Delta x \sum_\alpha \tilde{b}_\alpha (p^0|_{(\Delta t, \tilde{c}_\alpha \Delta x)} - p^0|_{(0, \tilde{c}_\alpha \Delta x)}) + \Delta t \sum_i b_i (p^1|_{(c_i \Delta t, \Delta x)} - p^1|_{(c_i \Delta t, 0)}) \\
&\quad + \Delta t \Delta x \sum_{i,\alpha} \frac{\partial H}{\partial \phi}(\phi, p^0, p^1)|_{(c_i \Delta t, \tilde{c}_\alpha \Delta x)}.
\end{aligned}$$

Consider the multisymplectic partitioned Runge–Kutta method (2.16a)-(2.16k); if we multiply equation (2.16d) by $\tilde{b}_\alpha$ and sum over α, multiply equation (2.16h) by b_i and sum over i, and add the resulting equations together, we have

$$0 = \Delta x \sum_\alpha \tilde{b}_\alpha (\pi^0_{1[\alpha]} - \pi^1_{0[\alpha]}) + \Delta t \sum_i b_i (\pi^1_{[i]1} - \pi^1_{[i]0}) + \Delta t \Delta x \sum_{i,\alpha} b_i \tilde{b}_\alpha \frac{\partial H}{\partial \phi} (\Phi_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}), \quad (2.18)$$

where we used $X^{i\alpha} + Y^{i\alpha} = \partial H / \partial \phi (\Phi_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha})$. Comparing these two, we see that the discrete method satisfies an approximation of the integral form of the De Donder–Weyl equation (2.17a) and that the error in the approximation of the field equations is directly related to the quadrature error and the field and momenta expansions. Similar statements can be made about the other De Donder–Weyl equations, (2.17b) and (2.17c).

Now, let's write our approximation (2.18) of the integral De Donder–Weyl equations as a difference equation. For a quantity f defined on the nodes of the edges $\{0\} \times [0, \Delta x]$ and $\{\Delta t\} \times [0, \Delta x]$ (and similarly a quantity g defined on the nodes of the edges $[0, \Delta t] \times \{0\}$ and $[0, \Delta t] \times \{\Delta x\}$), define

$$\delta^0_{[\alpha]} f = f_{1[\alpha]} - f_{0[\alpha]},$$
$$\delta^1_{[i]} g = g_{[i]1} - g_{[i]0}.$$

Define the discrete difference operators

$$\partial^\square_0 = \frac{1}{\Delta t} \sum_\alpha \tilde{b}_\alpha \delta^0_{[\alpha]},$$
$$\partial^\square_1 = \frac{1}{\Delta x} \sum_i b_i \delta^1_{[i]}.$$

Dividing equation (2.18) by $\Delta t \Delta x$, we see that it satisfies

$$\partial^\square_0 \pi^0 + \partial^\square_1 \pi^1 = - \sum_{i\alpha} b_i \tilde{b}_\alpha \frac{\partial H}{\partial \phi} (\Phi_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}) \equiv - \left\langle \frac{\partial H}{\partial \phi} \right\rangle_\square,$$

where $\langle \frac{\partial H}{\partial \phi} \rangle_\square$ denotes our quadrature approximation of the average value of $\partial H/\partial \phi$ on $\square$. Similarly, the other discrete equations satisfy

$$\partial_0^\square \varphi = \left\langle \frac{\partial H}{\partial p^0} \right\rangle_\square,$$
$$\partial_1^\square \varphi = \left\langle \frac{\partial H}{\partial p^1} \right\rangle_\square.$$

These difference equations correspond to our discretization of (the integral form) of the DDW equations $\partial_0 p^0 + \partial_1 p^1 = -\partial H/\partial \phi$, $\partial_\mu \phi = \partial H/p^\mu$. As mentioned in Section 2.1.3, a method is called multisymplectic if the difference operators used in the discretization of the field equations are the same difference operators which appear in the discrete multisymplectic form formula that the method admits. In our case, if we divide the discrete multisymplectic form formula (2.4) by $\Delta t \Delta x$, we see that it satisfies

$$\partial_0^\square \omega^0 + \partial_1^\square \omega^1 = 0$$

(when evaluated on discrete first variations), where $\omega^0 = d\varphi \wedge d\pi^0, \omega^1 = d\varphi \wedge d\pi^1$. Hence, our method is multisymplectic in the sense that the difference operators which appear in the difference equation that the discrete solution satisfies over $\square \in \mathscr{T}(X)$ are the same difference operators which appear in the discrete multisymplectic form formula.

2.3 Numerical Example

For our numerical example, we will study the $(1+1)-$dimensional sine–Gordon equation,

$$\partial_0^2 \phi(t,x) - \partial_1^2 \phi(t,x) = -\sin \phi(t,x). \tag{3.1}$$

The Hamiltonian for this equation is given by

$$H(\phi, p^0, p^1) = \frac{1}{2}(p^0)^2 - \frac{1}{2}(p^1)^2 - \cos \phi. \tag{3.2}$$

The De Donder–Weyl equations corresponding to this Hamiltonian are

$$\partial_0 \phi = \partial H / \partial p^0 = p^0, \tag{3.3a}$$

$$\partial_1 \phi = \partial H / \partial p^1 = -p^1, \tag{3.3b}$$

$$\partial_0 p^0 + \partial_1 p^1 = -\partial H / \partial \phi = -\sin \phi. \tag{3.3c}$$

Note that substituting (3.3a) and (3.3b) into (3.3c) recovers (3.1).

With this example, we aim to qualitatively show the preservation of multisymplecticity by considering the family of soliton solutions,

$$\phi_v(t,x) = 4 \arctan\left(\exp\left(\frac{x - vt}{\sqrt{1-v^2}} \right) \right), \tag{3.4}$$

where the family of solutions is indexed by a parameter $v \in (0,1)$. Consider the following curve on the space of sections of the restricted dual jet bundle

$$v \mapsto (\phi_v, p_v^0, p_v^1) \equiv (\phi_v, \partial_0 \phi_v, -\partial_1 \phi_v)$$

and note that it is differentiable for $v \in (0,1)$. Thus, the associated vector field, given by differentiating the above map with respect to v, defines a vector field on the space of sections of the restricted dual jet bundle. The associated vector field is a first variation on the space of soliton solutions, since its flow maps soliton solutions to other soliton solutions.

To visualize multisymplecticity for this example, we observe the following. Each soliton solution (3.4) propagates to the right at speed v in time, without changing form. Thus, the shape of a soliton solution in the (ϕ, p^0) plane does not change with respect to time. Hence, for a family of soliton solutions, the associated area in the (ϕ, p^0) plane will not expand or contract as the system evolves in time. In other words, restricting to the above first variations, this means that

$$\partial_0 \omega^0 = 0.$$

By the multisymplectic form formula $\partial_0 \omega^0 + \partial_1 \omega^1 = 0$, we also have that

$$\partial_1 \omega^1 = 0,$$

and hence the family of soliton solutions, occupying an area in the (ϕ, p^1) plane, will not expand or contract as the system evolves in space. This example then provides an intuitive way to visualize multisymplecticity as symplecticity in each spacetime direction, since the multisymplectic conservation law splits into two symplectic conservation laws, for this given family of solutions. This is a multisymplectic analogue of the visualization of symplecticity in the literature for symplectic integrators, where one evolves a family of initial conditions occupying an area in phase space; for symplectic integrators, this area is preserved under the flow of the integrator, unlike a generic method (see, for example, Hairer et al. [51]).

Explicit Methods for Separable Hamiltonians. Recall that in the above derivation of the multisymplectic partitioned Runge–Kutta method, we used that the Runge–Kutta matrices $a, \tilde{a}$ were invertible and hence the variational construction in Section 2.2.3 does not directly apply to explicit Runge–Kutta matrices a and $\tilde{a}$ (since explicit Runge–Kutta methods have strictly lower triangular Runge–Kutta matrices and hence are non-invertible). Since equation (3.1) is nonlinear, using an implicit method would be computationally expensive and hence an explicit method would be preferable. However, for separable Hamiltonians of the form $H(\phi, p^\mu) = K(p^\mu) + V(\phi)$ (as is the case for the sine–Gordon Hamiltonian (3.2)), we can derive an explicit method as follows. Let a be an explicit Runge–Kutta matrix such that its symplectic pair $a^{(2)}$ is invertible, where again the symplectic pair is given by

$$a^{(2)}_{ij} = \frac{b_j b_i - b_j a_{ji}}{b_i}.$$

Then, it follows that the symplectic pair of the symplectic pair of a equals a, i.e., $(a^{(2)})^{(2)} = a$, since

$$(a^{(2)})^{(2)}_{ij} = \frac{b_j b_i - b_j a^{(2)}_{ji}}{b_i} = \frac{b_j b_i - b_j \frac{b_i b_j - b_i a_{ij}}{b_j}}{b_i} = a_{ij}.$$

Thus, we can choose a to instead be $a^{(2)}$, so that the symplectic pair of a becomes an explicit Runge–Kutta matrix. The variational construction now applies with this choice of a, since it is invertible. For a separable Hamiltonian, the integration scheme splits and the system can be evolved explicitly in time.

Numerical Scheme. We take a one-stage Runge–Kutta matrix in the temporal direction $a = 1$ (with $b = 1$, $c = 1$) so that $a^{(2)} = 0$, and similarly in the spatial direction $\tilde{a} = 1$ (with $\tilde{b} = 1$, $\tilde{c} = 1$) so that $\tilde{a}^{(2)} = 0$. Let $\Phi_{a,b}, P^0_{a,b}, P^1_{a,b}, V_{a,b}, W_{a,b}, X_{a,b}, Y_{a,b}$ denote the internal stages associated to $\square_{ab} = \{t_a, t_a + \Delta t\} \times \{x_b, x_b + \Delta x\}$. Letting $\varphi_{a,b}$ denote the value of φ at $\{t_a, x_b\}$ (and similarly for the momenta), the multisymplectic partitioned Runge–Kutta method (2.16a)-(2.16k) gives, with the choice of the sine–Gordon Hamiltonian (3.2),

$$P^0_{a,b} = \pi^0_{a,b+1}, \tag{3.5a}$$

$$\varphi_{a+1,b+1} = \varphi_{a,b+1} + \Delta t V_{a,b} = \Phi_{a,b}, \tag{3.5b}$$

$$\pi^0_{a+1,b+1} = \pi^0_{a,b+1} + \Delta t X_{a,b}, \tag{3.5c}$$

$$P^1_{a,b} = \pi^1_{a+1,b}, \tag{3.5d}$$

$$\varphi_{a+1,b+1} = \varphi_{a+1,b} + \Delta x W_{a,b}, \tag{3.5e}$$

$$\pi^1_{a+1,b+1} = \pi^1_{a+1,b} + \Delta x Y_{a,b}, \tag{3.5f}$$

$$V_{a,b} = \frac{\partial H}{\partial p^0}(\Phi_{a,b}, P^0_{a,b}, P^1_{a,b}) = P^0_{a,b}, \tag{3.5g}$$

$$W_{a,b} = \frac{\partial H}{\partial p^1}(\Phi_{a,b}, P^0_{a,b}, P^1_{a,b}) = -P^1_{a,b}, \tag{3.5h}$$

$$X_{a,b} + Y_{a,b} = \frac{\partial H}{\partial \phi}(\Phi_{a,b}, P^0_{a,b}, P^1_{a,b}) = -\sin(\Phi_{a,b}). \tag{3.5i}$$

Eliminating the internal stage variables, equations (3.5g) and (3.5i) can be expressed as an integration scheme in time

$$\frac{\varphi_{a+1,b}-\varphi_{a,b}}{\Delta t} = \pi^0_{a,b},$$
$$\frac{\pi^0_{a+1,b}-\pi^0_{a,b}}{\Delta t} + \frac{\pi^1_{a+1,b}-\pi^1_{a+1,b-1}}{\Delta x} = -\sin(\varphi_{a+1,b})$$

(where we shifted $b \mapsto b-1$). Further eliminating the π^1 variables using (3.5d), (3.5e), (3.5h), the second equation above can be expressed as

$$\frac{\pi^0_{a+1,b}-\pi^0_{a,b}}{\Delta t} - \frac{\varphi_{a+1,b+1}-2\varphi_{a+1,b}+\varphi_{a+1,b-1}}{\Delta x^2} = -\sin(\varphi_{a+1,b}).$$

Thus, the corresponding numerical scheme is

$$\varphi_{a+1,b} = \varphi_{a,b} + \Delta t\, \pi^0_{a,b}, \tag{3.6a}$$
$$\pi^0_{a+1,b} = \pi^0_{a,b} + \Delta t \frac{\varphi_{a+1,b+1}-2\varphi_{a+1,b}+\varphi_{a+1,b-1}}{\Delta x^2} - \Delta t \sin(\varphi_{a+1,b}). \tag{3.6b}$$

The scheme corresponds to discretizing the first-order formulation of the sine–Gordon equation,

$$\partial_0 p^0 = \partial_1^2 \phi - \sin\phi,$$
$$\partial_0 \phi = p^0,$$

in space using the standard discrete Laplacian and in time using the (adjoint) symplectic Euler method. We refer to the method (3.6a)-(3.6b) as MSE (multisymplectic Euler).

As discussed in Section 2.2.1, this scheme can be computed in a time marching fashion, given supplied initial conditions for φ and π^0, as well as spatial boundary conditions. This scheme is explicit, since the values of the field can first be updated using (3.6a), followed by updating the temporal momenta using (3.6b). For the numerical experiment, we will compare this scheme to the scheme which uses the standard discrete Laplacian in space and the forward Euler method in time,

$$\varphi_{a+1,b} = \varphi_{a,b} + \Delta t\, \pi^0_{a,b}, \tag{3.7a}$$

$$\pi^0_{a+1,b} = \pi^0_{a,b} + \Delta t \frac{\varphi_{a,b+1} - 2\varphi_{a,b} + \varphi_{a,b-1}}{\Delta x^2} - \Delta t \sin(\varphi_{a,b}). \tag{3.7b}$$

We refer to the method (3.7a)-(3.7b) as FE (forward Euler).

For our numerical experiment, we consider a family of initial conditions given by interpolating the soliton solutions $(\varphi_v(x), \pi^0_v(x)) = (\phi_v(0,x), \partial_0 v(0,x))$ onto the spatial grid, for several values of v ($v = 0.50, 0.47, 0.45$), on a spatial domain $[-L, L]$. We choose Neumann boundary conditions $\pi^1(-L) = 0 = \pi^1(L)$ and choose L sufficiently large so that the Neumann conditions are satisfied initially, up to a desired level of error (since $\pi^1(x) = -\partial_1 \phi_v(0,x)$ decays monotonically to 0 as $|x|$ increases), say $L = 20$ (so that $\pi^1(L) = \pi^1(-L) \sim 10^{-10}$). To demonstrate the robustness of MSE, we take a large spatial step $\Delta x = 0.1$ and a time step $\Delta t = \Delta x/2$; the experiment is run until a final time $T = 20$.

The initial (p^0, ϕ) phase space distribution is shown in Figure 2.5. The (p^0, ϕ) phase space distribution at $t = 20$ is shown in Figures 2.6 and 2.7 for MSE and FE, respectively. Comparison of Figures 2.5 and 2.6 shows the preservation of symplecticity in the temporal direction for the method MSE, whereas it is clearly not preserved for FE.

Similarly, Figures 2.8 and 2.9 shown the preservation of symplecticity in the x direction for MSE.

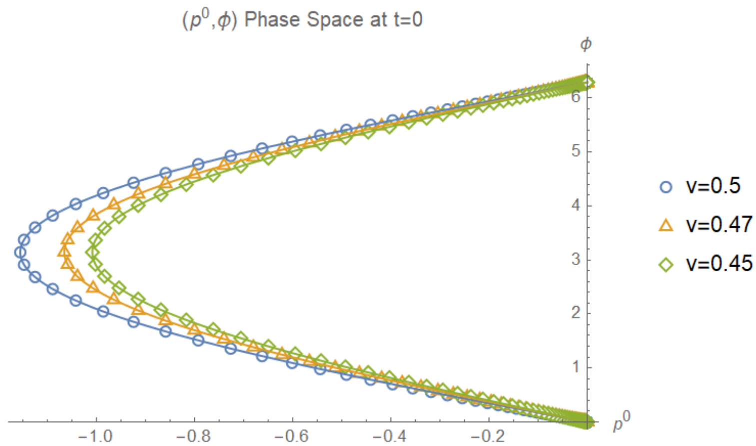

Figure 2.5. The (p^0, ϕ) phase space distribution of the initial conditions (running over all spatial nodes in $[-L, L]$). The solid curves indicate the exact distribution.

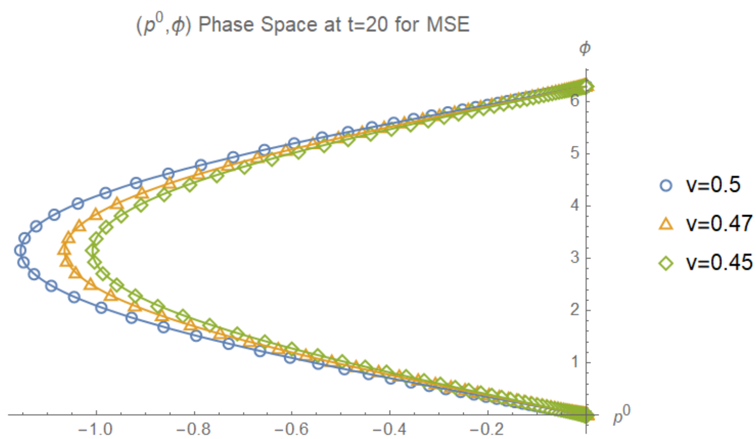

Figure 2.6. The (p^0, ϕ) phase space distribution at $t = 20$ using MSE (running over all spatial nodes in $[-L, L]$). The solid curves indicate the exact distribution.

2.4 Conclusion and Future Directions

In this paper, we extended the construction of Hamiltonian variational integrators to the setting of multisymplectic Hamiltonian PDEs. Our construction is based on a discrete approximation of the boundary Hamiltonian, introduced in Vankerschaver et al. [116]. Through the Type II variational principle, this discrete boundary Hamiltonian is a generating function for the discrete Hamilton's equations that define our multisymplectic integrator. The discrete variational principle automatically yields integrators which are multisymplectic and satisfy

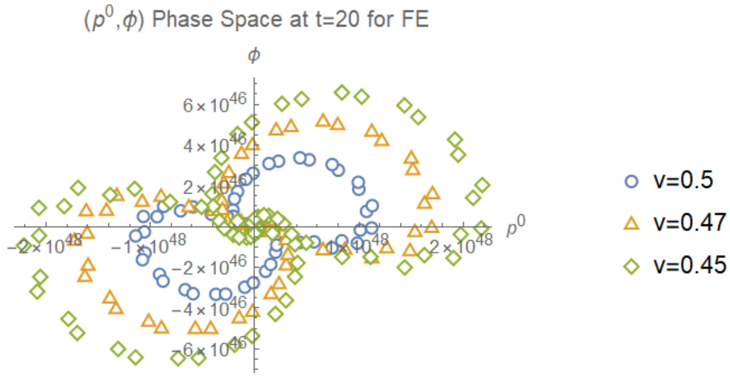

Figure 2.7. The (p^0, ϕ) phase space distribution at $t = 20$ using FE (running over all spatial nodes in $[-L, L]$).

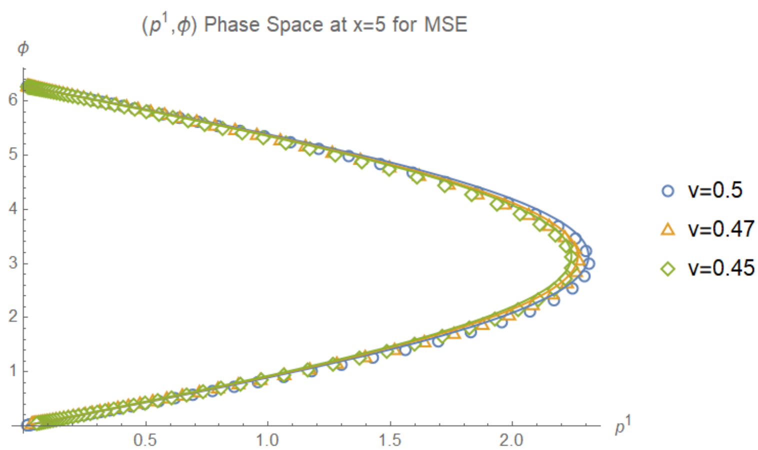

Figure 2.8. The (p^1, ϕ) phase space distribution at $x = 5$ using MSE (running over all timesteps in $[0, T]$). The solid curves indicate the exact distribution.

a discrete Noether's theorem for group-invariant discretizations. As an application of this variational framework, we derived the class of multisymplectic partitioned Runge–Kutta methods; however, our construction is more general and is not limited to this class of multisymplectic integrators. Finally, we showed that the discrete multisymplecticity which arose from the discrete variational principle agrees with the notion of discrete multisymplecticity introduced in Bridges and Reich [20].

Perhaps the most natural research direction is to establish a variational error analysis result which demonstrates that a computable discrete Hamiltonian that approximates the boundary

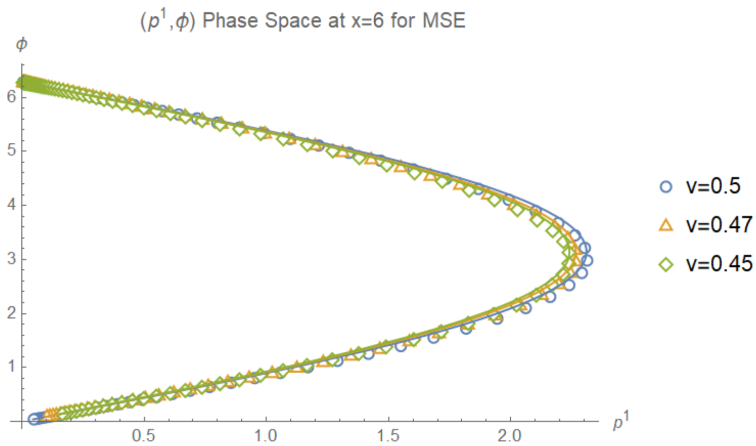

Figure 2.9. The (p^1, ϕ) phase space distribution at $x = 6$ using MSE (running over all timesteps in $[0, T]$). The solid curves indicate the exact distribution.

Hamiltonian to a given order of accuracy will result in a numerical method for the Hamiltonian partial differential equation with the same order of accuracy. It should be observed that this poses two main challenges as compared to the case for ordinary differential equations. The first is that the boundary of the spacetime domain is in general curved, and the space of boundary data (and boundary momentum) is infinite-dimensional. As such, one would first have to approximate the spacetime domain with a spacetime mesh, and choose a finite-dimensional subspace for sections of the dual jet bundle that is subordinate to this spacetime mesh. Then, the error between the computable discrete Hamiltonian and the boundary Hamiltonian can be decomposed into three terms, the first of which can be bounded by assuming that the boundary-value problem is well-posed and therefore has continuous dependence on the boundary data, the second is associated with the variational crime of replacing the spacetime domain with a spacetime mesh, and the third is a term that is analogous to what arises in the usual variational error analysis for ordinary differential equations.

The second natural direction would be to establish a quasi-optimality result which demonstrates that the variational error in the construction of a Galerkin boundary Hamiltonian is bounded from above by a multiple of the best approximation error of the finite-dimensional function space used to approximate sections of the configuration bundle.

Finally, it was established in McLachlan and Stern [90] that many hybridizable discontinuous Galerkin methods are multisymplectic when applied to semilinear elliptic PDEs in mixed form, and it would be interesting to see the kind of multisymplectic Hamiltonian variational integrators that would arise for Hamiltonian time-evolution PDEs when using spacetime discontinuous Galerkin finite element spaces to discretize the dual jet bundle.

2.5 Acknowledgements

Chapter 2, in full, is a reprint of the material as it appears in ”Multisymplectic Hamiltonian Variational Integrators” (2022). Tran, Brian; Leok, Melvin, *International Journal of Computer Mathematics (Special Issue on Geometric Numerical Integration, Twenty-Five Years Later)*, 99(1), 113-157. The dissertation author was the primary investigator and first author of this paper.

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2.6 Chapter Appendix

2.6.1 Higher Spacetime Dimensions

In this appendix, we treat the case of a spacetime tensor product (hyper)rectangular mesh in $(n+1)$-spacetime dimensions, where the coordinates on spacetime are given by $\{x^\mu\}_{\mu=0}^n$. Let $\mathscr{T}(X)$ be a regular (hyper)rectangular mesh, with Δx^μ the spacing in the x^μ direction. We index the nodes of this mesh by $x_a^\mu = a\Delta x^\mu$ (where a is an integer) and consider $\square_{a^0\ldots a^n} \in \mathscr{T}(X)$ given by $\square_{a^0\ldots a^n} = \prod_{\mu=0}^n [x^\mu_{a^\mu}, x^\mu_{a^\mu} + \Delta x^\mu]$, where $\prod$ denotes the (ordered) Cartesian product. Fix a spacetime direction x^μ. For this direction, there are two $(n-1)$-dimensional faces of $\square_{a^0\ldots a^n}$, located along the hyperplanes $x^\mu = x^\mu_{a^\mu}$ and $x^\mu = x^\mu_{a^\mu+1}$, to which the unit vector in the x^μ direction is normal. To each pair of such faces, we associate a quadrature rule (for simplicity, we consider the case of one quadrature point). The field values at this pair of quadrature points are denoted $\varphi_{[a^0]\ldots[a^{\mu-1}]a^\mu[a^{\mu+1}]\ldots[a^n]}$ and $\varphi_{[a^0]\ldots[a^{\mu-1}]a^\mu+1[a^{\mu+1}]\ldots[a^n]}$, where the unbracketed indices a^μ and $a^\mu+1$ indices denote the faces with smaller and larger x^μ, respectively. Similarly, the corresponding normal momenta to these faces are denoted $\pi^\mu_{[a^0]\ldots[a^{\mu-1}]a^\mu[a^{\mu+1}]\ldots[a^n]}$ and $\pi^\mu_{[a^0]\ldots[a^{\mu-1}]a^\mu+1[a^{\mu+1}]\ldots[a^n]}$. Note that, in the $(1+1)$-dimensional case, this notation agrees with the notation that we used in Section 2.2.1 (where $a^0 = a, a^1 = b$).

We take $B(\Box_{a^0\ldots a^n})$ to consist of the "forward" faces; that is, $B(\Box_{a^0\ldots a^n})$ is the union, over all μ, of the face in the x^μ direction with larger x^μ coordinate, $x^\mu = x^\mu_{a^\mu+1}$ (and similarly $A(\Box_{a^0\ldots a^n})$ is the union, over all μ of the face in the x^μ direction with smaller x^μ coordinate, $x^\mu = x^\mu_{a^\mu}$). For brevity in the following equations, let

$$\begin{aligned}
\pi^\mu_{]a^\mu[} &\equiv \pi^\mu_{[a^0]\ldots[a^{\mu-1}]a^\mu[a^{\mu+1}]\ldots[a^n]},\\
\varphi_{]a^\mu[} &\equiv \varphi_{[a^0]\ldots[a^{\mu-1}]a^\mu[a^{\mu+1}]\ldots[a^n]},\\
\pi^\mu_{]a^\mu+1[} &\equiv \pi^\mu_{[a^0]\ldots[a^{\mu-1}]a^\mu+1[a^{\mu+1}]\ldots[a^n]},\\
\varphi_{]a^\mu+1[} &\equiv \varphi_{[a^0]\ldots[a^{\mu-1}]a^\mu+1[a^{\mu+1}]\ldots[a^n]},
\end{aligned}$$

where we implicitly understand that $(a^0,\ldots,a^n)$ are fixed. Then the quadrature approximation of the integral over B is given by

$$\sum\!\!\!\!\!\!\int_{B(\Box_{a^0\ldots a^n})} \pi_B \varphi_B = \sum_{\mu=0}^{n} \left[\pi^\mu_{]a^\mu+1[}\varphi_{]a^\mu+1[}\Delta^n x_\mu \right],$$

where $\Delta^n x_\mu \equiv \prod_{\nu\neq\mu} \Delta x^\nu$. Letting φ_A denote the collection of values of φ on the quadrature points on $A(\Box_{a^0\ldots a^n})$ (and similarly for π_B), the associated discrete boundary Hamiltonian is

$$H_d^+(\varphi_A,\pi_B) = \text{ext}\left(\sum_{\mu=0}^{n}\left[\pi^{\mu}_{]a^\mu+1[}\varphi_{]a^\mu+1[}\Delta^n x_\mu\right] - S_d^{\Box_{a^0\ldots a^n}}[\phi,p]\right),$$

where $S_d^{\Box_{a^0\ldots a^n}}$ is some discrete approximation of the action and the extremization is over all (ϕ,p) in the discrete approximating space satisfying the prescribed (φ_A,π_B) boundary conditions. The Type II variational principle yields the discrete forward Hamilton's equations: for each μ,

$$\pi^{\mu}_{]a^\mu[} = \frac{1}{\Delta^n x_\mu} D_{\varphi,A,\mu} H_d^+(\varphi_A,\pi_B),$$
$$\varphi_{]a^\mu+1[} = \frac{1}{\Delta^n x_\mu} D_{\pi,B,\mu} H_d^+(\varphi_A,\pi_B),$$

where $D_{\phi,A,\mu}$ denotes differentiation with respect to the value of φ on the node on A in the μ direction, i.e., $\partial/\partial\varphi_{]a^\mu[}$ (and similarly $D_{\pi,B,\mu} = \partial/\partial\pi^{\mu}_{]a^\mu+1[}$).

Analogous results to the main body of the paper can be derived for the case of higher spacetime dimensions. For example, the multisymplectic conservation law $d^2H_d^+ = 0$ (when evaluated on first variations) gives

$$\sum_\mu \left(d\varphi_{]a^\mu+1[}\wedge d\pi^{\mu}_{]a^\mu+1[} - d\varphi_{]a^\mu[}\wedge d\pi^{\mu}_{]a^\mu[}\right)\Delta^n x_\mu = 0$$

(which formally is the quadrature approximation to $\int_{\Box_{a^0\ldots a^n}} \omega^\mu(\cdot,\cdot)d^n x_\mu = 0$).

Similarly, the generalization to multiple quadrature points is straight-forward; for each pair of forward and backward $(n-1)$-dimensional faces in the μ direction, we can choose multiple quadrature points and weights on the faces (the quadrature rules on the forward and backward faces in the same direction must be the same, but the quadrature rules can differ among the spacetime directions, as was the case in $(1+1)$-spacetime dimensions). Associated to these quadrature points are the field and normal momenta values. Then, the discrete forward Hamilton's equations just states that the value of φ on a quadrature node in B is given by differentiating H_d^+ with respect to the normal momenta π on that node, divided by the product of $\Delta^n x_\mu$ and the quadrature weight at that node (and similarly, the value of the normal momenta π on a quadrature node in A is given by differentiating H_d^+ with respect to the field value on that node, divided by the product of $\Delta^n x_\mu$ and the quadrature weight at that node). As one can verify, in the $(1+1)$-dimensional case, this precisely reproduces (2.3a)-(2.3d).

One can then proceed as we did in the main body of the paper, in using the Galerkin construction as a discrete approximation for the action. Utilizing analogous expansions to those in the main body of the paper (with an expansion in each spacetime direction), the resulting variational integrator would then give a multisymplectic partitioned Runge–Kutta method, where the integrator would formally be a symplectic partitioned Runge–Kutta method in each spacetime direction with the internal stages satisfying the De Donder–Weyl equations.

Finally, it is worth noting that, at the start of Section 2.2.1, we laid a general formulation for unstructured meshes, arbitrary finite element spaces, and arbitrary spacetime dimensions. However, in general, the form of the discrete Hamilton's equations arising from the Type II variational principle can not be written explicitly, which is why we specialized to the case of spacetime tensor product (hyper)rectangular meshes. It would be interesting to determine the form of the discrete forward Hamilton's equations in other settings for particular choices of meshes, finite element spaces, and spacetime dimensions. For example, although a fully unstructured spacetime mesh would be challenging, one could consider a spacetime tensor product mesh which is the tensor product of an unstructured spatial mesh and a regular temporal mesh. Even in the case of a (hyper)rectangular mesh, it would be interesting to consider finite element spaces of differential forms (such as the $Q_r^- \Lambda^k$ spaces arising in finite element exterior calculus [7]), which could be interesting in physical applications such as lattice field theory.

2.6.2 Relation to Galerkin Lagrangian Variational Integrators

In this appendix, we discuss the relation between Galerkin Hamiltonian and Lagrangian variational integrators. From the Lagrangian perspective, the appropriate generating functional is the boundary Lagrangian (see Vankerschaver et al. [116]),

$$L_{\partial U}(\varphi) = \int_U L(\phi, \partial_\mu \phi) d^{n+1}x,$$

where the expression on the right hand side is extremized over all ϕ such that $\phi|_{\partial U} = \varphi$. In general, methods derived from discretizing the boundary Hamiltonian and boundary Lagrangian are not expected to be equivalent, even in the hyperregular case, as was shown in Schmitt and Leok [107] for the case of mechanics (where the boundary Hamiltonian and boundary Lagrangian are referred to as the exact discrete Hamiltonian and the exact discrete Lagrangian, respectively).

However, for the case of Galerkin Lagrangian variational integrators on a 2-dimensional rectangular mesh, they are equivalent (in the hyperregular case), for a suitable choice of discrete boundary Lagrangian and using the same (Galerkin based) expansions that we utilized in our construction of Galerkin Hamiltonian variational integrators. We assume the same field expansions that we used in Section 2.2.3 (when discussing independent internal stages). Unlike the boundary Hamiltonian where φ is specified on A and π is specified on B, the Lagrangian perspective specifies φ on both A and B. One can define a discrete boundary Lagrangian as

$$\begin{aligned}
L_d^{\partial\Box}(\varphi_A, \varphi_B) &= \underset{\phi|_A=\varphi_A, \phi|_B=\varphi_B}{\operatorname{ext}^{\phi}} \Delta t \Delta x \sum_{i\alpha} L\big(\phi(c_i\Delta t, \tilde{c}_\alpha \Delta x), \partial_0\phi(c_i\Delta t, \tilde{c}_\alpha \Delta x), \partial_1\phi(c_i\Delta t, \tilde{c}_\alpha \Delta x)\big) \\
&= \operatorname{ext}_{V^{i\alpha}, W^{i\alpha}, \lambda_\alpha, \lambda_i, \lambda_{i\alpha}} \Delta t \Delta x \Bigg[\sum_{i,\alpha} b_i \tilde{b}_\alpha L(\Phi^\theta_{i\alpha}, V^{i\alpha}, W^{i\alpha}) \\
&\qquad + \sum_\alpha \lambda_\alpha \left(\varphi_{1[\alpha]} - \varphi_{0[\alpha]} - \Delta t \sum_j b_j V^{j\alpha} \right) \\
&\qquad + \sum_i \lambda_i \left(\varphi_{[i]1} - \varphi_{[i]0} - \Delta x \sum_\beta \tilde{b}_\beta W^{i\beta} \right) \\
&\qquad + \sum_{i,\alpha} \lambda_{i\alpha} (\Phi_{i\alpha} + \tilde{\Phi}_{i\alpha}) \Bigg],
\end{aligned}$$

where in the first line, the right hand side is extremized over the finite-dimensional function space chosen in the Galerkin construction (to obtain a discrete boundary Lagrangian instead of the exact discrete boundary Lagrangian which extremizes over an infinite-dimensional space). The second equality follows from substituting the chosen expansion and explicitly enforcing that the boundary condition $\phi|_B = \varphi_B$ are satisfied by the Lagrange multipliers λ_α and λ_i. The normal momenta are then obtained by enforcing the variational principle, which gives the normal momenta π_A, π_B in terms of the derivatives of $L_d^{\partial\Box}$ with respect to φ_A, φ_B. This defines a Galerkin Lagrangian variational integrator.

Proposition 2.6.1. *If the continuous Hamiltonian H is hyperregular and the associated Lagrangian L is constructed by the Legendre transform, then the Galerkin Hamiltonian variational integrator and the Galerkin Lagrangian variational integrator are equivalent, for the same choice of expansion (i.e., specified by the basis functions ψ_i, $\tilde{\psi}_\beta$ and quadrature rules).*

Proof. The proof follows from using the Legendre transform to express

$$\partial_\mu \phi = \frac{\partial H(\phi, p^0, p^1)}{\partial p^\mu},$$

which is invertible by assumption of hyperregularity (i.e., one can express the momenta in terms of the field and their derivatives). The computation then follows analogously to the 1-dimensional (mechanics) case, as shown in Leok and Zhang [76], noting that the Legendre transform holds at the internal stages. □

It is expected that this equivalence holds in the case of higher-dimensional spacetime tensor product (hyper)rectangular meshes, although it is still unclear to what degree this holds for general unstructured spacetime meshes and general finite element spaces. We aim to explore this in future work.

Chapter 3

Geometric Methods for Adjoint Systems

3.1 Introduction

3.1.1 Applications of the Adjoint Equations

The solution of many nonlinear problems involves successive linearization, and as such variational equations and their adjoints play a critical role in a variety of applications. Adjoint equations are of particular interest when the parameter space is significantly higher dimension than that of the output or objective. In particular, the simulation of adjoint equations arise in sensitivity analysis [25; 26], adaptive mesh refinement [80], uncertainty quantification [118], automatic differentiation [47], superconvergent functional recovery [96], optimal control [102], optimal design [41], optimal estimation [93], and deep learning viewed as an optimal control problem [12].

The study of geometric aspects of adjoint systems arose from the observation that the combination of any system of differential equations and its adjoint equations are described by a formal Lagrangian [57; 58]. This naturally leads to the question of when the formation of adjoints and discretization commutes [110], and prior work on this include the Ross–Fahroo lemma [103], and the observation by Sanz-Serna [106] that the adjoints and discretization commute if and only if the discretization is symplectic.

3.1.2 Symplectic and Presymplectic Geometry

Throughout the paper, we will assume that all manifolds and maps are smooth, unless otherwise stated. Let (P,Ω) be a (finite-dimensional) symplectic manifold, i.e., Ω is a closed nondegenerate two-form on P. Given a Hamiltonian $H : P \to \mathbb{R}$, the Hamiltonian system is defined by

$$i_{X_H}\Omega = dH,$$

where the vector field X_H is a section of the tangent bundle to P. By nondegeneracy, the vector field X_H exists and is uniquely determined. For an open interval $I \subset \mathbb{R}$, we say that a curve $z : I \to P$ is a solution of Hamilton's equations if z is an integral curve of X_H, i.e., $\dot{z}(t) = X_H(z(t))$ for all $t \in I$.

A particularly important example for our purposes is when the symplectic manifold is the cotangent bundle of a manifold, $P = T^*M$, equipped with the canonical symplectic form $\Omega = dq \wedge dp$ in natural coordinates (q, p) on T^*M. A Hamiltonian system has the coordinate expression

$$\begin{aligned}
\dot{q} &= \frac{\partial H(q,p)}{\partial p}, \\
\dot{p} &= -\frac{\partial H(q,p)}{\partial q}.
\end{aligned}$$

By Darboux's theorem, any symplectic manifold is locally symplectomorphic to a cotangent bundle equipped with its canonical symplectic form. As such, any Hamiltonian system can be locally expressed in the above form (even when P is not a cotangent bundle), using Darboux coordinates.

We now consider the generalization of Hamiltonian systems where we relax the condition that Ω is nondegenerate, i.e., presymplectic geometry. Let (P,Ω) be a presymplectic manifold, i.e., Ω is a closed two-form on P with constant rank. As before, given a Hamiltonian $H : P \to \mathbb{R}$, we define the associated Hamiltonian system as

$$i_{X_H}\Omega = dH.$$

Note that since Ω is now degenerate, X_H is not guaranteed to exist and if it does, it need not be unique and in general is only partially defined on a submanifold of P. Again, we say a curve on P is a solution to Hamilton's equations if it is an integral curve of X_H. Using Darboux coordinates (q, p, r) adapted to (P, Ω), where $\Omega = dq \wedge dp$ and $\ker(\Omega) = \text{span}\{\partial/\partial r\}$, the local expression for Hamilton's equations is given by

$$\begin{aligned}
\dot{q} &= \frac{\partial H(q,p,r)}{\partial p}, \\
\dot{p} &= -\frac{\partial H(q,p,r)}{\partial q}, \\
0 &= \frac{\partial H(q,p,r)}{\partial r}.
\end{aligned}$$

The third equation above is interpreted as a constraint equation which any solution curve must satisfy. We will assume that the constraint defines a submanifold of P. It is clear that in order for a solution vector field X_H to exist, it must be restricted to lie on this submanifold. However, in order for its flow to remain on the submanifold, it must be tangent to this submanifold, which further restricts where X can be defined. Alternating restriction in order to satisfy these two constraints yields the presymplectic constraint algorithm of Gotay et al. [43]. The presymplectic constraint algorithm begins with the observation that for any X satisfying the above system, so does $X + Z$, where $Z \in \ker(\Omega)$. In order to obtain such a vector field X, one considers the subset P_1 of P such that $Z_p(H) = 0$ for any $Z \in \ker(\Omega), p \in P_1$. We will assume that the set P_1 is a submanifold of P. We refer to P_1 as the primary constraint manifold. In order for the flow of the resulting Hamiltonian vector field X to remain on P_1, one further requires that X is tangent to P_1. The set of points satisfying this property defines a subsequent secondary constraint submanifold

P_2. Iterating this process, one obtains a sequence of submanifolds

$$\cdots \to P_k \to \cdots \to P_1 \to P_0 \equiv P,$$

defined by

$$P_{k+1} = \{p \in P_k : Z_p(H_k) = 0 \text{ for all } Z \in \ker(\Omega_k)\}, \tag{1.1}$$

where

$$\Omega_{k+1} = \Omega_k|_{P_{k+1}},$$
$$H_{k+1} = H_k|_{P_{k+1}}.$$

If there exists a nontrivial fixed point in this sequence, i.e., a submanifold P_k of P such that $P_k = P_{k+1}$, we refer to P_k as the final constraint manifold. If such a fixed point exists, we denote by ν_P the minimum integer such that $P_{\nu_P} = P_{\nu_P+1}$, i.e., ν_P is the number of steps necessary for the presymplectic constraint algorithm to terminate. If such a final constraint manifold P_{ν_P} exists, there always exists a solution vector field X defined on and tangent to P_{ν_P} such that $i_X\Omega_{\nu_P} = dH_{\nu_P}$ and X is unique up to the kernel of Ω_{ν_P}. Furthermore, such a final constraint manifold is maximal in the sense that if there exists a submanifold N of P which admits a vector field X defined on and tangent to N such that $i_X\Omega|_N = dH|_N$, then $N \subset P_{\nu_P}$ (Gotay and Nester [42]).

3.1.3 Main Contributions

In this paper, we explore the geometric properties of adjoint systems associated with ordinary differential equations (ODEs) and differential-algebraic equations (DAEs). For a discussion of adjoint systems associated with ODEs and DAEs, see Sanz-Serna [106] and Cao et al. [26], respectively. In particular, we utilize the machinery of symplectic and presymplectic geometry as a basis for understanding such systems.

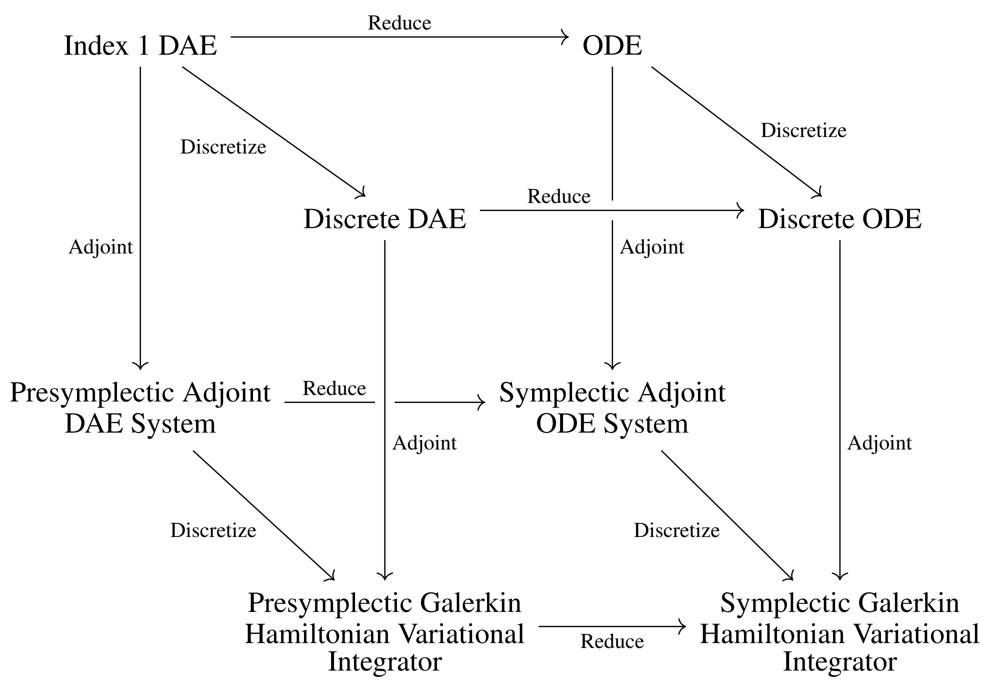
In Section 3.2.1, we review the notion of adjoint equations associated with ODEs over vector spaces. We show that the quadratic conservation law, which is the key to adjoint sensitivity analysis, arises from the symplecticity of the flow of the adjoint system. In Section 3.2.2, we investigate the symplectic geometry of adjoint systems associated with ODEs on manifolds. We additionally discuss augmented adjoint systems, which are useful in the adjoint sensitivity of running cost functions. In Section 3.2.3, we investigate the presymplectic geometry of adjoint systems associated with DAEs on manifolds. We investigate the relation between the index of the base DAE and the index of the associated adjoint system, using the notions of DAE reduction and the presymplectic constraint algorithm. We additionally consider augmented systems for such adjoint DAE systems. For the various adjoint systems that we consider, we derive various quadratic conservation laws which are useful in adjoint sensitivity analysis of terminal and running cost functions. We additionally discuss symmetry properties and present variational characterizations of such systems that provide a useful perspective for constructing geometric numerical methods for these systems.

In Section 3.3, we discuss applications of the various adjoint systems to adjoint sensitivity and optimal control. In Section 3.3.1, we show how the quadratic conservation laws developed in Section 3.2 can be used for adjoint sensitivity analysis of running and terminal cost functions, subject to ODE or DAE constraints. In Section 3.3.2, we construct structure-preserving discretizations of adjoint systems using the Galerkin Hamiltonian variational integrator construction of Leok and Zhang [76]. For adjoint DAE systems, we introduce a presymplectic analogue of the Galerkin Hamiltonian variational integrator construction. We show that such discretizations admit discrete analogues of the aforementioned quadratic conservation laws and hence are suitable for the numerical computation of adjoint sensitivities. Furthermore, we show that such discretizations are natural when applied to DAE systems, in the sense that reduction, forming the adjoint system, and discretization all commute (for particular choices of these processes). As an application of this naturality, we derive a variational error analysis result for the resulting presymplectic variational integrator for adjoint DAE systems. Finally, in Section 3.3.3, we discuss adjoint systems in the context of optimal control problems, where we prove a similar naturality result, in that suitable choices of reduction, extremization, and discretization commute.

By developing a geometric theory for adjoint systems, the application areas that utilize such adjoint systems can benefit from the existing work on geometric and structure-preserving methods.

3.1.4 Main Results

In this paper, we prove that, starting with an index 1 DAE, appopriate choices of reduction, discretization, and forming the adjoint system commute. That is, the following diagram commutes.



In order to prove this result, we develop along the way the definitions of the various vertices and arrows in the above diagram. Roughly speaking, the four "Adjoint" arrows are defined by forming the appropriate continuous or discrete action and enforcing the variational principle; the four "Reduce" arrows are defined by solving the algebraic variables in terms of the kinematic variables through the continuous or discrete constraint equations; the two "Discretize" arrows on the top face are given by a Runge–Kutta method, while the two "Discretize" arrows on the bottom face are given by the associated symplectic partitioned Runge–Kutta method. The above commutative diagram can be understood as an extension of the result of Sanz-Serna [106] (that discretization and forming the adjoint of an ODE commute when the discretization is a symplectic Runge–Kutta method) by adding the reduction operation. In order to appropriately define this reduction operation, we will show that the presymplectic adjoint DAE system has index 1 if the base DAE has index 1, so that the reduction of the presymplectic adjoint DAE system results in a symplectic adjoint ODE system; the tool for this will be the presymplectic constraint algorithm.

In the process of defining the ingredients in the above diagram, we will additionally prove various properties of adjoint systems associated with ODEs and DAEs. The key properties that we will prove for such adjoint systems are the adjoint variational quadratic conservation laws, Propositions 3.2.3, 3.2.6, 3.2.9, 3.2.10. As we will show, these conservation laws can be used to compute adjoint sensitivities of running and terminal cost functions under the flow of an ODE or DAE. In order to prove these conservation laws, we will need to define the variational equations associated with an adjoint system. We will define them as the linearization of the base ODE or DAE; for the DAE case, we will show that the variational equations have the same index as the base DAE so that they have the same (local) solvability.

3.2 Adjoint Systems

3.2.1 Adjoint Equations on Vector Spaces

In this section, we review the notion of adjoint equations on vector spaces and their properties, as preparation for adjoint systems on manifolds.

Let Q be a finite-dimensional vector space and consider the ordinary differential equation on Q given by

$$\dot{q} = f(q), \tag{2.1}$$

where $f : Q \to Q$ is a differentiable vector field on Q. Let $Df(q)$ denote the linearization of f at $q \in Q$, $Df(q) \in L(Q,Q)$. Denoting its adjoint by $[Df(q)]^* \in L(Q^*,Q^*)$, the adjoint equation associated with (2.1) is given by

$$\dot{p} = -[Df(q)]^* p, \tag{2.2}$$

where p is a curve on Q^*.

Let q^A be coordinates for Q and let p_A be the associated dual coordinates for Q^*, so that the duality pairing is given by $\langle p,q\rangle = p_A q^A$. The linearization of f at q is given in coordinates by

$$(Df(q))^A_B = \frac{\partial f^A(q)}{\partial q^B},$$

where its action on $v \in Q$ in coordinates is

$$(Df(q)v)^A = \frac{\partial f^A(q)}{\partial q^B} v^B.$$

Its adjoint then acts on $p \in Q^*$ by

$$([Df(q)]^* p)_A = \frac{\partial f^B(q)}{\partial q^A} p_B.$$

Thus, the ODE and its adjoint can be expressed in coordinates as

$$\begin{aligned} \dot{q}^A &= f^A(q), \\ \dot{p}_A &= -\frac{\partial f^B(q)}{\partial q^A} p_B. \end{aligned}$$

Next, we recall that the combined system (2.1)-(2.2), which we refer to as the adjoint system, arises from a variational principle. Letting $\langle\cdot,\cdot\rangle$ denote the duality pairing between Q^*

and Q, we define the Hamiltonian

$$H : Q \times Q^* \to \mathbb{R},$$
$$(q,p) \mapsto H(q,p) \equiv \langle p, f(q) \rangle.$$

The associated action, defined on the space of curves on $Q \times Q^*$ covering some interval (t_0,t_1), is given by

$$S[q,p] = \int_{t_0}^{t_1} (\langle p, \dot{q} \rangle - H(q,p))\, dt = \int_{t_0}^{t_1} (\langle p, \dot{q} \rangle - \langle p, f(q) \rangle)\, dt.$$

Proposition 3.2.1. *The variational principle $\delta S = 0$, subject to variations $(\delta q, \delta p)$ which fix the initial position $\delta q(t_0) = 0$ and the final momenta $\delta p(t_1) = 0$, yields the adjoint system* (2.1)-(2.2).

Remark 3.2.1. *We defer the proof of the above proposition until Proposition 3.2.11, where we prove the more general case for manifolds.*

The conditions $\delta q(t_0) = 0$ and $\delta p(t_1) = 0$ correspond to boundary conditions $q(t_0) = q_0$ and $p(t_1) = p_1$, which are the boundary conditions used in adjoint sensitivity analysis.

The variational principle utilized above is formulated so that the stationarity condition $\delta S = 0$ is equivalent to Hamilton's equations, where we view $Q \times Q^* \cong T^*Q$ with the canonical symplectic form on the cotangent bundle $\Omega = dq \wedge dp$ and with the corresponding Hamiltonian $H : T^*Q \to \mathbb{R}$ given as above. It then follows that the flow of the adjoint system is symplectic.

The symplecticity of the adjoint system is a key feature of the system. In fact, the symplecticity of the adjoint system implies that a certain quadratic invariant is preserved along the flow of the system. This quadratic invariant is the key ingredient to the use of adjoint equations for sensitivity analysis. To state the quadratic invariant, consider the variational equation associated with equation (2.1),

$$\frac{d}{dt} \delta q = Df(q) \delta q, \tag{2.3}$$

which corresponds to the linearization of (2.1) at $q \in Q$. For solution curves p and δq to (2.2) and (2.3), respectively, over the same curve q, one has that the quantity $\langle p, \delta q \rangle$ is preserved along the flow of the system, since

$$\begin{aligned}
\frac{d}{dt}\langle p, \delta q \rangle &= \langle \dot{p}, \delta q \rangle + \langle p, \frac{d}{dt}\delta q \rangle = \langle -[Df(q)]^* p, \delta q \rangle + \langle p, Df(q)\delta q \rangle \\
&= -\langle p, Df(q)\delta q \rangle + \langle p, Df(q)\delta q \rangle = 0.
\end{aligned}$$

To see that symplecticity implies the preservation of this quantity, recall that symplecticity is the statement that, along a solution curve of the adjoint system (2.1)-(2.2), one has

$$\frac{d}{dt}\Omega(V,W) = 0,$$

where V and W are first variations to the adjoint system (i.e., that the flow of V and W on solutions are again solutions). Infinitesimally, first variations V and W correspond to solutions of the linearization of the adjoint system (2.1)-(2.2). At a solution (q, p) to the adjoint system, the linearization of the system is given by

$$\begin{aligned}
\frac{d}{dt}\delta q &= Df(q)\delta q, \\
\frac{d}{dt}\delta p &= -[Df(q)]^* \delta p.
\end{aligned}$$

Note that the first equation is just the variational equation (2.3) while the second equation is the adjoint equation (2.2), with p replaced by δp, since the adjoint equation is linear in p. The first variation vector field V corresponding to a solution $(\delta q, \delta p)$ of this linearized system is

$$V = \delta q \frac{\partial}{\partial q} + \delta p \frac{\partial}{\partial p}.$$

Now, we make two choices for the first variations V and W. For W, we take the solution $\delta q = 0$,

$\delta p = p$ of the linearized system, which gives $W = p\,\partial/\partial p$. For V, we take the solution $\delta q = \delta q$, $\delta p = 0$ of the linearized system, which gives $V = \delta q\,\partial/\partial q$. Inserting these into Ω gives

$$\Omega(V,W) = p\frac{\partial}{\partial p} \lrcorner \left(\delta q \frac{\partial}{\partial q} \lrcorner (dq \wedge dp)\right) = \langle p, \delta q\rangle.$$

Thus, symplecticity $\frac{d}{dt}\Omega(V,W) = 0$ with this particular choice of first variations V,W gives the preservation of the quadratic invariant $\langle p, \delta q\rangle$.

3.2.2 Adjoint Systems on Manifolds

We now extend the notion of the adjoint system to the case where the configuration space of the base ODE is a manifold. We will provide a symplectic characterization of these adjoint systems, prove the associated adjoint variational quadratic conservation laws, and additionally discuss symmetries and variational principles associated with these systems.

Let M be a manifold and consider the ODE on M given by

$$\dot{q} = f(q), \tag{2.4}$$

where f is a vector field on M. Letting $\pi : TM \to M$ denote the tangent bundle projection, we recall that a vector field f is a map $f : M \to TM$ which satisfies $\pi \circ f = \mathbf{1}_M$, i.e., f is a section of the tangent bundle.

Analogous to the adjoint system on vector spaces, we will define the adjoint system on a manifold as an ODE on the cotangent bundle T^*M which covers (2.4), such that the time evolution of the momenta in the fibers of T^*M are given by an adjoint linearization of f.

To do this, in analogy with the vector space case, consider the Hamiltonian $H : T^*M \to \mathbb{R}$ given by $H(q, p) = \langle p, f(q)\rangle_q$ where $\langle\cdot,\cdot\rangle_q$ is the duality pairing of T_q^*M with T_qM. When there is no possibility for confusion of the base point, we simply denote this duality pairing as $\langle\cdot,\cdot\rangle$. Recall that the cotangent bundle T^*M possesses a canonical symplectic form $\Omega = -d\Theta$ where Θ

is the tautological one-form on T^*M. With coordinates $(q,p) = (q^A, p_A)$ on T^*M, this symplectic form has the coordinate expression $\Omega = dq \wedge dp \equiv dq^A \wedge dp_A$.

We define the adjoint system as the ODE on T^*M given by Hamilton's equations, with the above choice of Hamiltonian H and the canonical symplectic form. Thus, the adjoint system is given by the equation

$$i_{X_H}\Omega = dH,$$

whose solution curves on T^*M are the integral curves of the Hamiltonian vector field X_H. As is well-known, for the particular choice of Hamiltonian $H(q,p) = \langle p, f(q)\rangle$, the Hamiltonian vector field X_H is given by the cotangent lift $\widehat{f}$ of f, which is a vector field on T^*M that covers f (see, for example, Bullo and Lewis [23]). With coordinates $z = (q,p)$ on T^*M, the adjoint system is the ODE on T^*M given by

$$\dot{z} = \widehat{f}(z). \tag{2.5}$$

To be more explicit, recall that the cotangent lift of f is constructed as follows. Let $\Phi_\varepsilon : M \to M$ denote the one-parameter family of diffeomorphisms generated by f. Then, we consider the cotangent lifted diffeomorphisms given by $(\Phi_{-\varepsilon})^* : T^*M \to T^*M$. This covers Φ_ε in the sense that $\pi_{T^*M} \circ (\Phi_{-\varepsilon})^* = \Phi_\varepsilon \circ \pi_{T^*M}$ where $\pi_{T^*M} : T^*M \to M$ is the cotangent projection. The cotangent lift $\widehat{f}$ is then defined to be the infinitesimal generator of the cotangent lifted flow,

$$\widehat{f}(z) = \frac{d}{d\varepsilon}\Big|_{\varepsilon=0} (\Phi_{-\varepsilon})^*(z).$$

We can directly verify that $\widehat{f}$ is the Hamiltonian vector field for H, which follows from

$$i_{\widehat{f}}\Omega = -i_{\widehat{f}}d\Theta = -\mathscr{L}_{\widehat{f}}\Theta + d(i_{\widehat{f}}\Theta) = d(i_{\widehat{f}}\Theta) = dH,$$

where $\mathscr{L}_{\widehat{f}}\Theta = 0$ follows from the fact that cotangent lifted flows preserve the tautological one-form and $H = i_{\widehat{f}}\Theta$ follows from a direct computation (where $i_{\widehat{f}}\Theta$ is interpreted as a function on the cotangent bundle which maps (q,p) to $\langle \Theta(q,p), \widehat{f}(q,p) \rangle$)

The adjoint system (2.5) covers (2.4) in the following sense.

Proposition 3.2.2. *Integral curves to the adjoint system* (2.5) *lift integral curves to the system* (2.4).

Proof. Let $z=(q,p)$ be coordinates on T^*M. Let $(\dot{q},\dot{p}) \in T_{(q,p)}T^*M$. Then, $T\pi_{T^*M}(\dot{q},\dot{p}) = \dot{q}$ where $T\pi_{T^*M}$ is the pushforward of the cotangent projection. Furthermore,

$$\begin{aligned} T\pi_{T^*M}\hat{f}(q,p) = T\pi_{T^*M}\frac{d}{d\varepsilon}\Big|_{\varepsilon=0}(\Phi_{-\varepsilon})^*(q,p) &= \frac{d}{d\varepsilon}\Big|_{\varepsilon=0}(\pi_{T^*M}\circ(\Phi_{-\varepsilon})^*)(q,p) \\ = \frac{d}{d\varepsilon}\Big|_{\varepsilon=0}(\Phi_\varepsilon \circ \pi_{T^*M})(q,p) &= \frac{d}{d\varepsilon}\Big|_{\varepsilon=0}\Phi_\varepsilon(q) = f(q). \end{aligned}$$

Thus, the pushforward of the cotangent projection applied to (2.5) gives (2.4). It then follows that integral curves of (2.5) lift integral curves of (2.4). □

Remark 3.2.2. *This can also be seen explicitly in coordinates. Recalling that $i_{\widehat{f}}\Omega = dH$, one has*

$$dH = d(p_A f^A(q)) = f^A(q)dp_A + p_B\frac{\partial f^B(q)}{\partial q^A}dq^A,$$

and, on the other hand, denoting $\widehat{f}(q,p) = X^A(q,p)\partial/\partial q^A + Y_A(q,p)\partial/\partial p_A$,

$$i_{\widehat{f}}\Omega = (X^A(q,p)\partial_{q^A} + Y_A(q,p)\partial_{p_A}) \lrcorner (dq^B \wedge dp_B) = X^A(q,p)dp_A - Y_A(q,p)dq^A.$$

Equating these two gives the coordinate expression for the cotangent lift $\widehat{f}$,

$$\widehat{f}(q,p) = f^A(q)\frac{\partial}{\partial q^A} - p_B\frac{\partial f^B(q)}{\partial q^A}\frac{\partial}{\partial p_A}.$$

Thus, the system $\dot{z} = \widehat{f}(z)$ can be expressed in coordinates as

$$\dot{q}^A = f^A(q), \tag{2.6a}$$

$$\dot{p}_A = -p_B \frac{\partial f^B(q)}{\partial q^A}, \tag{2.6b}$$

which clearly covers the original ODE $\dot{q}^A = f^A(q)$. Also, note that this coordinate expression for the adjoint system recovers the coordinate expression for the adjoint system in the vector space case.

Analogous to the vector space case, the adjoint system possesses a quadratic invariant associated with the variational equations of (2.4). The variational equation is given by considering the tangent lifted vector field on TM, $\widetilde{f}: TM \to TTM$, which is defined in terms of the flow Φ_ε generated by f by

$$\widetilde{f}(q, \delta q) = \frac{d}{d\varepsilon}\Big|_{\varepsilon=0} T\Phi_\varepsilon(q, \delta q),$$

where $(q, \delta q)$ are coordinates on TM. That is, $\widetilde{f}$ is the infinitesimal generator of the tangent lifted flow. The variational equation associated with (2.4) is the ODE associated with the tangent lifted vector field. In coordinates,

$$\frac{d}{dt}(q, \delta q) = \widetilde{f}(q, \delta q). \tag{2.7}$$

Proposition 3.2.3. *For integral curves (q, p) of* (2.5) *and $(q, \delta q)$ of* (2.7)*, which cover the same curve q,*

$$\frac{d}{dt}\Big\langle (q(t), p(t)), (q(t), \delta q(t)) \Big\rangle_{q(t)} = 0. \tag{2.8}$$

Proof. Note that $(q(t), p(t)) \in T^*_{q(t)}M$ and $(q(t), \delta q(t)) \in T_{q(t)}M$ so the duality pairing is well-defined. Then,

$$\begin{aligned}
\Big\langle (q(t),p(t)),(q(t),\delta q(t)) \Big\rangle_{q(t)} &= \Big\langle (\Phi_{-t})^*(q(0),p(0)), T\Phi_t(q(0),\delta q(0)) \Big\rangle_{q(t)} \\
&= \Big\langle (q(0),p(0)), T\Phi_{-t} \circ T\Phi_t(q(0),\delta q(0)) \Big\rangle_{q(0)} \\
&= \Big\langle (q(0),p(0)), T(\Phi_{-t} \circ \Phi_t)(q(0),\delta q(0)) \Big\rangle_{q(0)} \\
&= \Big\langle (q(0),p(0)), (q(0),\delta q(0)) \Big\rangle_{q(0)},
\end{aligned}$$

so the pairing is constant. □

Remark 3.2.3. *In the vector space case, we saw that the preservation of the quadratic invariant is implied by symplecticity. The above result is analogously implied by symplecticity, noting that the flow of the adjoint system is symplectic since $\widehat{f}$ is a Hamiltonian vector field.*

Another conserved quantity for the adjoint system (2.5) is the Hamiltonian, since the adjoint system corresponds to a time-independent Hamiltonian flow, $\frac{d}{dt}H = \Omega(X_H, X_H) = 0$.

Additionally, conserved quantities for adjoint systems are generated, via cotangent lift, by symmetries of the original ODE (2.4), where we say that a vector field g is a symmetry of the ODE $\dot{x} = h(x)$ if $[g,h] = 0$.

Proposition 3.2.4. *Let g be a symmetry of* (2.4)*, i.e.,* $[g,f] = 0$*. Then, its cotangent lift $\widehat{g}$ is a symmetry of* (2.5) *and additionally, the function*

$$\langle \Theta, \widehat{g} \rangle$$

on T^*M is preserved along the flow of $\widehat{f}$, i.e., under the flow of the adjoint system (2.5).

Proof. We first show that $\widehat{g}$ is a symmetry of (2.5), i.e., that $[\widehat{g}, \widehat{f}] = 0$. To see this, we recall that the cotangent lift of the Lie bracket of two vector fields equals the Lie bracket of their cotangent lifts,

$$\widehat{[g,f]} = [\widehat{g},\widehat{f}].$$

Then, since $[g,f] = 0$ by assumption, $[\widehat{g},\widehat{f}] = \widehat{[g,f]} = \widehat{0} = 0$.

To see that $\langle \Theta, \widehat{g} \rangle$ is preserved along the flow of $\widehat{f}$, we have

$$\mathscr{L}_{\widehat{f}} \langle \Theta, \widehat{g} \rangle = \langle \mathscr{L}_{\widehat{f}} \Theta, \widehat{g} \rangle + \langle \Theta, \mathscr{L}_{\widehat{f}} \widehat{g} \rangle = \langle 0, \widehat{g} \rangle + \langle \Theta, [\widehat{f},\widehat{g}] \rangle = 0,$$

where we used that $\mathscr{L}_{\widehat{f}} \Theta = 0$ since $\widehat{f}$ is a cotangent lifted vector field. □

Remark 3.2.4. *The above proposition states when* $[f,g] = 0$*, the Hamiltonian for the adjoint system associated with g,* $\langle \Theta, \widehat{g} \rangle$*, is preserved along the Hamiltonian flow corresponding to the Hamiltonian for the adjoint system associated with f,* $\langle \Theta, \widehat{f} \rangle$*, and vice versa. Note,* $\langle \Theta, \widehat{g} \rangle$ *can be interpreted as the momentum map corresponding to the action on* T^*M *given by the flow of* $\widehat{g}$*.*

The above proposition shows that (at least some) symmetries of the adjoint system (2.5) *can be found by cotangent lifting symmetries of the original ODE* (2.4)*. Additionally, the above proposition states that such cotangent lifted symmetries give rise to conserved quantities.*

In light of the above proposition, it is natural to ask the following question. Given a symmetry G of the adjoint system (2.5) (i.e., $[G,\widehat{f}] = 0$), does it arise from a cotangent lifted symmetry in the sense of Proposition 3.2.4? In general, the answer is no. However, for a projectable vector field G which is a symmetry of the adjoint system, its projection by $T\pi_{T^*M}$ to a vector field on M does satisfy the assumptions of Proposition 3.2.4. This gives the following partial converse to the above proposition.

Proposition 3.2.5. *Let G be a projectable vector field on the bundle* $\pi_{T^*M} : T^*M \to M$ *which is a symmetry of* (2.5)*, i.e.,* $[G,\widehat{f}] = 0$*. Then, the pushforward vector field* $g = T\pi_{T^*M}(G)$ *on M satisfies the assumptions of Proposition 3.2.4 and* $T\pi_{T^*M}\widehat{g} = T\pi_{T^*M}G$*.*

Proof. Since G is a projectable vector field on the cotangent bundle, $g = T\pi_{T^*M}G$ defines a well-defined vector field on M. Thus,

$$[g,f] = [T\pi_{T^*M}G, T\pi_{T^*M}\widehat{f}] = T\pi_{T^*M}[G,\widehat{f}] = T\pi_{T^*M}0 = 0,$$

so g is a symmetry of (2.4). Furthermore, we also have

$$T\pi_{T^*M}\widehat{g} = T\pi_{T^*M}(\widehat{T\pi_{T^*M}G}) = T\pi_{T^*M}G.$$

□

The preceding proposition shows that, for the class of projectable symmetries of the adjoint system (2.5), it is always possible to find an associated symmetry of the original ODE (2.4) which, by Proposition 3.2.4, corresponds to a Hamiltonian symmetry. Note that this implies that we can associate a conserved quantity $\langle \Theta, \widehat{g} \rangle$ to G, where $g = T\pi_{T^*M}G$. Furthermore, since $T\pi_{T^*M}\widehat{g} = T\pi_{T^*M}G$ and the canonical form Θ is a horizontal one-form, this implies that $\langle \Theta, G \rangle$ equals $\langle \Theta, \widehat{g} \rangle$ and hence, is conserved.

These two propositions show that symmetries of an ODE can be identified with equivalence classes of projectable symmetries of the associated adjoint system, where two projectable symmetries are equivalent if their difference lies in the kernel of $T\pi_{T^*M}$.

Adjoint Systems with Augmented Hamiltonians

In this section, we consider a class of modified adjoint systems, where some function on the base manifold M is added to the Hamiltonian of the adjoint system. More precisely, let $H : T^*M \to \mathbb{R}, H(q,p) = \langle p, f(q) \rangle$ be the Hamiltonian of the previous section, corresponding to the ODE $\dot{q} = f(q)$. Let $L : M \to \mathbb{R}$ be a function on M. We identify L with its pullback through

$\pi_{T^*M} : T^*M \to M$. Then, we define the augmented Hamiltonian

$$\begin{aligned} H_L \equiv H + L : T^*M &\to \mathbb{R} \\ (q,p) &\mapsto H(q,p) + L(q) = \langle p, f(q) \rangle + L(q). \end{aligned}$$

We define the augmented adjoint system as the Hamiltonian system associated with H_L relative to the canonical symplectic form Ω on T^*M,

$$i_{X_{H_L}} \Omega = dH_L. \tag{2.9}$$

Remark 3.2.5. *The motivation for such systems arises from adjoint sensitivity analysis and optimal control. For adjoint sensitivity analysis of a running cost function, one is concerned with the sensitivity of some functional*

$$\int_0^t L(q)dt$$

along the flow of the ODE $\dot{q} = f(q)$. In the setting of optimal control, the goal is to minimize such a functional, constrained to curves satisfying the ODE (see, for example, Aguiar et al. [3]). We will discuss such applications in more detail in Section 3.3.

In coordinates, the augmented adjoint system (2.9) takes the form

$$\dot{q}^A = \frac{\partial H}{\partial p_A} = f^A(q), \tag{2.10a}$$

$$\dot{p}_A = -\frac{\partial H}{\partial q^A} = -p_B \frac{\partial f^B(q)}{\partial q^A} - \frac{\partial L(q)}{\partial q^A}. \tag{2.10b}$$

We now prove various properties of the augmented adjoint system, analogous to the previous section. To start, first note that we can decompose the Hamiltonian vector field X_{H_L} as follows. Let $\widehat{f}$ be the cotangent lift of f. Let $X_L \equiv X_{H_L} - \widehat{f}$. Then, observe that

$$i_{X_L}\Omega = i_{X_{H_L}}\Omega - i_{\widehat{f}}\Omega = dH_L - dH = dL.$$

Thus, we have the decomposition $X_{H_L} = \widehat{f} + X_L$, where $\widehat{f}$ and X_L are the Hamiltonian vector fields for H and L, respectively. In coordinates,

$$X_L = -\frac{\partial L}{\partial q^A}\frac{\partial}{\partial p_A}.$$

From the coordinate expression, we see that X_L is a vertical vector field over the bundle $T^*M \to M$. We can also see this intrinsically, since dL is a horizontal one-form on T^*M, X_L satisfies $i_{X_L}\Omega = dL$, and Ω restricts to an isomorphism from vertical vector fields on T^*M to horizontal one-forms on T^*M. Thus, it is immediate to see intrinsically that an analogous statement to Proposition 3.2.2 holds, since the flow of $\widehat{f}$ lifts the flow of f, while the flow of X_L is purely vertical. That is, since $T\pi_{T^*M}X_L = 0$,

$$T\pi_{T^*M}X_{H_L} = T\pi_{T^*M}\widehat{f} = f.$$

We can of course also see that the augmented adjoint system lifts the original ODE from the coordinate expression for the augmented adjoint system, (2.10a)-(2.10b).

We now prove analogous statements to Propositions 3.2.3 and 3.2.4, modified appropriately for the presence of L in the augmented Hamiltonian.

Proposition 3.2.6. *Let* (q,p) *be an integral curve of the augmented adjoint system* (2.9) *and let* $(q,\delta q)$ *be an integral curve of the variational equation* (2.7)*, covering the same curve q. Then,*

$$\frac{d}{dt}\langle p,\delta q\rangle = -\langle dL,\delta q\rangle.$$

Remark 3.2.6. *Note that the variational equation associated with the above system is the same as in the nonaugmented case, equation* (2.7)*, since augmenting L to the Hamiltonian system only shifts the Hamiltonian vector field in the vertical direction.*

Proof. We will prove this in coordinates. We have the equations

$$\dot{p}_A = -p_B \frac{\partial f^B}{\partial q^A} - \frac{\partial L}{\partial q^A},$$
$$\frac{d}{dt}\delta q^B = \frac{\partial f^B}{\partial q^A}\delta q^A.$$

Then,

$$\begin{aligned}
\frac{d}{dt}\langle p, \delta q\rangle &= \frac{d}{dt} p_A \delta q^A = \dot{p}_A \delta q^A + p_B \frac{d}{dt}\delta q^B \\
&= -p_B \frac{\partial f^B}{\partial q^A}\delta q^A - \frac{\partial L}{\partial q^A}\delta q^A + p_B \frac{\partial f^B}{\partial q^A}\delta q^A \\
&= -\frac{\partial L}{\partial q^A}\delta q^A = -\langle dL, \delta q\rangle.
\end{aligned}$$

□

Remark 3.2.7. *Interestingly, the above proposition states that in the augmented case,* $\langle p, \delta q\rangle$ *is no longer preserved but rather, its change measures the change of* L *with respect to the variation* δq*. This may at first seem contradictory since both the augmented and nonaugmented Hamiltonian vector fields,* X_{H_L} *and* X_H*, preserve* Ω*, and as we noted previously in Remark 3.2.3, the preservation of the quadratic invariant is implied by symplecticity. However, upon closer inspection, there is no contradiction because the two cases have different first variations, where recall a first variation is a symmetry vector field of the Hamiltonian system and symplecticity can be stated as*

$$\frac{d}{dt}\Omega(V, W) = 0,$$

for first variation vector fields V *and* W*. In the nonaugmented case, the equations satisfied by the first variation of the momenta* p *can be identified with* p *itself, since the adjoint equation for* p *is linear in* p*. On the other hand, in the augmented case, the adjoint equation for* p*,* (2.10b)*, is no longer linear in* p*, rather, it is affine in* p*. Furthermore, the failure of this equation to be linear in* p *is given precisely by* $-dL$*. Thus, in the augmented case, first variations in* p *can no longer* *be identified with p, and this leads to the additional term* $-\langle dL, \delta q\rangle$ *in the above proposition.*

To prove an analogous statement to Proposition 3.2.4, we need the additional assumption that the symmetry vector field g leaves L invariant, $\mathscr{L}_g L = 0$.

Proposition 3.2.7. *Let g be a symmetry of the ODE* $\dot{q} = f(q)$*, i.e.,* $[g, f] = 0$*. Additionally, assume that g is a symmetry of L, i.e.,* $\mathscr{L}_g L = 0$*. Then, its cotangent lift* $\widehat{g}$ *is a symmetry of the augmented adjoint system,* $[\widehat{g}, X_{H_L}] = 0$ *and additionally, the function*

$$\langle \Theta, \widehat{g}\rangle$$

on T^*M *is preserved along the flow of* X_{H_L}*.*

Proof. To see that $[\widehat{g}, X_{H_L}] = 0$, note that with the decomposition $X_{H_L} = \widehat{f} + X_L$, we have

$$[\widehat{g}, X_{H_L}] = [\widehat{g}, \widehat{f}] + [\widehat{g}, X_L] = [\widehat{g}, X_L],$$

where we used that $[\widehat{g}, \widehat{f}] = \widehat{[g, f]} = 0$. To see that $[\widehat{g}, X_L] = 0$, we note that $[\widehat{g}, X_L]$ can be expressed

$$[\widehat{g}, X_L] = \mathscr{L}_{\widehat{g}} X_L = \mathscr{L}_{\widehat{g}}(\Omega^{-1}(dL)),$$

where we interpret $\Omega : T(T^*M) \to T^*(T^*M)$. Then, note that $\widehat{g}$ preserves Ω since $\widehat{g}$ is a cotangent lift and it also preserves L (where, since we identify L with its pullback through π_{T^*M}, this is equivalent to g preserving L). More precisely, since we are identifying L with its pullback $(\pi_{T^*M})^* L$, we have

$$\mathscr{L}_{\widehat{g}}((\pi_{T^*M})^* L) = \langle (\pi_{T^*M})^* dL, \widehat{g}\rangle = \langle dL, T\pi_{T^*M}\widehat{g}\rangle = \langle dL, g\rangle = \mathscr{L}_g L = 0.$$

Hence, $\mathscr{L}_{\widehat{g}}(\Omega^{-1}(dL)) = 0$. One can also verify this in coordinates, and a direct computation yields

$$[\widehat{g}, X_L] = \frac{\partial}{\partial q^A}\left(g^B(q)\frac{\partial L}{\partial q^B}\right)\frac{\partial}{\partial p_A},$$

which vanishes since $\mathscr{L}_g L = 0$.

Now, to show that $\langle \Theta, \widehat{g}\rangle$ is preserved along the flow of X_{H_L}, compute

$$\mathscr{L}_{X_{H_L}}\langle \Theta, \widehat{g}\rangle = \mathscr{L}_{\widehat{f}}\langle \Theta, \widehat{g}\rangle + \mathscr{L}_{X_L}\langle \Theta, \widehat{g}\rangle = \mathscr{L}_{X_L}\langle \Theta, \widehat{g}\rangle,$$

where we used that $\mathscr{L}_{\widehat{f}}\langle \Theta, \widehat{g}\rangle = 0$ by Proposition 3.2.4. Now, we have

$$\begin{aligned}
\mathscr{L}_{X_{H_L}}\langle \Theta, \widehat{g}\rangle &= \mathscr{L}_{X_L}\langle \Theta, \widehat{g}\rangle = \langle \mathscr{L}_{X_L}\Theta, \widehat{g}\rangle + \langle \Theta, \mathscr{L}_{X_L}\widehat{g}\rangle = \langle \mathscr{L}_{X_L}\Theta, \widehat{g}\rangle + \langle \Theta, \underbrace{[X_L, \widehat{g}]}_{=0}\rangle \\
&= \langle i_{X_L} d\Theta + d(i_{X_L}\Theta), \widehat{g}\rangle = \langle -i_{X_L}\Omega, \widehat{g}\rangle + \langle d(i_{X_L}\Theta), \widehat{g}\rangle \\
&= -\langle dL, \widehat{g}\rangle + \langle d(i_{X_L}\Theta), \widehat{g}\rangle.
\end{aligned}$$

The first term above vanishes since $\mathscr{L}_g L = 0$. Furthermore, $\langle d(i_{X_L}\Theta), \widehat{g}\rangle = 0$ since X_L is a vertical vector field while Θ is a horizontal one-form. Hence, $\mathscr{L}_{X_{H_L}}\langle \Theta, \widehat{g}\rangle = 0$. □

3.2.3 Adjoint Systems for DAEs via Presymplectic Mechanics

In this section, we generalize the notion of adjoint system to the case where the base equation is a (semi-explicit) DAE. We will prove analogous results to the ODE case. However, more care is needed than the ODE case, since the DAE constraint introduces issues with solvability. As we will see, the adjoint system associated with a DAE is a presymplectic system, so we will approach the solvability of such systems through the presymplectic constraint algorithm.

We consider the following setup for a differential-algebraic equation. Let M_d and M_a be two manifolds, where we regard M_d as the configuration space of the "dynamical" or "differential" variables and M_a as the configuration space of the "algebraic" variables. Let $\pi_\Phi : \Phi \to M_d \times M_a$ be a vector bundle over $M_d \times M_a$. Furthermore, let $\pi_d : M_d \times M_a \to M_d$ be the projection onto the first factor and let $\pi_{\overline{TM}_d} : \overline{TM}_d \to M_d \times M_a$ be the pullback bundle of the tangent bundle $\pi_{TM_d} : TM_d \to M_d$ by π_d, i.e., $\overline{TM}_d = \pi_d^*(TM_d)$. Then, a (semi-explicit) DAE is specified by a section $f \in \Gamma(\overline{TM}_d)$ and a section $\phi \in \Gamma(\Phi)$, via the system

$$\dot{q} = f(q,u), \tag{2.11a}$$

$$0 = \phi(q,u), \tag{2.11b}$$

where (q,u) are coordinates on $M_d \times M_a$. We refer to $\overline{TM}_d$ as the differential tangent bundle, with coordinates (q,u,v) and to Φ as the constraint bundle.

Remark 3.2.8. *For the local solvability of* (2.11a)-(2.11b)*, regard ϕ locally as a map $\mathbb{R}^{\dim(M_d)} \times \mathbb{R}^{\dim(M_a)} \to \mathbb{R}^{\operatorname{rank}(\Phi)}$. If $\partial\phi/\partial u$ is an isomorphism at a point (q_0,u_0) where $\Phi(q_0,u_0) = 0$, then by the implicit function theorem, one can locally solve $u = u(q)$ about (q_0,u_0) such that $\phi(q,u(q)) = 0$, and subsequently solve the unconstrained differential equation $\dot{q} = f(q,u(q))$ locally. This is the case for semi-explicit index* 1 *DAEs.*

In order for the $\operatorname{rank}(\Phi) \times \dim(M_a)$ *matrix $\partial\phi/\partial u(q_0,u_0)$ to be an isomorphism, it is necessary that* $\operatorname{rank}(\Phi) = \dim(M_a)$*. However, we will make no such assumption, so as to treat the theory in full generality, allowing for, e.g., nonunique solutions.*

Now, let $\overline{T^*M}_d$ be the pullback bundle of the cotangent bundle T^*M_d by π_d, with coordinates (q,u,p), which we refer to as the differential cotangent bundle. Furthermore, let Φ^* be the dual vector bundle to Φ, with coordinates (q,u,λ). Let $\overline{T^*M}_d \oplus \Phi^*$ be the Whitney sum of these two vector bundles over $M_d \times M_a$ with coordinates (q,u,p,λ), which we refer to as the generalized phase space bundle. We define a Hamiltonian on the generalized phase space,

$$H : \overline{T^*M}_d \oplus \Phi^* \to \mathbb{R},$$
$$H(q,u,p,\lambda) = \langle p, f(q,u)\rangle + \langle \lambda, \phi(q,u)\rangle.$$

Let Ω_d denote the canonical symplectic form on T^*M_d, with coordinate expression $\Omega_d = dq \wedge dp$.

We define a presymplectic form Ω_0 on $\overline{T^*M}_d \oplus \Phi^*$ as follows: the pullback bundle admits the map $\tilde{\pi}_d : \overline{T^*M}_d \to T^*M_d$ which covers π_d and acts as the identity on fibers and furthermore, the generalized phase space bundle admits the projection $\Pi : \overline{TM}^*_d \oplus \Phi^* \to \overline{TM}^*_d$, since the Whitney sum has the structure of a double vector bundle. Hence, we can pullback Ω_d along the sequence of maps

$$\overline{T^*M}_d \oplus \Phi^* \xrightarrow{\Pi} \overline{T^*M}_d \xrightarrow{\tilde{\pi}_d} T^*M_d,$$

which allows us to define a two-form $\Omega_0 \equiv \Pi^* \circ \tilde{\pi}_d^*(\Omega_d)$ on the generalized phase space bundle. Clearly, Ω_0 is closed as the pullback of a closed form. In general, Ω_0 will be degenerate except in the trivial case where M_a is empty and the fibers of Φ are the zero vector space. Hence, Ω_0 is a presymplectic form. Note that since Π acts by projection and $\tilde{\pi}_d$ acts as the identity on fibers, the coordinate expression for Ω_0 on $\overline{T^*M}_d \oplus \Phi^*$ with coordinates (q,u,p,λ) is the same as the coordinate expression for Ω_d, $\Omega_0 = dq \wedge dp$. The various spaces and their coordinates are summarized in the diagram below, Figure 3.1.

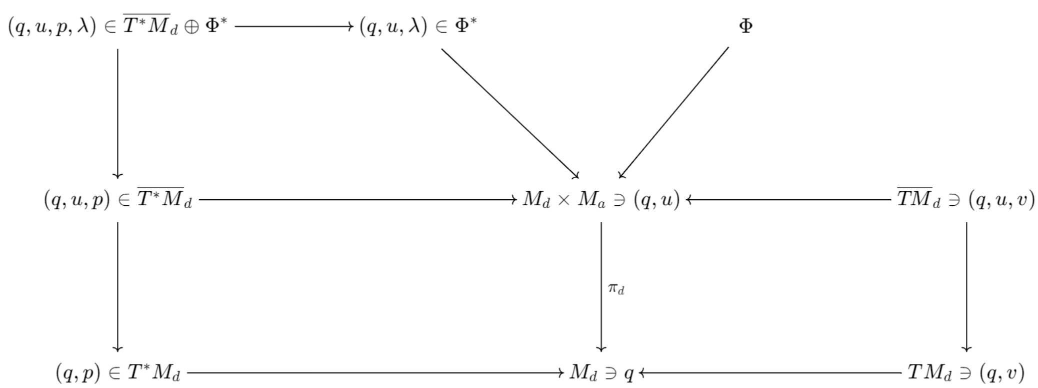


Figure 3.1. Projection maps and coordinates on the generalized phase space bundle

We now define the adjoint system associated with the DAE (2.11a)-(2.11b) as the Hamiltonian system

$$i_X \Omega_0 = dH. \tag{2.12}$$

Given a (generally, partially defined) vector field X on the generalized phase space satisfying

(2.12), we say a curve $(q(t),u(t),p(t),\lambda(t))$ is a solution curve of (2.12) if it is an integral curve of X.

Let us find a coordinate expression for the above system. Expressing our coordinates with indices (q^i,u^a,p_j,λ_A), the left hand side of (2.12) along a solution curve has the expression

$$\begin{aligned} i_X\Omega_0 &= \left(\dot{q}^i\frac{\partial}{\partial q^i}+\dot{u}^a\frac{\partial}{\partial u^a}+\dot{p}_j\frac{\partial}{\partial p_j}+\dot{\lambda}_A\frac{\partial}{\partial \lambda_A}\right)\lrcorner\, dq^k\wedge dp_k \\ &= \dot{q}^i dp_i - \dot{p}_j dq^j. \end{aligned}$$

On the other hand, the right hand side of (2.12) has the expression

$$\begin{aligned} dH &= d\Big(p_i f^i(q,u)+\lambda_A\phi^A(q,u)\Big) \\ &= f^i(q,u)dp_i + \left(p_i\frac{\partial f^i}{\partial q^j}+\lambda_A\frac{\partial \phi^A}{\partial q^j}\right)dq^j + \phi^A(q,u)d\lambda_A + \left(p_i\frac{\partial f^i}{\partial u^a}+\lambda_A\frac{\partial \phi^A}{\partial u^a}\right)du^a. \end{aligned}$$

Equating these expressions gives the coordinate expression for the adjoint DAE system,

$$\dot{q}^i = f^i(q,u), \tag{2.13a}$$

$$\dot{p}_j = -p_i\frac{\partial f^i}{\partial q^j}-\lambda_A\frac{\partial \phi^A}{\partial q^j}, \tag{2.13b}$$

$$0 = \phi^A(q,u), \tag{2.13c}$$

$$0 = p_i\frac{\partial f^i}{\partial u^a}+\lambda_A\frac{\partial \phi^A}{\partial u^a}. \tag{2.13d}$$

Remark 3.2.9. *As mentioned in Remark 3.2.8, in the index* 1 *case, one can locally solve the original DAE* (2.13a) *and* (2.13c)*. Viewing such a solution* (q,u) *as fixed, one can subsequently locally solve for* λ *in equation* (2.13d) *as a function of p, since* $\partial\phi/\partial u$ *is locally invertible. Substituting this into* (2.13b) *gives an ODE solely in the variable p, which can be solved locally.*

Stated another way, if the original DAE (2.11a)-(2.11b) *is an index* 1 *system, then the adjoint DAE system* (2.13a)-(2.13d) *is an index* 1 *system with dynamical variables* (q,p) *and* *algebraic variables* (u,λ)*. To see this, if one denotes the constraints for the adjoint system* (2.13c) *and* (2.13d) *as*

$$0 = \tilde{\phi}(q,u,p,\lambda) \equiv \begin{pmatrix} \phi^A(q,u) \\ p_i \frac{\partial f^i}{\partial u^a} + \lambda_A \frac{\partial \phi^A}{\partial u^a} \end{pmatrix},$$

then the matrix derivative of $\tilde{\phi}$ *with respect to the algebraic variables* (u,λ) *can be locally expressed in block form as*

$$\begin{pmatrix} \partial\phi/\partial u & A \\ 0 & \partial\phi/\partial u \end{pmatrix},$$

where the block A has components given by the derivative of the right hand side of (2.13d) *with respect to u. It is clear from the block triangular form of this matrix that it is pointwise invertible if* $\partial\phi/\partial u$ *is.*

Remark 3.2.10. *It is clear from the coordinate expression* (2.13a)-(2.13d) *that a solution curve of the adjoint DAE system, if it exists, covers a solution curve of the original DAE system.*

We now prove several results regarding the structure of the adjoint DAE system.

First, we show that the constraint equations (2.13c)-(2.13d) can be interpreted as the statement that the Hamiltonian H has the same time dependence as the "dynamical" Hamiltonian,

$$H_d : \overline{T^*M}_d \oplus \Phi^* \to \mathbb{R},$$
$$H_d(q,u,p,\lambda) = \langle p, f(q,u)\rangle,$$

when evaluated along a solution curve.

Proposition 3.2.8. *For a solution curve* (q,u,p,λ) *of* (2.12)*,*

$$\frac{d}{dt}H(q(t),u(t),p(t),\lambda(t)) = \frac{d}{dt}H_d(q(t),u(t),p(t),\lambda(t)).$$

Proof. For brevity, all functions below are appropriately evaluated along the solution curve. We have

$$\begin{aligned}\frac{d}{dt}H &= \frac{\partial H}{\partial q^i}\dot{q}^i + \frac{\partial H}{\partial p_j}\dot{p}_j + \frac{\partial H}{\partial u^a}\dot{u}^a + \frac{\partial H}{\partial \lambda_A}\dot{\lambda}_A \\ &= \frac{\partial H}{\partial q^i}\dot{q}^i + \frac{\partial H}{\partial p_j}\dot{p}_j + \left(p_i\frac{\partial f^i}{\partial u^a} + \lambda_A\frac{\partial \phi^A}{\partial u^a}\right)\dot{u}^a + \phi^A\dot{\lambda}_A \\ &= \frac{\partial H}{\partial q^i}\dot{q}^i + \frac{\partial H}{\partial p_j}\dot{p}_j \\ &= \frac{\partial H_d}{\partial q^i}\dot{q}^i + \frac{\partial H_d}{\partial p_j}\dot{p}_j = \frac{d}{dt}H_d,\end{aligned}$$

where in the third equality, we used (2.13c) and (2.13d). □

Remark 3.2.11. *A more geometric way to view the above proposition is as follows: note that if a partially-defined vector field X exists such that $i_X\Omega_0 = dH$, then the change of H in a given direction Y, at any point where X is defined, can be computed as $dH(Y) = \Omega_0(X,Y)$. Observe that the kernel of Ω_0 is locally spanned by $\partial/\partial u$, $\partial/\partial\lambda$, i.e., it is spanned by the coordinate vectors in the algebraic coordinates. Hence, the change of H in the algebraic coordinate directions is zero. This justifies referring to (u,λ) as "algebraic" variables.*

We now prove a result regarding the conservation of a quadratic invariant, analogous to the case of cotangent lifted adjoint systems in the ODE case. To do this, we define the variational equations as the linearization of the DAE (2.11a)-(2.11b). The coordinate expressions for the variational equations are obtained by taking the variation of equations (2.11a)-(2.11b) with respect to variations $(\delta q, \delta u)$,

$$\dot{q}^i = f^i(q,u), \tag{2.14a}$$

$$0 = \phi^A(q,u), \tag{2.14b}$$

$$\frac{d}{dt}\delta q^i = \frac{\partial f^i(q,u)}{\partial q^j}\delta q^j + \frac{\partial f^i(q,u)}{\partial u^a}\delta u^a, \tag{2.14c}$$

$$0 = \frac{\partial \phi^A(q,u)}{\partial q^j}\delta q^j + \frac{\partial \phi^A(q,u)}{\partial u^a}\delta u^a. \tag{2.14d}$$

Proposition 3.2.9. *For a solution* (q,u,p,λ) *of the adjoint DAE system* (2.13a)-(2.13d) *and a solution* $(q,u,\delta q,\delta u)$ *of the variational equations* (2.14a)-(2.14d)*, covering the same curve* (q,u)*, one has*

$$\frac{d}{dt}\langle p(t),\delta q(t)\rangle = 0.$$

Proof. This follows from a direct computation,

$$\begin{aligned}
\frac{d}{dt}\langle p,\delta q\rangle &= \frac{d}{dt}\left(p_i\delta q^i\right) = \dot{p}_j\delta q^j + p_i\frac{d}{dt}\delta q^i \\
&= -p_i\frac{\partial f^i}{\partial q^j}\delta q^j - \lambda_A\frac{\partial \phi^A}{\partial q^j}\delta q^j + p_i\frac{\partial f^i}{\partial q^j}\delta q^j + p_i\frac{\partial f^i}{\partial u^a}\delta u^a \\
&= -\lambda_A\frac{\partial \phi^A}{\partial q^j}\delta q^j + p_i\frac{\partial f^i}{\partial u^a}\delta u^a \\
&= \left(\lambda_A\frac{\partial \phi^A}{\partial u^a} + p_i\frac{\partial f^i}{\partial u^a}\right)\delta u^a = 0,
\end{aligned}$$

where we used (2.13b), (2.14c), (2.14d), and (2.13d). □

Remark 3.2.12. *Although we proved the previous proposition in coordinates, it can be understood intrinsically through the presymplecticity of the adjoint DAE flow. To see this, assume a partially-defined vector field* X *exists such that* $i_X\Omega_0 = dH$*. Then, the flow of* X *preserves* Ω_0*, which follows from*

$$\mathscr{L}_X\Omega_0 = i_X d\Omega_0 + d(i_X\Omega_0) = d(i_X\Omega_0) = d^2H = 0.$$

The coordinate expression for the preservation of the presymplectic form $\Omega_0 = dq^i\wedge dp_i$*, with the appropriate choice of first variations, gives the previous proposition, analogous to the argument that we made in the symplectic (unconstrained) case.*

Additionally, as we will see in Section 3.3.1, Proposition 3.2.9 will provide a method for computing adjoint sensitivities.

These two observations are interesting when constructing numerical methods to compute adjoint sensitivities, since if we can construct integrators that preserve the presymplectic form, *then it will preserve the quadratic invariant and hence, be suitable for computing adjoint sensitivities efficiently.*

Remark 3.2.13. *For an index 1 DAE* (2.11a)-(2.11b)*, since $\partial\phi/\partial u$ is (pointwise) invertible for a fixed curve (q,u), one can solve for δu as a function of δq in the variational equation* (2.14d) *and substitute this into* (2.14c) *to obtain an explicit ODE for δq. Hence, in the index 1 case, given a solution (q,u) of the DAE* (2.11a)-(2.11b) *and an initial condition $\delta q(0)$ in the tangent fiber over $q(0)$, there is a corresponding (at least local) unique solution of the variational equations.*

DAE Index and the Presymplectic Constraint Algorithm

In this section, we relate the index of the DAE (2.11a)-(2.11b) to the number of steps for convergence in the presymplectic constraint algorithm associated with the adjoint DAE system (2.12). In particular, we show that for an index 1 DAE, the presymplectic constraint algorithm for the associated adjoint DAE system converges after $\nu_P = 1$ step. Subsequently, we discuss how one can formally handle the more general index ν DAE case.

We consider again the presymplectic system given by the adjoint DAE system, $P = \overline{T^*M_d} \oplus \Phi^*$ equipped with the presymplectic form $\Omega_0 = dq \wedge dp$ and Hamiltonian $H(q,u,p,\lambda) = \langle p, f(q,u)\rangle + \langle \lambda, \phi(q,u)\rangle$, as discussed in the previous section. Our goal is to bound the number of steps in the presymplectic constraint algorithm ν_P for this presymplectic system in terms of the index ν of the underlying DAE (2.11a)-(2.11b).

Recall the presymplectic constraint algorithm discussed in Section 3.1.2. We first determine the primary constraint manifold P_1. Observe that since $\Omega_0 = dq \wedge dp$, we have the local expression $\ker(\Omega_0)|_{(q,u,p,\lambda)} = \text{span}\{\partial/\partial u, \partial/\partial\lambda\}$. Thus, we require that

$$\frac{\partial H}{\partial u} = 0,$$
$$\frac{\partial H}{\partial \lambda} = 0,$$

i.e., P_1 consists of the points (q,u,p,λ) such that

$$0 = \frac{\partial H(q,u,p,\lambda)}{\partial u^a} = p_i \frac{\partial f^i(q,u)}{\partial u^a} + \lambda_A \frac{\partial \phi^A(q,u)}{\partial u^a},$$
$$0 = \frac{\partial H(q,u,p,\lambda)}{\partial \lambda^A} = \phi^A(q,u).$$

These are of course the constraint equations (2.13c)-(2.13d) of the adjoint DAE system.

We now consider first the case when the DAE system (2.11a)-(2.11b) has index $\nu = 1$ and subsequently, consider the general case $\nu \geq 1$.

The Presymplectic Constraint Algorithm for $\nu = 1$. For the case $\nu = 1$, we will show that the presymplectic constraint algorithm terminates after 1 step, i.e., $\nu_P = \nu = 1$.

Now, assume that the DAE system (2.11a)-(2.11b) has index $\nu = 1$, i.e., for each $(q,u) \in M_d \times M_a$ such that $\phi(q,u) = 0$, the matrix with A^{th} row and a^{th} column entry

$$\frac{\partial \phi^A(q,u)}{\partial u^a}$$

is invertible. Observe that the definition of the presymplectic constraint algorithm, equation (1.1), is local and hence, we seek a local coordinate expression for $\Omega_1 \equiv \Omega_0|_{P_1}$ and its kernel.

Let $(q,u,p,\lambda) \in P_1$. In particular, $\phi(q,u) = 0$. Since $\partial\phi(q,u)/\partial u$ is invertible, by the implicit function theorem, one can locally solve for u as a function of q, which we denote $u = u(q)$, such that $\phi(q,u(q)) = 0$. Then, one can furthermore locally solve for λ as a function of q and p from the second constraint equation,

$$\lambda_A(q,p) = -\left[\left(\frac{\partial \phi(q,u(q))}{\partial u}\right)^{-1}\right]^a_A p_i \frac{\partial f^i(q,u(q))}{\partial u^a}.$$

Thus, we can coordinatize P_1 via coordinates (q',p'), where the inclusion $i_1 : P_1 \hookrightarrow P$ is given by the coordinate expression

$$i_1 : (q', p') \mapsto (q', u(q'), p', \lambda(q', p')).$$

Then, one obtains the local expression for Ω_1,

$$\Omega_1 = i_1^* \Omega_0 = i_1^*(dq) \wedge i_1^*(dp) = dq' \wedge dp'.$$

This is clearly nondegenerate, i.e., $Z_p = 0$ for any $Z \in \ker(\Omega_1), p \in P_1$, so the presymplectic constraint algorithm terminates, $P_2 = P_1$. We conclude that $\nu_P = 1$.

To conclude the discussion of the index 1 case, we obtain coordinate expressions for the resulting nondegenerate Hamiltonian system. The Hamiltonian on P_1 can be expressed as

$$H_1(q', p') = H(i_1(q', p')) = \langle p', f(q', u(q')) \rangle + \langle \lambda(q', p'), \phi(q', u(q')) \rangle = \langle p', f(q', u(q')) \rangle.$$

Thus, with the coordinate expression $X = \dot{q}'^i \partial/\partial q'^i + \dot{p}'_i \partial/\partial p'_i$, Hamilton's equations $i_X \Omega_1 = dH_1$ can be expressed as

$$\begin{aligned} \dot{q}'^i &= \frac{\partial H_1}{\partial p'_i} = f^i(q', u(q')), \\ \dot{p}'_i &= -\frac{\partial H_1}{\partial q'^i} = -p'_j \frac{\partial f^j(q', u(q'))}{\partial q^i} - p'_j \frac{\partial f^j(q', u(q'))}{\partial u^a} \frac{\partial u^a(q')}{\partial q'^i}. \end{aligned}$$

We will now show explicitly that this Hamiltonian system solves (2.13a)-(2.13d) along the submanifold P_1. Clearly, the latter two equations (2.13c)-(2.13d) are satisfied, by definition of P_1. So, we want to show that the first two equations (2.13a)-(2.13b) are satisfied. Using the second constraint equation (2.13d), we have

$$-p'_j \frac{\partial f^j(q', u(q'))}{\partial u^a} = \lambda_A(q', p') \frac{\partial \phi^A(q', u(q'))}{\partial u^a}.$$

Substituting this into the equation for $\dot{p}'_i$ above gives

$$\dot{p}'_i = -p'_j \frac{\partial f^j(q', u(q'))}{\partial q^i} + \lambda_A(q', p') \frac{\partial \phi^A(q', u(q'))}{\partial u^a} \frac{\partial u^a(q')}{\partial q'^i}.$$

By the implicit function theorem, one has

$$\frac{\partial \phi^A(q', u(q'))}{\partial u^a} \frac{\partial u^a(q')}{\partial q'^i} = -\frac{\partial \phi^A(q', u(q'))}{\partial q^i}.$$

Hence, the Hamiltonian system on P_1 can be equivalently expressed as

$$\begin{aligned}
\dot{q}'^i &= f^i(q', u(q')), \\
\dot{p}'_i &= -p'_j \frac{\partial f^j(q', u(q'))}{\partial q^i} - \lambda_A(q', p') \frac{\partial \phi^A(q', u(q'))}{\partial q^i}.
\end{aligned}$$

Thus, we have explicitly verified that (2.13a)-(2.13d) are satisfied along P_1. Note that since the presymplectic constraint algorithm terminates at $v_P = 1$, X is guaranteed to be tangent to P_1. One can also verify this explicitly by computing the pushforward $Ti_1(X)$ and verifying that it annihilates the constraint functions whose zero level set defines P_1,

$$\begin{aligned}
(q, u, p, \lambda) &\mapsto \phi^A(q, u), \\
(q, u, p, \lambda) &\mapsto p_i \frac{\partial f^i(q, u)}{\partial u^a} + \lambda_A \frac{\partial \phi^A(q, u)}{\partial u^a}.
\end{aligned}$$

Remark 3.2.14. *It is interesting to note that the Hamiltonian system $i_X \Omega_1 = dH_1$, which we obtained by forming the adjoint system of the underlying index 1 DAE and subsequently, reducing the index of the adjoint DAE system through the presymplectic constraint algorithm, can be equivalently obtained (at least locally) by first reducing the index of the underlying DAE and then forming the adjoint system.*

More precisely, if one locally solves $\phi(q, u) = 0$ for $u = u(q)$, then the index 1 DAE can *be reduced to an ODE,*

$$\dot{q} = f(q, u(q)).$$

Subsequently, we can form the adjoint system to this ODE, as discussed in Section 3.2.2. The corresponding Hamiltonian is $H(q,p) = \langle p, f(q,u(q))\rangle$, which is the same as H_1.

Thus, for the index 1 case, the process of forming the adjoint system and reducing the index commute.

Remark 3.2.15. *In the language of the presymplectic constraint algorithm, Proposition 3.2.8 can be restated as the statement that the Hamiltonian H and its first derivatives, restricted to the primary constraint manifold, agrees with the dynamical Hamiltonian H_1 and its first derivatives.*

Remark 3.2.16. *An alternative view of the solution theory of the presymplectic adjoint DAE system* (2.13a)-(2.13d) *is through singular perturbation theory (see, for example, Berglund [13] and Chen and Trenn [32]). We proceed by writing* (2.13a)-(2.13d) *as*

$$\begin{aligned}
\dot{q} &= \frac{\partial H}{\partial p} = f(q,u), \\
\dot{p} &= -\frac{\partial H}{\partial q} = -[D_q f(q,u)]^* p - [D_q \phi(q,u)]^* \lambda, \\
0 &= \frac{\partial H}{\partial \lambda} = \phi(q,u), \\
0 &= -\frac{\partial H}{\partial u} = -[D_u f(q,u)]^* p - [D_u \phi(q,u)]^* \lambda.
\end{aligned}$$

Applying a singular perturbation to the constraint equations yields the system

$$\begin{aligned}
\dot{q} &= \frac{\partial H}{\partial p}, \\
\dot{p} &= -\frac{\partial H}{\partial q}, \\
\varepsilon \dot{u} &= \frac{\partial H}{\partial \lambda}, \\
\varepsilon \dot{\lambda} &= -\frac{\partial H}{\partial u},
\end{aligned}$$

where $\varepsilon > 0$. Observe that this is a nondegenerate Hamiltonian system with $H(q,u,p,\lambda)$ as previously defined but with the modified symplectic form $\Omega_\varepsilon = dq \wedge dp + \varepsilon\, du \wedge d\lambda$. Then, the above system can be expressed $i_{X_H}\Omega_\varepsilon = dH$. In the language of perturbation theory, the primary constraint manifold for the presymplectic system is precisely the slow manifold of the singularly perturbed system. One can utilize techniques from singular perturbation theory to develop a solution theory for this system, using Tihonov's theorem, whose assumptions for this particular system depend on the eigenvalues of the algebraic Hessian $D^2_{u,\lambda}H$ (see, Berglund [13]). Although we will not elaborate on this here, this could be an interesting approach for the existence, stability, and approximation theory of such systems. In particular, the slow manifold integrators introduced in Burby and Klotz [24] may be relevant to their discretization. It is also interesting to note that for a solution $(q_\varepsilon, p_\varepsilon, u_\varepsilon, \lambda_\varepsilon)$ of the singularly perturbed system and a solution $(\delta q_\varepsilon, \delta u_\varepsilon)$ of the variational equations,

$$\begin{aligned} \frac{d}{dt}\delta q_\varepsilon &= D_q f(q_\varepsilon,u_\varepsilon)\delta q_\varepsilon + D_u f(q_\varepsilon,u_\varepsilon)\delta u_\varepsilon, \\ \varepsilon\frac{d}{dt}\delta u_\varepsilon &= D_q \phi(q_\varepsilon,u_\varepsilon)\delta q_\varepsilon + D_u \phi(q_\varepsilon,u_\varepsilon)\delta u_\varepsilon, \end{aligned}$$

one has the perturbed adjoint variational quadratic conservation law

$$\frac{d}{dt}\Big(\langle p_\varepsilon, \delta q_\varepsilon\rangle + \varepsilon\langle \lambda_\varepsilon, \delta u_\varepsilon\rangle\Big) = 0,$$

which follows immediately from the preservation of Ω_ε under the symplectic flow.

The Presymplectic Constraint Algorithm for General $\nu \geq 1$. Note that for the general case, we assume that the index of the DAE is finite, $1 \leq \nu < \infty$.

In this case, there are two possible approaches to reduce the adjoint system: either form the adjoint system associated with the index ν DAE and then successively apply the presymplectic constraint algorithm or, alternatively, reduce the index of the DAE, form the adjoint system, and then apply the presymplectic constraint algorithm as necessary.

Since we have already worked out the presymplectic constraint algorithm for the index 1 case, we will take the latter approach. Namely, we reduce an index ν DAE to an index 1 DAE, and subsequently, apply the presymplectic constraint algorithm to the reduced index 1 DAE. Given an index ν DAE, it is generally possible to reduce the DAE to an index 1 DAE using the algorithm introduced in Mattsson and Söderlind [89]. The process of index reduction is given by differentiating the equations of the DAE to reveal hidden constraints. Geometrically, the process of index reduction can be understood as the successive jet prolongation of the DAE and subsequent projection back onto the first jet (see, Reid et al. [100]).

Thus, given an index ν DAE $\dot{x} = \tilde{f}(x,y)$, $\tilde{\phi}(x,y) = 0$, we can, after $\nu - 1$ reduction steps, transform it into an index 1 DAE of the form $\dot{q} = f(q,u)$, $\phi(q,u) = 0$. Subsequently, we can form the adjoint DAE system and apply one iteration of the presymplectic constraint algorithm to obtain the underlying nondegenerate dynamical system. If we let the $\nu_{R,P}$ denote the minimum number of DAE index reduction steps plus presymplectic constraint algorithm iterations necessary to take an index ν DAE and obtain the underlying nondegenerate Hamiltonian system associated with the adjoint, we have $\nu_{R,P} \leq \nu$.

Remark 3.2.17. *Note that we could have reduced the index ν DAE to an explicit ODE after ν reduction steps, and subsequently, formed the adjoint. While this is formally equivalent to the above procedure by Remark 3.2.14, we prefer to keep the DAE in index 1 form. This is especially preferable from the viewpoint of numerics: if one reduces an index 1 DAE to an ODE and attempts to apply a numerical integrator, it is generically the case that the discrete flow drifts off the constraint manifold. For this reason, it is preferable to develop numerical integrators for the index 1 adjoint DAE system directly to prevent constraint violation.*

Example 3.2.1 (Hessenberg Index 2 DAE)**.** *Consider a Hessenberg index 2 DAE, i.e., a DAE of* *the form*

$$\dot{q} = f(q,u),$$
$$0 = g(q),$$

where $(q,u) \in \mathbb{R}^n \times \mathbb{R}^m$*,* $f : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^n$*,* $g : \mathbb{R}^n \to \mathbb{R}^m$*, and* $\frac{\partial g}{\partial q}\frac{\partial f}{\partial u}$ *is pointwise invertible. We reduce this to an index 1 DAE* (2.11a)-(2.11b) *as follows. Let* $M_d = g^{-1}(\{0\})$ *be the dynamical configuration space which we will assume is a submanifold of* $\mathbb{R}^n$*. For example, this is true if g is a constant rank map. Furthermore, let* $M_a = \mathbb{R}^m$ *be the algebraic configuration space. To reduce the index, we differentiate the constraint* $g(q) = 0$ *with respect to time. This is equivalent to enforcing that the dynamics are tangent to* M_d*. This gives*

$$0 = \frac{\partial g^A(q)}{\partial q^i}\dot{q}^i = \frac{\partial g^A(q)}{\partial q^i} f^i(q,u) \equiv \phi^A(q,u).$$

Hence, we can form the semi-explicit index 1 system on $M_d \times M_a$ *given by*

$$\dot{q} = f(q,u),$$
$$0 = \phi(q,u).$$

The above system is an index 1 DAE since $\frac{\partial \phi}{\partial u} = \frac{\partial g}{\partial q}\frac{\partial f}{\partial u}$ *is pointwise invertible.*

We now form the adjoint DAE system associated with this index 1 DAE, (2.13a)-(2.13d).

Expressing the constraint in terms of g and f, instead of ϕ, gives

$$\dot{q}^i = f^i(q,u),$$
$$\dot{p}_j = -p_i \frac{\partial f^i(q,u)}{\partial q^j} - \lambda_A \left(\frac{\partial^2 g^A(q)}{\partial q^j \partial q^i} f^i(q,u) + \frac{\partial g^A(q)}{\partial q^i} \frac{\partial f^i(q,u)}{\partial q^j} \right),$$
$$0 = \frac{\partial g^A(q)}{\partial q^i} f^i(q,u),$$
$$0 = p_i \frac{\partial f^i(q,u)}{\partial u^a} + \lambda_A \left(\frac{\partial g^A(q)}{\partial q^i} \frac{\partial f^i(q,u)}{\partial u^a} \right).$$

We can then apply one iteration of the presymplectic constraint algorithm, as discussed above in the index $\nu = 1$ case, to obtain the underlying nondegenerate Hamiltonian dynamics. Restricting to the primary constraint manifold, using the first constraint equation to solve for $u = u(q)$ by the implicit function theorem and subsequently, using the second constraint equation to solve for $\lambda = \lambda(q,p)$ by inverting $\left(\frac{\partial g}{\partial q}\frac{\partial f}{\partial u}\right)^T$, gives the Hamiltonian system

$$\dot{q}'^i = f^i(q', u(q')),$$
$$\dot{p}'_j = -p'_i \frac{\partial f^i(q', u(q'))}{\partial q^j} - \lambda_A(q',p') \left(\frac{\partial^2 g^A(q')}{\partial q^j \partial q^i} f^i(q', u(q')) + \frac{\partial g^A(q')}{\partial q^i} \frac{\partial f^i(q', u(q'))}{\partial q^j} \right).$$

Adjoint Systems for DAEs with Augmented Hamiltonians

In Section 3.2.2, we augmented the adjoint ODE Hamiltonian by some function L. In this section, we do analogously for the adjoint DAE system.

To begin, let $H(q,u,p,\lambda) = \langle p, f(q,u)\rangle + \langle \lambda, \phi(q,u)\rangle$ be the Hamiltonian on the generalized phase space bundle corresponding to the DAE $\dot{q} = f(q,u)$, $0 = \phi(q,u)$, and let $L : M_d \times M_a \to \mathbb{R}$ be the function that we would like to augment. We identify L with its pullback through $\overline{T^*M}_d \oplus \Phi^* \to M_d \times M_a$. Then, we define the augmented Hamiltonian

$$H_L \equiv H + L : \overline{T^*M}_d \oplus \Phi^* \to \mathbb{R}$$
$$(q,u,p,\lambda) \mapsto H(q,u,p,\lambda) + L(q,u).$$

We define the augmented adjoint DAE system as the presymplectic system

$$i_{X_{H_L}}\Omega_0 = dH_L. \tag{2.15}$$

A direct calculation yields the coordinate expression, along an integral curve of such a (generally, partially-defined) vector field X_{H_L},

$$\dot{q}^i = f^i(q,u), \tag{2.16a}$$
$$\dot{p}_j = -p_i \frac{\partial f^i}{\partial q^j} - \lambda_A \frac{\partial \phi^A}{\partial q^j} - \frac{\partial L}{\partial q^j}, \tag{2.16b}$$
$$0 = \phi^A(q,u), \tag{2.16c}$$
$$0 = p_i \frac{\partial f^i}{\partial u^a} + \lambda_A \frac{\partial \phi^A}{\partial u^a} + \frac{\partial L}{\partial u^a}. \tag{2.16d}$$

Remark 3.2.18. *Observe that if the base DAE* (2.11a)-(2.11b) *has index 1, then the above system has index 1 by the exact same argument given in the nonaugmented case. After reduction by applying the presymplectic constraint algorithm and solving for u as a function of q and λ as a function of (q,p), the underlying nondegenerate Hamiltonian system on the primary (final) constraint manifold corresponds to the Hamiltonian*

$$(H_L)_1(q',p') = \langle p', f(q',u(q'))\rangle + L(q',u(q')),$$

which is the adjoint Hamiltonian for the ODE $\dot{q}' = f(q',u(q'))$, augmented by $L(q',u(q'))$.

However, as we will discuss in Section 3.3.3, it is not uncommon in optimal control *problems for $\partial\phi/\partial u$ to be singular, but the presence of $\int L dt$ in the minimization objective may uniquely specify the singular degrees of freedom.*

We now prove an analogous proposition to Proposition 3.2.9, modified by the presence of L in the Hamiltonian. We again consider the variational equations (2.14a)-(2.14d) associated with the base DAE (2.11a)-(2.11b), which for simplicity we express in matrix derivative notation as

$$\dot{q} = f(q,u), \tag{2.17a}$$

$$0 = \phi(q,u), \tag{2.17b}$$

$$\frac{d}{dt}\delta q = D_q f(q,u)\delta q + D_u f(q,u)\delta u, \tag{2.17c}$$

$$0 = D_q \phi(q,u)\delta q + D_u \phi(q,u)\delta u. \tag{2.17d}$$

Proposition 3.2.10. *For a solution (q,u,p,λ) of the augmented adjoint DAE system* (2.16a)-(2.16d) *and a solution $(q,u,\delta q,\delta u)$ of the variational equations* (2.17a)-(2.17d)*, covering the same solution (q,u) of the base DAE* (2.11a)-(2.11b)*,*

$$\frac{d}{dt}\langle p,\delta q\rangle = -\langle \nabla_q L,\delta q\rangle - \langle \nabla_u L,\delta u\rangle. \tag{2.18}$$

Proof. This follows from a direct computation:

$$\begin{aligned}
\frac{d}{dt}\langle p,\delta q\rangle &= \langle \dot{p},\delta q\rangle + \langle p,\frac{d}{dt}\delta q\rangle \\
&= -\langle [D_q f]^* p,\delta q\rangle - \langle [D_q\phi]^*\lambda,\delta q\rangle - \langle \nabla_q L,\delta q\rangle + \langle p,D_q f\delta q\rangle + \langle p,D_u f\delta u\rangle \\
&= -\langle \lambda,D_q\phi\delta q\rangle - \langle \nabla_q L,\delta q\rangle + \langle p,D_u f\delta u\rangle \\
&= \langle \lambda,D_u\phi\delta u\rangle - \langle \nabla_q L,\delta q\rangle + \langle p,D_u f\delta u\rangle \\
&= -\langle \nabla_q L,\delta q\rangle + \langle [D_u\phi]^*\lambda + [D_u f]^* p,\delta u\rangle \\
&= -\langle \nabla_q L,\delta q\rangle - \langle \nabla_u L,\delta u\rangle,
\end{aligned}$$

where in the fourth equality above we used (2.17d) and in the sixth equality above we used (2.16d). □

Remark 3.2.19. *Analogous to the ODE case discussed in Remark 3.2.7, we remark that for the nonaugmented adjoint DAE system* (2.13a)-(2.13d)*, we have preservation of* $\langle p, \delta q \rangle$ *by virtue of presymplecticity. On the other hand, for the augmented adjoint DAE system, despite preserving the same presymplectic form, the change of* $\langle p, \delta q \rangle$ *now measures the change in L with respect to variations in q and u. This can be understood from the fact that the adjoint equations for* (p, λ) *in the nonaugmented case,* (2.13b) *and* (2.13d)*, are linear in* (p, λ)*, so that one can identify first variations in* (p, λ) *with* (p, λ)*; whereas, in the augmented case, equations* (2.16b) *and* (2.16d) *are affine in* (p, λ)*, so such an identification cannot be made. Furthermore, the failure of* (2.16b) *and* (2.16d) *to be linear in* (p, λ) *are given precisely by* $\nabla_q L$ *and* $\nabla_u L$*, respectively. Thus, in the augmented case, this leads to the additional terms* $-\langle \nabla_u L, \delta q \rangle - \langle \nabla_q L, \delta u \rangle$ *in equation* (2.18).

3.2.4 An Intrinsic Type II Variational Principle for Adjoint Systems

We now show that the adjoint system (2.9) arises from an intrinsic Type II variational principle. In coordinates, the type II variational principle corresponds to fixed initial position $q(t_0) = q_0$ and fixed final momenta $p(t_1) = p_1$, which are the boundary conditions used in adjoint sensitivity analysis, as we will discuss in Section 3.3.1.

Consider the augmented adjoint system

$$\dot{q} = \partial H_L / \partial p = f(q),$$
$$\dot{p} = -\partial H_L / \partial q = -[Df(q)]^* p - dL(q),$$

where H_L is the augmented Hamiltonian. Recall that H_L is intrinsically defined by $H_L = i_{\widehat{f}} \Theta + \pi_{T^*M}^* L$, where Θ is the tautological one-form on T^*M, $\pi_{T^*M} : T^*M \to M$ is the cotangent bundle projection, and $L : M \to \mathbb{R}$.

We would like to show that the above system arises from a variational principle. We consider the action

$$S[\psi] = \int_{t_0}^{t_1} \psi^* (\Theta - H_L\, dt),$$

where $\psi : (t_0, t_1) \to T^*M$ is a curve on T^*M.

In order to derive the augmented adjoint system from a variational principle, we have to place boundary conditions on the curve ψ. Note that Type I boundary conditions, given by fixing the position endpoints, $\pi_{T^*M}(\psi(t_0)) = q_0$ and $\pi_{T^*M}(\psi(t_1)) = q_1$, are in general incompatible with the adjoint system. To see this, recall that the augmented adjoint system lifts an ODE on M, given by $\dot{q} = f(q)$. For the base ODE on M, once one specifies $q(t_0) = q_0$, this determines $q(t_1)$ as $q(t_1) = \Phi_{t_1 - t_0}(q(t_0))$, where Φ_t denotes the time-t flow of f, assuming that the flow Φ_t is defined for time $t = t_1 - t_0$. Thus, one cannot in general impose boundary conditions for q at two different times for the base ODE on M. Since the adjoint system lifts this ODE to an ODE on T^*M, it follows that one cannot in general place Type I boundary conditions for the adjoint system.

On the other hand, Type II boundary conditions, $q(t_0) = q_0$ and $p(t_1) = p_1$, do not have the aforementioned inconsistency. However, Type II boundary conditions for Hamiltonian systems, in general, suffer the drawback that they do not make intrinsic sense on a manifold, since one cannot specify a covector $p(t_1) = p_1$ without specifying the basepoint $q(t_1)$. Fortunately, for Hamiltonian systems which are adjoint systems, Type II boundary conditions do make intrinsic sense, due to the fact they cover an ODE on the base manifold M. To see this, if we fix the boundary condition $q(t_0) = q_0$, the time $t_1 - t_0$ flow of f, assuming it exists for this time, fixes the basepoint $q(t_1) = \Phi_{t_1 - t_0}(q(t_0))$. In terms of the curve ψ, this means that once we fix $\pi_{T^*M}(\psi(t_0)) = q_0$, we have $\psi(t_1) \in T^*_{q(t_1)}M$, where $q(t_1) = \Phi_{t_1 - t_0}(q(t_0))$. Thus, it then makes sense to specify a boundary condition on $\psi(t_1) \in T^*_{q(t_1)}M$ of the form $\psi(t_1) = p_1$, for any $p_1 \in T^*_{q(t_1)}M$. Figure 3.2 illustrates Type II boundary conditions for an adjoint system; the flow of f on the base manifold evolves the initial condition q_0 forward to q_1 and subsequently, the vertical component of the lifted vector field X_{H_L} evolves the final momenta p_1, based at q_1, backwards to the initial momenta p_0. As we will see in Section 3.3.1, p_1 can be chosen by taking $p_1 = dC|_{q_1}$ to compute the sensivity of a terminal cost function $C : M \to \mathbb{R}$ with a non-augmented Hamiltonian $H_L = H$ or by taking $p_1 = 0$ to compute the sensivity of a running cost function L with an augmented Hamiltonian $H_L = H + L$.

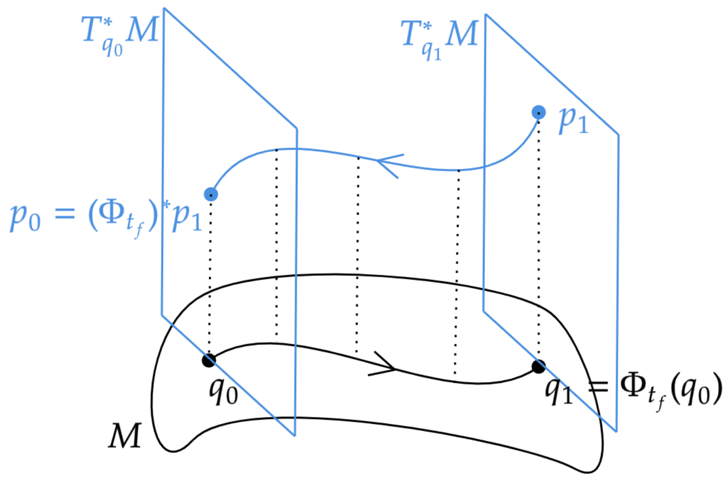


Figure 3.2. Type II boundary conditions for adjoint systems

Remark 3.2.20. *It is interesting to note that the reason for which Type I boundary conditions for adjoint systems are generally inconsistent (namely, that they cover an ODE on the base manifold) is precisely the reason that one can make intrinsic sense of Type II boundary conditions for adjoint systems. That is, Type II boundary conditions are consistent while Type I boundary conditions are generally inconsistent precisely because an adjoint system is a Hamiltonian system which covers an ODE on the base manifold. Conversely, every Hamiltonian system on T^*M which covers an ODE on the base manifold M is locally an adjoint system. To see this, if a Hamiltonian system covers an ODE on the base manifold, then Hamilton's equation in the position variable $\dot{q} = \partial H/\partial p$ must equal $f(q)$ for some vector field f on M. Thus, we have*

$\partial H/\partial p = f(q)$. *Integrating this equation yields a coordinate expression for the Hamiltonian*

$$H(q,p) = \langle p, f(q)\rangle + L(q),$$

where the "constant of integration" (constant with respect to the p variable) $L(q)$ is some arbitrary function of q. This is precisely the form of the Hamiltonian for an augmented adjoint system.

To state an intrinsic Type II variational principle for adjoint systems, we regard the integrand of the above action (before pulling back by ψ) as a contact form on the extended phase space $I \times T^*M$. Namely, given an interval $I = (t_0,t_1) \subset \mathbb{R}$, $t_0 \neq t_1$, let $\pi_{I\times T^*M} : I \times T^*M \to T^*M$ denote the projection onto the second factor. Then, define the contact form

$$\Theta_H = \pi^*_{I\times T^*M}\Theta - Hdt,$$

where we have identified $H : T^*M \to \mathbb{R}$ with its pullback through $\pi_{I\times T^*M}$. In coordinates, $\Theta_H(q,p) = pdq - Hdt$. Additionally, we define the presymplectic form $\Omega_H = -d\Theta_H$. Furthermore, we identify curves on T^*M, of the form $\psi : I \to T^*M$, with curves on $I \times T^*M$ which cover the identity on I; in coordinates, this identification reads $\psi(t) = (t,q(t),p(t))$. The above action can then be expressed

$$S[\psi] = \int_I \psi^*\Theta_H.$$

To enforce Type II boundary conditions $\pi_{T^*Q}(\psi(t_0)) = q_0 \in M$ and $\psi(t_1) = p_1 \in T^*_{q_1}M$ where $q_1 = \Phi_{t_1-t_0}(q_0)$, we define the space of admissible variations with respect to these boundary conditions as the space of vector fields X on T^*M (identified with vertical vector fields on $I \times T^*M \to T^*M$) such that $(T\pi_{T^*M}X)(q_0) = 0$ and $X(\psi_1) = 0$, where $\psi_1 = (q_1, p_1) \in T^*_{q_1}M$. Intuitively, the first condition states that an admissible variation does not vary the initial position $q(t_0) = q_0$, whereas the second condition states that an admissible variation does not vary the final momenta ψ_1.

Proposition 3.2.11. *Fix an interval $I = (t_0, t_1) \subset \mathbb{R}$, $t_0 \neq t_1$. Consider the above augmented Hamiltonian, where we assume that the time $t_1 - t_0$ flow of the vector field f exists. Let $q_0 \in M$ and let $p_1 \in T^*_{q_1}M$ where $q_1 = \Phi_{t_1-t_0}(q_0)$. Then, the augmented adjoint system with Type II boundary conditions*

$$\begin{aligned} \dot{q} &= f(q), \\ \dot{p} &= -[Df(q)]^* p - dL(q), \\ q(t_0) &= q_0, \\ p(t_1) &= p_1, \end{aligned}$$

is intrinsically given by the variation principle: enforce the stationarity of the action

$$S[\psi] = \int_I \psi^* \Theta_H$$

with respect to admissible variations.

Proof. Let φ_ε denote the time-ε flow of an admissible variation X. Then, the variation principle for the action with respect to admissible variations is given by

$$\begin{aligned} 0 = dS[\psi] \cdot X = \frac{d}{d\varepsilon}\Big|_{\varepsilon=0} S[\varphi_\varepsilon \circ \psi] &= \int_I \psi^* \frac{d}{d\varepsilon}\Big|_0 \varphi_\varepsilon^* \Theta_H = \int_I \psi^* \mathscr{L}_X \Theta_H \\ = -\int_I \psi^*(i_X \Omega_H) + \int_I \psi^* d(i_X \Theta_H) &= -\int_I \psi^*(i_X \Omega_H) + \int_I d(\psi^* i_X \Theta_H). \end{aligned}$$

Observe that the boundary term $\int_I d(\psi^* i_X \Theta_H) = (\psi^* i_X \Theta_H)(t_1) - (\psi^* i_X \Theta_H)(t_0)$ vanishes by the fact that X is an admissible variation since $(\psi^* i_X \Theta_H)(t) = \langle p(t), (T\pi_{T^*M} X)(q(t))\rangle$. Hence, the stationarity condition is given by

$$\int_I \psi^*(i_X \Omega_H) = 0.$$

By the fundamental lemma of the calculus of variations, we have $\psi^*(i_X \Omega_H) = 0$, whose coordinate expression is precisely the adjoint system. □

Remark 3.2.21. *In our definition of the space of admissible variations, we set the conditions that the variation at q_0 is purely vertical, $(T\pi_{T^*M}X)(q_0) = 0$, whereas at q_1, we enforced that the variation is zero, $X(q_1, p_1) = 0$. In coordinates where*

$$X = \delta q \frac{\partial}{\partial q} + \delta p \frac{\partial}{\partial p},$$

the first condition reads $\delta q_0 = 0$ and the second condition reads $\delta q_1 = 0$, $\delta p_1 = 0$. It would thus seem that we are enforcing an overdetermined set of three boundary conditions $q(t_0) = q_0$, $q(t_1) = q_1$, $p(t_1) = p_1$. However, the resolution is that the variations δq_0 and δq_1 are not independent; fixing one to zero sets the other one to zero, by virtue of the fact that the adjoint system covers an ODE on M. Thus, with the chosen variational principle, we are only setting two independent boundary conditions, $q(t_0) = q_0, p(t_1) = p_1$.

Furthermore, in the above proof, by looking at the coordinate expression of the boundary term,

$$\psi^* i_X \Theta_H \Big|_{t_0}^{t_1} = \langle p(t_1), \delta q(t_1) \rangle - \langle p(t_0), \delta q(t_0) \rangle,$$

we see that we only used $\delta q_0 = 0$, $\delta q_1 = 0$. We did not need that $\delta p_1 = 0$ for the boundary terms to vanish. However, without setting $\delta p_1 = 0$, we only have the system

$$\begin{aligned} \dot{q} &= f(q), \\ \dot{p} &= -[Df(q)]^* p - dL(q), \\ q(t_0) &= q_0. \end{aligned}$$

Hence, this system is underdetermined; any curve $p(t)$ in the fibers of T^*M satisfying

$$\dot{p} = -[Df(q)]^* p - dL(q)$$

would suffice. Thus, to uniquely fix the system, we must also supply a boundary condition of the form $p(t_1) = p_1$. Thus, even though the condition $\delta p_1 = 0$ is not strictly necessary in the variational principle to derive the equations of motion, it is necessary to fix the curve $p(t)$ in the fibers that define the adjoint system with Type II boundary conditions.

Analogously the adjoint DAE system (2.16a)-(2.16d), for index 1 DAEs, can be derived by an intrinsic Type II variational principle, by considering variations V of the action

$$S[\psi] = \int_{t_0}^{t_1} pdq - (H(q,u,p,\lambda) + L(q,u))dt$$

such that $T\Pi_q V|_{t_0} = 0$ and $T\Pi_{(q,p)} V|_{t_1} = 0$ where $\Pi_q : (q,u,p,\lambda) \mapsto q$ and $\Pi_{(q,p)} : (q,u,p,\lambda) \mapsto (q,p)$ are the canonical bundle projections on $\overline{T^*M}_d \oplus \Phi^*$.

Remark 3.2.22. *We will use the Type II variational structures associated with the adjoint ODE and adjoint DAE systems to construct numerical integrators in Section 3.3.2.*

3.3 Applications

3.3.1 Adjoint Sensitivity Analysis for Semi-explicit Index 1 DAEs

In this section, we discuss how one can utilize adjoint systems to compute sensitivities. We will split this into four cases; namely, we want to compute sensitivities for ODEs or DAEs (we will focus on index 1 DAEs), and whether we are computing the sensitivity of a terminal cost or the sensitivity of a running cost.

The relevant adjoint system used to compute sensitivities in all four cases is summarized in Table 3.1.

Note that in our calculations below, the top row (the ODE case) can be formally obtained from the bottom row (the DAE case) simply by ignoring the algebraic variables (u,λ) and letting the constraint function ϕ be identically zero. Thus, we will focus on the bottom row, i.e., computing sensitivities of a terminal cost function and of a running cost function, subject to a

Table 3.1. Adjoint systems for sensitivity analysis of terminal and running cost functions subject to the dynamics of an ODE or DAE.

	Terminal Cost	Running Cost
ODE	Adjoint ODE System (2.6a)-(2.6b)	Augmented Adjoint ODE System (2.10a)-(2.10b)
DAE	Adjoint DAE System (2.13a)-(2.13d)	Augmented Adjoint DAE System (2.16a)-(2.16d)

DAE constraint. In both cases, we will first show how the adjoint sensitivity can be derived using a traditional variational argument. Subsequently, we will show how the adjoint sensitivity can be derived more simply by using Propositions 3.2.9 and 3.2.10.

Adjoint Sensitivity of a Terminal Cost. Consider the DAE $\dot{q} = f(q,u)$, $0 = \phi(q,u)$ as in Section 3.2.3. We will assume that M_d is a vector space and additionally, that the DAE has index 1. We would like to extract the gradient of a terminal cost function $C(q(t_f))$ with respect to the initial condition $q(0) = \alpha$, i.e., we want to extract the sensitivity of $C(q(t_f))$ with respect to an infinitesimal perturbation in the initial condition, given by $\nabla_\alpha C(q(t_f))$. Consider the functional J defined by

$$J = C(q(t_f)) - \langle p_0, q(0) - \alpha \rangle - \int_0^{t_f} [\langle p, \dot{q} - f(q,u) \rangle - \langle \lambda, \phi(q,u) \rangle] dt.$$

Observe that for (q,u) satisfying the given DAE with initial condition $q(0) = \alpha$, J coincides with $C(q(t_f))$. We think of p_0 as a free parameter. For simplicity, we will use matrix derivative notation instead of indices. Computing the variation of J yields

$$\begin{aligned}\delta J = {} & \langle \nabla_q C(q(t_f)), \delta q(t_f) \rangle - \langle p_0, \delta q(0) - \delta\alpha \rangle \\ & - \int_0^{t_f} \Big[\langle p, \frac{d}{dt}\delta q - D_q f(q,u)\delta q \rangle \\ & \qquad - \langle p, D_u f(q,u)\delta u \rangle - \langle \lambda, D_q \phi(q,u)\delta q + D_u \phi(q,u)\delta u \rangle \Big] dt.\end{aligned}$$

Integrating by parts in the term containing $\frac{d}{dt}\delta q$ and restricting to a solution (q,u,p,λ) of the adjoint DAE system (2.13a)-(2.13d) yields

$$\delta J = \langle \nabla_q C(q(t_f)) - p(t_f), \delta q(t_f) \rangle - \langle p_0, \delta \alpha \rangle + \langle p(0) - p_0, \delta q(0) \rangle.$$

We enforce the endpoint condition $p(t_f) = \nabla_q C(q(t_f))$ and choose $p_0 = p(0)$, which yields

$$\delta J = \langle p(0), \delta \alpha \rangle.$$

Hence, the sensitivity of $C(q(t_f))$ is given by

$$p(0) = \nabla_\alpha J = \nabla_\alpha C(q(t_f)),$$

with initial condition $q(0) = \alpha$ and terminal condition $p(t_f) = \nabla_q C(q(t_f))$. Thus, the adjoint sensitivity can be computed by setting the terminal condition on $p(t_f)$ above and subsequently, solving for the momenta p at time 0. In order for this to be well-defined, we have to verify that the given initial and terminal conditions lie on the primary constraint manifold P_1. However, as discussed in Section 3.2.3, since the DAE has index 1, we can always solve for the algebraic variables $u = u(q)$ and $\lambda = \lambda(q, p)$ and thus, we are free to choose the initial and terminal values of q and p, respectively. For higher index DAEs, one has to ensure that these conditions are compatible with the final constraint manifold. For example, this is done in [26] in the case of Hessenberg index 2 DAEs. Alternatively, at least theoretically, for higher index DAEs, one can reduce the DAE to an index 1 DAE and then the above discussion applies, however, this reduction may fail in practice due to numerical cancellation.

Note that the above adjoint sensitivity result is also a consequence of the preservation of the quadratic invariant $\langle p, v \rangle$ as in Proposition 3.2.9. From this proposition, one has that

$$\langle p(t_f), \delta q(t_f) \rangle = \langle p(0), \delta q(0) \rangle,$$

where δq satisfies the variational equations. Setting $p(t_f) = \nabla_q C(q(t_f))$ and $\delta q(0) = \delta\alpha$ gives the same result. As mentioned in Remark 3.2.12, this quadratic invariant arises from the presymplecticity of the adjoint DAE system. Thus, a numerical integrator which preserves the presymplectic structure is desirable for computing adjoint sensitivities, as it exactly preserves the quadratic invariant that allows the adjoint sensitivities to be accurately and efficiently computed. We will discuss this in more detail in Section 3.3.2.

Adjoint Sensitivity of a Running Cost. Again, consider an index 1 DAE $\dot{q} = f(q,u)$, $0 = \phi(q,u)$. We would like to extract the sensitivity of a running cost function

$$\int_0^{t_f} L(q,u)dt,$$

where $L : M_d \times M_a \to \mathbb{R}$, with respect to an infinitesimal perturbation in the initial condition $q(0) = \alpha$. Consider the functional J defined by

$$J = -\langle p_0, q(0) - \alpha\rangle + \int_0^{t_f} [L(q,u) + \langle p, f(q,u) - \dot{q}\rangle + \langle \lambda, \phi(q,u)\rangle]dt.$$

Observe that when the DAE is satisfied with initial condition $q(0) = \alpha$, $J = \int_0^{t_f} Ldt$. Now, we would to compute the implicit change in $\int_0^{t_f} Ldt$ with respect to a perturbation $\delta\alpha$ in the initial condition. Taking the variation in J yields

$$\begin{aligned}
\delta J = &-\langle p_0, \delta q(0) - \delta\alpha\rangle \\
&+ \int_0^{t_f} \Big[\langle \nabla_q L, \delta q\rangle + \langle \nabla_u L, \delta u\rangle + \langle p, D_q f \delta q - \frac{d}{dt}\delta q\rangle \\
&\qquad + \langle p, D_u f \delta u\rangle + \langle \lambda, D_q\phi\delta q + D_u\phi\delta u\rangle\Big] dt \\
= &-\langle p_0, \delta q(0) - \delta\alpha\rangle - \langle p(t_f), \delta q(t_f)\rangle + \langle p(0), \delta q(0)\rangle \\
&+ \int_0^{t_f} \Big[\langle \nabla_q L + [D_q f]^* p + [D_q\phi]^*\lambda + \dot{p}, \delta q\rangle + \langle \nabla_u L + [D_u f]^* p + [D_u\phi]^*\lambda, \delta u\rangle\Big] dt.
\end{aligned}$$

Restricting to a solution (q,u,p,λ) of the augmented adjoint DAE system (2.16a)-(2.16d), setting the terminal condition $p(t_f) = 0$, and choosing $p_0 = p(0)$ gives $\delta J = \langle p(0), \delta\alpha \rangle$. Hence, the implicit sensitivity of $\int_0^{t_f} L dt$ with respect to a change $\delta\alpha$ in the initial condition is given by

$$p(0) = \delta_\alpha J = \delta_\alpha \int_0^{t_f} L(q,u)dt.$$

Thus, the adjoint sensitivity of a running cost functional with respect to a perturbation in the initial condition can be computed by using the augmented adjoint DAE system (2.16a)-(2.16d) with terminal condition $p(t_f) = 0$ to solve for the momenta p at time 0.

Note that the above adjoint sensitivity result can be obtained from Proposition 3.2.10 as follows. We write equation (2.18) as

$$\frac{d}{dt}\langle p, \delta q \rangle = -\langle dL, (\delta q, \delta u) \rangle,$$

to highlight that the right hand side measures the total induced variation of L. Now, we integrate this equation from 0 to t_f, which gives

$$\langle p(t_f), \delta q(t_f) \rangle - \langle p(0), \delta q(0) \rangle = -\int_0^{t_f} \langle dL, (\delta q, \delta u) \rangle dt.$$

Since we want to determine the change in the running cost functional with respect to a perturbation in the initial condition, we set $p(t_f) = 0$ which yields

$$\langle p(0), \delta q(0) \rangle = \int_0^{t_f} \langle dL, (\delta q, \delta u) \rangle dt.$$

The right hand side is the total change induced on the running cost functional, whereas the left hand side tells us how this change is implicitly induced from a perturbation $\delta q(0)$ in the initial condition. Note that a perturbation in the initial condition $\delta q(0)$ will generally induce perturbations in both q and u, according to the variational equations. Such a curve $(\delta q, \delta u)$ satisfying the variational equations exists in the index 1 case as noted in Remark 3.2.13. Thus, we arrive at the same conclusion as the variational argument: $p(0)$ is the desired adjoint sensitivity.

To summarize, adjoint sensitivities for terminal and running costs can be computed using the properties of adjoint systems, such as the various aforementioned propositions regarding $\frac{d}{dt}\langle p, \delta q\rangle$, which is zero in the nonaugmented case and measures the variation of L in the augmented case. In the case of a terminal cost, one sets an inhomogeneous terminal condition $p(t_f) = \nabla_q C(q(t_f))$ and backpropagates the momenta through the nonaugmented adjoint DAE system (2.13a)-(2.13d) to obtain the sensitivity $p(0)$. On the other hand, in the case of a running cost, one sets a homogeneous terminal condition $p(t_f) = 0$ and backpropagates the momenta through the augmented adjoint DAE system (2.16a)-(2.16d) to obtain the sensitivity $p(0)$.

The various propositions used to derive the above adjoint sensitivity results are summarized in Table 3.2. We also include the ODE case, since it follows similarly.

Table 3.2. Quadratic adjoint variational conservation laws corresponding to adjoint sensitivity analysis of terminal and running cost functions subject to the dynamics of an ODE or DAE.

	Terminal Cost	Running Cost
ODE	Proposition 3.2.3, $\frac{d}{dt}\langle p, \delta q\rangle = 0$	Proposition 3.2.6, $\frac{d}{dt}\langle p, \delta q\rangle = -\langle dL, \delta q\rangle$
DAE	Proposition 3.2.9, $\frac{d}{dt}\langle p, \delta q\rangle = 0$	Proposition 3.2.10, $\frac{d}{dt}\langle p, \delta q\rangle = -\langle dL, (\delta q, \delta u)\rangle$

In Section 3.3.2, we will construct integrators that admit discrete analogues of the above propositions, and hence, are suitable for computing discrete adjoint sensitivities.

3.3.2 Structure-Preserving Discretizations of Adjoint Systems

In this section, we utilize the Galerkin Hamiltonian variational integrators of Leok and Zhang [76] to construct structure-preserving integrators which admit discrete analogues of Propositions 3.2.3, 3.2.6, 3.2.9, and 3.2.10, and are therefore suitable for numerical adjoint sensitivity analysis. For brevity, the proofs of these discrete analogues can be found in Appendix 3.6.1.

We start by recalling the construction of Galerkin Hamiltonian variational integrators as introduced in Leok and Zhang [76]. We assume that the base manifold Q is a vector space and thus, we have the identification $T^*Q \cong Q \times Q^*$. To construct a variational integrator for a Hamiltonian system on T^*Q, one starts with the exact Type II generating function

$$H^+_{d,\text{exact}}(q_0, p_1) = \text{ext}\left[\langle p_1, q_1\rangle - \int_0^{\Delta t} [\langle p, \dot{q}\rangle - H(q,p)]dt\right],$$

where one extremizes over C^2 curves on the cotangent bundle satisfying $q(0) = q_0, p(\Delta t) = p_1$. This is a Type II generating function in the sense that it defines a symplectic map $(q_0, p_1) \mapsto (q_1, p_0)$ by $q_1 = D_2 H^+_{d,\text{exact}}(q_0, p_1)$, $p_0 = D_1 H^+_{d,\text{exact}}(q_0, p_1)$.

To approximate this generating function, one approximates the integral above using a quadrature rule and extremizes the resulting expression over a finite-dimensional subspace satisfying the prescribed boundary conditions. This yields the Galerkin discrete Hamiltonian

$$H^+_d(q_0, p_1) = \text{ext}\left[\langle p_1, q_1\rangle - \Delta t \sum_i b_i \Big(\langle P^i, V^i\rangle - H(Q^i, P^i)\Big)\right],$$

where $\Delta t > 0$ is the timestep, q_0, q_1, p_0 and p_1 are numerical approximations to $q(0), q(\Delta t), p(0)$ and $p(\Delta t)$, respectively, $b_i > 0$ are quadrature weights corresponding to quadrature nodes $c_i \in [0,1]$, Q^i and P^i are internal stages representing $q(c_i\Delta t), p(c_i\Delta t)$, respectively, and V is related to Q by $Q^i = q_0 + \Delta t \sum_j a_{ij} V^j$, where the coefficients a_{ij} arise from the choice of function space. The expression above is extremized over the internal stages Q^i, P^i and subsequently, one applies the discrete right Hamilton's equations

$$q_1 = D_2 H^+_d(q_0, p_1),$$
$$p_0 = D_1 H^+_d(q_0, p_1),$$

to obtain a Galerkin Hamiltonian variational integrator. The extremization conditions and the discrete right Hamilton's equations can be expressed as

$$q_1 = q_0 + \Delta t \sum_i b_i D_p H(Q^i, P^i), \tag{3.1a}$$

$$Q^i = q_0 + \Delta t \sum_j a_{ij} D_p H(Q^j, P^j), \tag{3.1b}$$

$$p_1 = p_0 - \Delta t \sum_i b_i D_q H(Q^i, P^i), \tag{3.1c}$$

$$P^i = p_0 - \Delta t \sum_j \tilde{a}_{ij} D_q H(Q^i, P^i), \tag{3.1d}$$

where we interpret a_{ij} as Runge–Kutta coefficients and $\tilde{a}_{ij} = (b_i b_j - b_j a_{ji})/b_i$ as the symplectic adjoint of the a_{ij} coefficients. Thus, (3.1a)-(3.1d) can be viewed as a symplectic partitioned Runge–Kutta method.

We will consider such methods in four cases: adjoint systems corresponding to a base ODE or DAE, and whether or not the corresponding system is augmented. Note that in the DAE case, we will have to modify the above construction because the system is presymplectic. Furthermore, we will assume that all of the relevant configuration spaces are vector spaces.

Nonaugmented Adjoint ODE System. The simplest case to consider is the nonaugmented adjoint ODE system (2.6a)-(2.6b). Since the quadratic conservation law in Proposition 3.2.3,

$$\frac{d}{dt}\langle p, \delta q\rangle = 0,$$

arises from symplecticity, a structure-preserving discretization can be obtained by applying a symplectic integrator. This case is already discussed in Sanz-Serna [106], so we will only outline it briefly.

Applying the Galerkin Hamiltonian variational integrator (3.1a)-(3.1d) to the Hamiltonian for the adjoint ODE system, $H(q,p) = \langle p, f(q)\rangle$, yields

$$q_1 = q_0 + \Delta t \sum_i b_i f(Q^i), \tag{3.2a}$$

$$Q^i = q_0 + \Delta t \sum_j a_{ij} f(Q^j), \tag{3.2b}$$

$$p_1 = p_0 - \Delta t \sum_i b_i [Df(Q^i)]^* P^i, \tag{3.2c}$$

$$P^i = p_0 - \Delta t \sum_j \tilde{a}_{ij} [Df(Q^j)]^* P^j. \tag{3.2d}$$

In the setting of adjoint sensitivity analysis of a terminal cost function, the appropriate boundary condition to prescribe on the momenta is $p_1 = \nabla_q C(q(t_f))$, as discussed in Section 3.3.1.

Since the above integrator is symplectic, we have the symplectic conservation law,

$$dq_1 \wedge dp_1 = dq_0 \wedge dp_0,$$

when evaluated on discrete first variations of (3.2a)-(3.2d). In this setting, a discrete first variation can be identified with solutions of the linearization of (3.2a)-(3.2d). For the linearization of the equations in the position variables, (3.2a)-(3.2b), we have

$$\delta q_1 = \delta q_0 + \Delta t \sum_i b_i Df(Q^i) \delta Q^i, \tag{3.3a}$$

$$\delta Q^i = \delta q_0 + \Delta t \sum_j a_{ij} Df(Q^j) \delta Q^j. \tag{3.3b}$$

As observed in Sanz-Serna [106], while we obtained this by linearizing the discrete equations, one could also obtain this by first linearizing (2.1) and subsequently, applying the Runge–Kutta scheme to the linearization. For the linearization of the equations for the adjoint variables, (3.2c)-(3.2d), observe that they are already linear in the adjoint variables, so we can identify the linearization with itself. Thus, we can choose for first variations vector fields V as the first variation corresponding to the solution of the linearized position equation and W as the first variation corresponding to the solution of the adjoint equation itself. With these choices, the above symplectic conservation law yields

$$0 = dq_1 \wedge dp_1(V,W)|_{(q_1,p_1)} - dq_0 \wedge dp_0(V,W)|_{(q_0,p_0)} = \langle p_1, \delta q_1 \rangle - \langle p_0, \delta q_0 \rangle.$$

This is of course a discrete analogue of Proposition 3.2.3. Note that one can derive the conservation law $\langle p_1, \delta q_1 \rangle = \langle p_0, \delta q_0 \rangle$ directly by starting with the expression $\langle p_1, \delta q_1 \rangle$ and substituting the discrete equations where appropriate. We will do this in the more general augmented case below.

Augmented Adjoint ODE System. We now consider the case of the augmented adjoint ODE system (2.10a)-(2.10b). In the continuous setting, we have from Proposition 3.2.6,

$$\frac{d}{dt}\langle p, \delta q \rangle = -\langle dL, \delta q \rangle.$$

We would like to construct an integrator which admits a discrete analogue of this equation. To do this, we apply the Galerkin Hamiltonian variational integrator, equations (3.1a)-(3.1d), to the augmented Hamiltonian $H_L(q,p) = \langle p, f(q) \rangle + L(q)$. This gives

$$q_1 = q_0 + \Delta t \sum_i b_i f(Q^i), \tag{3.4a}$$

$$Q^i = q_0 + \Delta t \sum_j a_{ij} f(Q^j), \tag{3.4b}$$

$$p_1 = p_0 - \Delta t \sum_i b_i([Df(Q^i)]^* P^i + dL(Q^i)), \tag{3.4c}$$

$$P^i = p_0 - \Delta t \sum_j \tilde{a}_{ij}([Df(Q^j)]^* P^j + dL(Q^j)). \tag{3.4d}$$

We now prove a discrete analogue of Proposition 3.2.6. To do this, we again consider the discrete variational equations for the position variables, (3.3a)-(3.3b).

Proposition 3.3.1. *With the above notation, the above integrator satisfies*

$$\langle p_1, \delta q_1 \rangle = \langle p_0, \delta q_0 \rangle - \Delta t \sum_i b_i \langle dL(Q^i), \delta Q^i \rangle. \tag{3.5}$$

Proof. See Appendix 3.6.1. □

Remark 3.3.1. *To see that this is a discrete analogue of $\frac{d}{dt}\langle p, \delta q \rangle = -\langle dL, \delta q \rangle$, we write it in integral form as*

$$\langle p_1, \delta q_1 \rangle = \langle p_0, \delta q_0 \rangle - \int_0^{\Delta t} \langle dL(q), \delta q \rangle dt.$$

Then, applying the quadrature rule on $[0, \Delta t]$ given by quadrature weights $b_i \Delta t$ and quadrature nodes $c_i \Delta t$, the above integral is approximated by

$$\int_0^{\Delta t} \langle dL(q), \delta q \rangle dt \approx \Delta t \sum_i b_i \langle dL(q(c_i \Delta t)), \delta q(c_i \Delta t) \rangle = \Delta t \sum_i b_i \langle dL(Q^i), \delta Q^i \rangle,$$

which yields equation (3.5)*. The discrete analogue is natural in the sense that the quadrature rule for which the discrete equation* (3.5) *approximates the continuous equation is the same as the quadrature rule used to approximate the exact discrete generating function. This occurs more generally for such Hamiltonian variational integrators, as noted in Tran and Leok [112] for the more general setting of multisymplectic Hamiltonian variational integrators.*

For adjoint sensitivity analysis of a running cost $\int L dt$, the appropriate boundary condition to prescribe on the momenta is $p_1 = 0$, as discussed in Section 3.3.1. With such a boundary condition, equation (3.5) reduces to

$$\langle p_0, \delta q_0 \rangle = \Delta t \sum_i b_i \langle dL(Q^i), \delta Q^i \rangle.$$

Thus, p_0 gives the discrete sensitivity, i.e., the change in the quadrature approximation of $\int L dt$ induced by a change in the initial condition along a discrete solution trajectory. One can compute this quantity directly via the direct method, where one needs to integrate the discrete variational equations for every desired search direction δq_0. On the other hand, by the above proposition, one can compute this quantity using the adjoint method: one integrates the adjoint equation with $p_1 = 0$ once to compute p_0 and subsequently, pair p_0 with any search direction δq_0 to obtain the sensitivity in that direction. By the above proposition, both methods give the same sensitivities. However, assuming the search space has dimension $n > 1$, the adjoint method is more efficient since it only requires $\mathscr{O}(1)$ integrations and $\mathscr{O}(n)$ vector-vector products, whereas the direct method requires $\mathscr{O}(n)$ integrations and $\mathscr{O}(ns)$ vector-vector products where $s \geq 1$ is the number of Runge–Kutta stages, since, in the direct method, one has to compute $\langle dL(Q^i), \delta Q^i \rangle$ for each i and for each choice of δq_0.

Nonaugmented Adjoint DAE System. We will now construct discrete Hamiltonian variational integrators for the adjoint DAE system (2.13a)-(2.13d), where we assume that the base DAE has index 1. To construct such a method, we have to modify the Galerkin Hamiltonian variational integrator (3.1a)-(3.1d), so that it is applicable to the presymplectic adjoint DAE system.

First, consider a general presymplectic system $i_X \Omega' = dH$. Note that, locally, any presymplectic system can be transformed to the canonical form (see, Cariñena et al. [27]),

$$
\begin{aligned}
\dot{q} &= D_p H(q,p,r), \\
\dot{p} &= -D_q H(q,p,r), \\
0 &= D_r H(q,p,r),
\end{aligned}
$$

where, in these coordinates, $\Omega' = dq \wedge dp$, so that $\ker(\Omega') = \operatorname{span}\{\partial/\partial r\}$. The action for this system is given by $\int_0^{\Delta t} (\langle p, \dot{q} \rangle - H(q,p,r)) dt$. We approximate this integral by quadrature, introduce internal stages for q, p as before, and additionally introduce internal stages $R^i = r(c_i h)$.

This gives the discrete generating function

$$H_d^+(q_0,p_1) = \text{ext}\Big[\langle p_1, q_1\rangle - \Delta t \sum_i b_i \left(\langle P^i, V^i\rangle - H(Q^i,P^i,R^i)\right)\Big],$$

where again V is related to the internal stages of Q by $Q^i = q_0 + \Delta t \sum_j a_{ij} V^j$ and the above expression is extremized over the internal stages Q^i, P^i, R^i. The discrete right Hamilton's equations are again given by

$$q_1 = H_d^+(q_0,p_1),\ p_0 = H_d^+(q_0,p_1),$$

which we interpret as the evolution equations of the system. There are no evolution equations for r due to the presymplectic structure and the absence of derivatives of r in the action. This gives the integrator

$$q_1 = q_0 + \Delta t \sum_i b_i D_p H(Q^i,P^i,R^i), \tag{3.6a}$$

$$Q^i = q_0 + \Delta t \sum_j a_{ij} D_p H(Q^i,P^i,R^i), \tag{3.6b}$$

$$p_1 = p_0 - \Delta t \sum_i b_i D_q H(Q^i,P^i,R^i), \tag{3.6c}$$

$$P^i = p_0 - \Delta t \sum_j \tilde{a}_{ij} D_q H(Q^i,P^i,R^i), \tag{3.6d}$$

$$0 = D_r H(Q^i,P^i,R^i), \tag{3.6e}$$

where (3.6b), (3.6d), (3.6e) arise from extremizing with respect to P^i, Q^i, R^i, respectively, while (3.6a) and (3.6c) arise from the discrete right Hamilton's equations. This integrator is presymplectic, in the sense that

$$dq_1 \wedge dp_1 = dq_0 \wedge dp_0,$$

when evaluated on discrete first variations. The proof is formally identical to the symplectic case. For this reason, we refer to (3.6a)-(3.6e) as a presymplectic Galerkin Hamiltonian variational integrator.

Remark 3.3.2. *In general, the system* (3.6a)-(3.6e) *evolves on the primary constraint manifold given implicitly by the zero level set of D_rH, however, it may not evolve on the final constraint manifold. This is not an issue for us since we are dealing with adjoint DAE systems for index 1 DAEs, for which we know the primary constraint manifold and the final constraint manifold coincide. For the general case, one may need to additionally differentiate the constraint equation $D_rH = 0$ to obtain hidden constraints.*

Thus, the method (3.6a)-(3.6e) *is generally only applicable to index 1 presymplectic systems, unless we add in further hidden constraints. In order for the continuous presymplectic system to have index 1, it is sufficient that the Hessian of H with respect to the algebraic variables, D_r^2H, is (pointwise) invertible on the primary constraint manifold. This is the case for the adjoint DAE system corresponding to an index 1 DAE.*

We now specialize to the adjoint DAE system (2.13a)-(2.13d), corresponding to an index 1 DAE, which is already in the above canonical form with $r = (u, \lambda)$ and $H(q,u,p,\lambda) = \langle p, f(q,u)\rangle + \langle \lambda, \phi(q,u)\rangle$. Note that we reordered the argument of H, $(q,p,r) = (q,p,u,\lambda) \to (q,u,p,\lambda)$, in order to be consistent with the previous notation used throughout. We label the internal stages for the algebraic variables as $R^i = (U^i, \Lambda^i)$. Applying the presymplectic Galerkin

Hamiltonian variational integrator to this particular system yields

$$q_1 = q_0 + \Delta t \sum_i b_i f(Q^i, U^i), \tag{3.7a}$$

$$Q^i = q_0 + \Delta t \sum_j a_{ij} f(Q^j, U^j), \tag{3.7b}$$

$$p_1 = p_0 - \Delta t \sum_i b_i \left([D_q f(Q^i, U^i)]^* P^i + [D_q \phi(Q^i, U^i)]^* \Lambda^i \right), \tag{3.7c}$$

$$P^i = p_0 - \Delta t \sum_j \tilde{a}_{ij} \left([D_q f(Q^j, U^j)]^* P^j + [D_q \phi(Q^j, U^j)]^* \Lambda^j \right), \tag{3.7d}$$

$$0 = \phi(Q^i, U^i), \tag{3.7e}$$

$$0 = [D_u f(Q^i, U^i)]^* P^i + [D_u \phi(Q^i, U^i)]^* \Lambda^i, \tag{3.7f}$$

where (3.7b), (3.7d), (3.7e), (3.7f) arise from extremizing over P^i, Q^i, Λ^i, U^i, respectively, while (3.7a), (3.7c) arise from the discrete right Hamilton's equations.

Remark 3.3.3. *In order for q_1 to appropriately satisfy the constraint, we should take the final quadrature point to be $c_s = 1$ (for an s-stage method), so that $\phi(q_1, U^s) = \phi(Q^s, U^s) = 0$. In this case, equation* (3.7a) *and equation* (3.7b) *with $i = s$ are redundant. Note that with the choice $c_s = 1$, they are still consistent (i.e., are the same equation), since in the Galerkin construction, the coefficients a_{ij} and b_i are defined as*

$$a_{ij} = \int_0^{c_i} \phi_j(\tau) d\tau, \; b_i = \int_0^1 \phi_j(\tau) d\tau,$$

where ϕ_j are functions on $[0,1]$ which interpolate the nodes c_j (see, Leok and Zhang [76]). Hence, $a_{sj} = b_j$, so that the two equations are consistent. However, we will write the system as above for conceptual clarity. Furthermore, even in the case where one does not take $c_s = 1$, the proposition that we prove below still holds, despite the possibility of constraint violations.

A similar remark holds for the adjoint variable p and the associated constraint (3.7f)*, except we think of p_0 as the unknown, instead of p_1.*

Note that (3.7a), (3.7b), (3.7e) is a standard Runge–Kutta discretization of an index 1 DAE $\dot{q} = f(q,u)$, $0 = \phi(q,u)$, where again, usually $c_s = 1$. Associated with these equations are the variational equations given by their linearization,

$$\delta q_1 = \delta q_0 + \Delta t \sum_i b_i (D_q f(Q^i, U^i)\delta Q^i + D_u f(Q^i, U^i)\delta U^i), \tag{3.8a}$$

$$\delta Q^i = \delta q_0 + \Delta t \sum_j a_{ij} (D_q f(Q^j, U^j)\delta Q^j + D_u f(Q^j, U^j)\delta U^j), \tag{3.8b}$$

$$0 = D_q \phi(Q^i, U^i)\delta Q^i + D_u \phi(Q^i, U^i)\delta U^i, \tag{3.8c}$$

which is the Runge–Kutta discretization of the continuous variational equations (2.14c) - (2.14d).

Proposition 3.3.2. *With the above notation, the above integrator satisfies*

$$\langle p_1, \delta q_1 \rangle = \langle p_0, \delta q_0 \rangle.$$

Proof. See Appendix 3.6.1. □

Thus, the above integrator admits a discrete analogue of Proposition 3.2.9 for the nonaugmented adjoint DAE system. By setting $p_1 = \nabla_q C(q(t_f))$, one can use this integrator to compute the sensitivity p_0 of a terminal cost function with respect to a perturbation in the initial condition. As discussed before, this only requires $\mathscr{O}(1)$ integrations instead of $\mathscr{O}(n)$ integrations via the direct method (for a dimension n search space). Furthermore, the adjoint method requires only $\mathscr{O}(1)$ numerical solves of the constraints, while the direct method requires $\mathscr{O}(n)$ numerical solves.

Remark 3.3.4. *Since we are assuming the DAE has index 1, it is always possible to prescribe an arbitrary initial condition q_0 (and δq_0) and terminal condition p_1, since the corresponding algebraic variables can always formally be solved for using the corresponding constraints. In practice, one generally has to solve the constraints to some tolerance, e.g., through an iterative* *scheme. If the constraints are only satisfied to a tolerance $\mathscr{O}(\varepsilon)$, then the above proposition holds to $\mathscr{O}(s\varepsilon)$, where s is the number of Runge–Kutta stages.*

Remark 3.3.5. *The above method* (3.7a)-(3.7f) *is presymplectic, since it is a special case of the more general presymplectic Galerkin Hamiltonian variational integrator* (3.6a)-(3.6e)*. Although we proved it directly, the above proposition could also have been proven from presymplecticity, with the appropriate choices of first variations.*

Augmented Adjoint DAE System. Finally, we construct a discrete Hamiltonian variational integrator for the augmented adjoint DAE system (2.16a)-(2.16d) associated with an index 1 DAE. To do this, we apply the presymplectic Galerkin Hamiltonian variational integrator (3.6a)-(3.6e) with $r = (u, \lambda)$ and with Hamiltonian given by the augmented adjoint DAE Hamiltonian,

$$H_L(q,u,p,\lambda) = \langle p, f(q,u)\rangle + \langle \lambda, \phi(q,u)\rangle + L(q,u).$$

The presymplectic integrator is then

$$q_1 = q_0 + \Delta t \sum_i b_i f(Q^i, U^i), \tag{3.9a}$$

$$Q^i = q_0 + \Delta t \sum_j a_{ij} f(Q^j, U^j), \tag{3.9b}$$

$$p_1 = p_0 - \Delta t \sum_i b_i \left([D_q f(Q^i,U^i)]^* P^i + [D_q \phi(Q^i,U^i)]^* \Lambda^i + D_q L(Q^i,U^i) \right), \tag{3.9c}$$

$$P^i = p_0 - \Delta t \sum_j \tilde{a}_{ij} \left([D_q f(Q^j,U^j)]^* P^j + [D_q \phi(Q^j,U^j)]^* \Lambda^j + D_q L(Q^i,U^i) \right), \tag{3.9d}$$

$$0 = \phi(Q^i, U^i), \tag{3.9e}$$

$$0 = [D_u f(Q^i,U^i)]^* P^i + [D_u \phi(Q^i,U^i)]^* \Lambda^i + D_u L(Q^i,U^i). \tag{3.9f}$$

The associated variational equations are again (3.8a)-(3.8c). Remarks analogous to the nonaugmented case regarding setting the quadrature node $c_s = 1$ and solvability of these systems under the index 1 assumption can be made.

Proposition 3.3.3. *With the above notation, the above integrator satisfies*

$$\langle p_1, \delta q_1 \rangle = \langle p_0, \delta q_0 \rangle - \Delta t \sum_i b_i \langle dL(Q^i, U^i), (\delta Q^i, \delta U^i) \rangle.$$

Proof. See Appendix 3.6.1. □

Remark 3.3.6. *Analogous to the remark in the augmented adjoint ODE case, the above proposition is a discrete analogue of Proposition 3.2.10, in integral form,*

$$\langle p_1, \delta q_1 \rangle - \langle p_0, \delta q_0 \rangle = -\int_0^{\Delta t} \langle dL(q,u), (\delta q, \delta u) \rangle dt.$$

The discrete analogue is natural in the sense that it is just quadrature applied to the right hand side of this equation, with the same quadrature rule used to discretize the generating function.

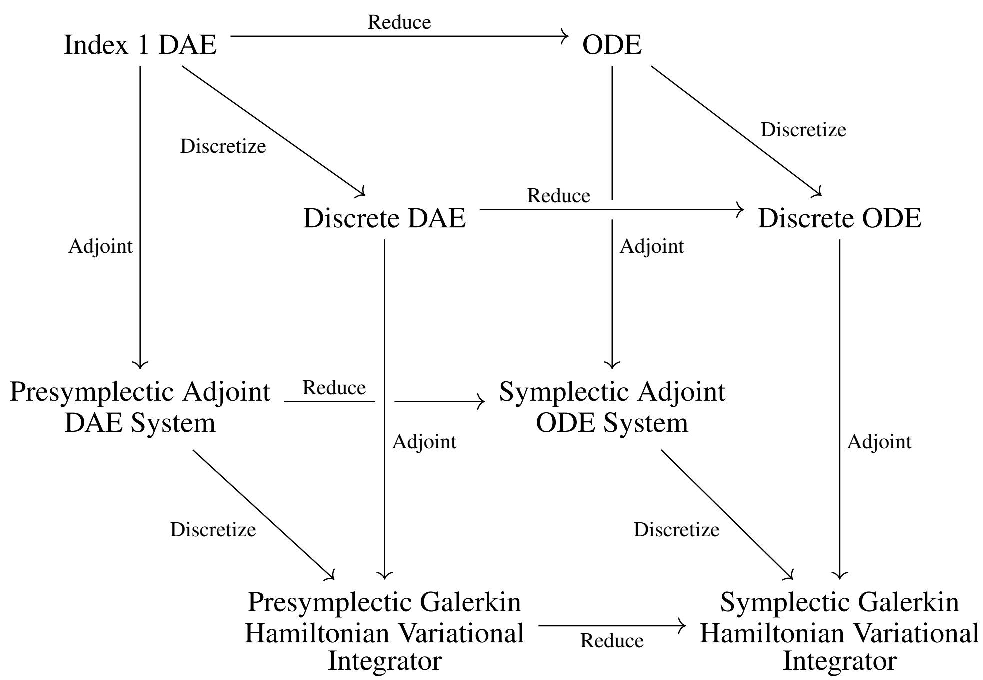
Remark 3.3.7. *As with the augmented adjoint ODE case, the above proposition allows one to compute numerical sensitivities of a running cost function by solving for p_0 with $p_1 = 0$, which is more efficient than the direct method.*

To summarize, we have utilized Galerkin Hamiltonian variational integrators to construct methods which admit natural discrete analogues of the various propositions used for sensitivity analysis. We summarize the results below.

	Terminal Cost	Running Cost
ODE	$\langle p_1, \delta q_1 \rangle = \langle p_0, \delta q_0 \rangle$	$\langle p_1, \delta q_1 \rangle = \langle p_0, \delta q_0 \rangle - \Delta t \sum_i b_i \langle dL(Q^i), \delta Q^i \rangle$
DAE	$\langle p_1, \delta q_1 \rangle = \langle p_0, \delta q_0 \rangle$	$\langle p_1, \delta q_1 \rangle = \langle p_0, \delta q_0 \rangle - \Delta t \sum_i b_i \langle dL(Q^i, U^i), (\delta Q^i, \delta U^i) \rangle$

Naturality of the Adjoint DAE System Discretization

To conclude our discussion of discretizing adjoint systems, we prove a discrete extension of the fact that, for an index 1 DAE, the process of index reduction and forming the adjoint system commute, as discussed in Section 3.2.3. Namely, we will show that, starting from an index 1 DAE (2.11a)-(2.11b), the processes of reduction, forming the adjoint system, and discretization all commute, for particular choices of these processes which we will define and choose below. This can be summarized in the following commutative diagram.



In the above diagram, we will use the convention that the "Discretize" arrows point forward, the "Adjoint" arrows point downward, and the "Reduce" arrows point to the right. For the "Discretize" arrows on the top face, we take the discretization to be a Runge–Kutta discretization (of a DAE on the left and of an ODE on the right, with the same Runge–Kutta coefficients in both cases). For the "Discretize" arrows on the bottom face, we take the discretization to be the symplectic partitioned Runge–Kutta discretization induced by the discretization of the base DAE or ODE, i.e., the momenta expansion coefficients $\tilde{a}_{ij}$ are the symplectic adjoint of the coefficients a_{ij} used on the top face. We have already defined the "Adjoint" arrows on the back face, as discussed in Section 3.2. For the "Adjoint" arrows on the front face, we define them as forming the discrete adjoint system corresponding to a discrete (and generally nonlinear) system of equations and we will review this notion where needed in the proof. We have already defined the “Reduce” arrows on the back face, as discussed in Section 3.2.3. For the “Reduce” arrows on the front face, we define this as solving for the discrete algebraic variables in terms of the discrete kinematic variables through the discrete constraint equations. With these choices, the above diagram commutes, as we will show. To prove this, it suffices to prove that the diagrams on each of the six faces commutes. To keep the exposition concise, we provide the proof in Appendix 3.6.2 and move on to discuss the implications of this result.

The previous discussion shows that the presymplectic Galerkin Hamiltonian variational integrator construction is natural for discretizing adjoint (index 1) DAE systems, in the sense that the integrator is equivalent to the integrator produced from applying a symplectic Galerkin Hamiltonian variational integrator to the underlying nondegenerate Hamiltonian system. Of course, in practice, one cannot generally determine the function $u = u(q)$ needed to reduce the DAE to an ODE. Therefore, one generally works with the presymplectic Galerkin Hamiltonian variational integrator instead, where one iteratively solves the constraint equations. However, although reduction then symplectic integration is often impractical, one can utilize this naturality to derive properties of the presymplectic integrator. For example, we will use this naturality to prove a variational error analysis result.

The basic idea for the variational error analysis result goes as follows: one utilizes the naturality to relate the presymplectic variational integrator to a symplectic variational integrator of the underlying nondegenerate Hamiltonian system and subsequently, applies the variational error analysis result in the symplectic case (Schmitt and Leok [107]). Recall the discrete generating function for the previously constructed presymplectic variational integrator,

$$H_d^+(q_0, p_1; \Delta t) = \text{ext}\Big[\langle p_1, q_1\rangle - \Delta t \sum_i b_i \left(\langle P^i, V^i\rangle - H(Q^i, U^i, P^i, \Lambda^i)\right)\Big],$$

where we have now explicitly included the timestep dependence in H_d^+ and H is the Hamiltonian for the adjoint DAE system (augmented or nonaugmented), corresponding to an index 1 DAE.

Proposition 3.3.4. *Suppose the discrete generating function $H_d^+(q_0, p_1; \Delta t)$ for the presymplectic* *variational integrator approximates the exact discrete generating function* $H_d^{+,E}(q_0, p_1; \Delta t)$ *to order r, i.e.,*

$$H_d^+(q_0, p_1; \Delta t) = H_d^{+,E}(q_0, p_1; \Delta t) + \mathscr{O}(\Delta t^{r+1}),$$

and the Hamiltonian H is continuously differentiable, then the Type II map $(q_0, p_1) \mapsto (q_1, p_0)$ *and the evolution map* $(q_0, p_0) \mapsto (q_1, p_1)$ *are order-r accurate.*

Proof. The proof follows from two simple steps. First, observe that the discrete generating function $H_d^+(q_0, p_1; \Delta t)$ for the presymplectic integrator is also the discrete generating function for the symplectic integrator for the underlying nondegenerate Hamiltonian system. This follows since in the definition of H_d^+, one extremizes over the algebraic variables U^i, Λ^i which enforces the constraints and hence, determines U^i, Λ^i as functions of the kinematic variables Q^i, P^i. Thus, the discrete (or continuous) Type II map determined by H_d^+ (or $H_d^{+,E}$, respectively), $(q_0, p_1) \mapsto (q_1, p_0)$, is the same as the Type II map for the underlying nondegenerate Hamiltonian system, which is just another consequence of the aforementioned naturality. One then applies the variational error analysis result in Schmitt and Leok [107]. □

Remark 3.3.8. *Another way to view this result is that the order of an implicit (partitioned) Runge–Kutta scheme for index 1 DAEs is the same as the order of an implicit (partitioned) Runge–Kutta scheme for ODEs (Roche [101]), since the aforementioned discretization generates a partitioned Runge–Kutta scheme. To be complete, we should determine the order for the full presymplectic flow, i.e., including also the algebraic variables. As discussed in Roche [101], as long as* $a_{si} = b_i$ *for each i, which, as we have discussed, is a natural choice and holds as long as* $c_s = 1$*, there is no order reduction arising from the algebraic variables. Thus, with this assumption, the presymplectic variational integrator in the previous proposition approximates the presymplectic flow, in both the kinematic and algebraic variables, to order r.*

Remark 3.3.9. *In the above proposition, we considered both the Type II map* $(q_0, p_1) \mapsto (q_1, p_0)$ *and the evolution map* $(q_0, p_0) \mapsto (q_1, p_1)$*. The latter is of course the traditional way to view the* *map corresponding to a numerical method, but the former is the form of the map used in adjoint sensitivity analysis.*

Furthermore, in light of this naturality, we can view Propositions 3.3.2 and 3.3.3 as following from the analogous propositions for symplectic Galerkin Hamiltonian variational integrators, applied to the underlying nondegenerate Hamiltonian system.

3.3.3 Optimal Control of DAE Systems

In this section, we derive the optimality conditions for an optimal control problem (OCP) subject to a semi-explicit DAE constraint. It is known that the optimality conditions can be described as a presymplectic system on the generalized phase space bundle (Delgado-Téllez and Ibort [35], Echeverría-Enríquez et al. [38]). We will subsequently consider a variational discretization of such OCPs and discuss the naturality of such discretizations.

Consider the following optimal control problem in Bolza form, subject to a DAE constraint, which we refer to as (OCP-DAE),

$$\begin{aligned}
&\min C(q(t_f)) + \int_0^{t_f} L(q,u)dt \\
&\text{subject to} \\
&\qquad \dot{q} = f(q,u), \\
&\qquad 0 = \phi(q,u), \\
&\qquad q_0 = q(0), \\
&\qquad 0 = \phi_f(q(t_f)),
\end{aligned}$$

where the DAE system $\dot{q} = f(q,u)$, $0 = \phi(q,u)$ is over $M_d \times M_a$ as described in Section 3.2.3, $C : M_d \to \mathbb{R}$ is the terminal cost, $L : M_d \times M_a \to \mathbb{R}$ is the running cost, the initial condition $q(0) = q_0$ is prescribed, and for generality, a terminal constraint $\phi_f(q(t_f)) = 0$ is also imposed, where ϕ_f is a map from M_d into some vector space V.

We assume a local optimum to (OCP-DAE). We then adjoin the constraints to J using adjoint variables, which gives the adjoined functional

$$\mathscr{J} = C(q(t_f)) + \langle \lambda_f, \phi_f(q(t_f)) \rangle + \int_0^{t_f} \left[L(q,u) + \langle p, f(q,u) - \dot{q} \rangle + \langle \lambda, \phi(q,u) \rangle \right] dt.$$

The optimality conditions are given by the condition that $\mathscr{J}$ is stationary about the local optimum, $\delta \mathscr{J} = 0$ (Biegler [15]). For simplicity in the notation, we will use matrix derivative instead of indices. Note also that we will implicitly leave out the variation of the adjoint variables, since those terms pair with the DAE constraints, which vanish at the local optimum. The optimality condition $\delta \mathscr{J} = 0$ is then

$$\begin{aligned}
0 = \delta \mathscr{J} &= \langle \nabla_q C(q(t_f)), \delta q(t_f) \rangle + \langle \lambda_f, D_q \phi_f(q(t_f)) \delta q(t_f) \rangle \\
&\quad + \int_0^{t_f} \Big[\langle \nabla_q L(q,u), \delta q \rangle + \langle \nabla_u L(q,u), \delta u \rangle + \langle p, D_q f(q,u) \delta q \rangle + \langle p, D_u f(q,u) \delta u \rangle \\
&\qquad - \langle p, \frac{d}{dt} \delta q \rangle + \langle \lambda, D_q \phi(q,u) \delta q \rangle + \langle \lambda, D_u \phi(q,u) \delta u \rangle \Big] dt \\
&= \langle \nabla_q C(q(t_f)) + [D_q \phi_f(q(t_f))]^* \lambda_f - p(t_f), \delta q(t_f) \rangle \\
&\quad + \int_0^{t_f} \Big[\langle \nabla_q L(q,u) + [D_q f(q,u)]^* p + \dot{p} + [D_q \phi(q,u)]^* \lambda, \delta q \rangle \\
&\qquad + \langle \nabla_u L(q,u) + [D_u f(q,u)]^* p + [D_u \phi(q,u)]^* \lambda, \delta u \rangle \Big] dt,
\end{aligned}$$

where we integrated by parts on the term $\langle p, \frac{d}{dt} \delta q \rangle$ and used $\delta q(0) = 0$ since the initial condition is fixed. Enforcing stationarity for all such variations gives the optimality conditions,

$$\dot{q} = f(q,u), \tag{3.10a}$$

$$\dot{p} = -[D_q f(q,u)]^* p - [D_q \phi(q,u)]^* \lambda - \nabla_q L(q,u), \tag{3.10b}$$

$$0 = \phi(q,u), \tag{3.10c}$$

$$0 = \nabla_u L(q,u) + [D_u f(q,u)]^* p + [D_u \phi(q,u)]^* \lambda, \tag{3.10d}$$

$$0 = \phi_f(q(t_f)), \tag{3.10e}$$

$$p(t_f) = \nabla_q C(q(t_f)) + [D_q \phi_f(q(t_f))]^* \lambda_f. \tag{3.10f}$$

The first four optimality conditions (3.10a)-(3.10d) are precisely the augmented adjoint DAE equations, (2.16a)-(2.16d). The last two optimality conditions (3.10e), (3.10f) are the terminal constraint and the associated transversality condition, respectively. Note that these conditions are only sufficient for a trajectory (q,u,p,λ) to be an extremum of the optimal control problem; whether or not the trajectory is optimal depends on the properties of the DAE constraint and cost function, e.g., convexity of L.

Regular Index 1 Optimal Control. In the literature, the problem (OCP-DAE) is usually formulated by making a distinction between algebraic variables and control variables, (q,y,u), instead of (q,u) (see, for example, Biegler [15] and Aguiar et al. [3]). This does not change any of the previous discussion of the optimality conditions, except that (3.10d) splits into two equations for y and u. That is, the distinction is not formally important for the previous discussion. It is of course important when actually solving such an optimal control problem. For example, the constraint function $\phi(q,y,u)$ may have a singular matrix derivative with respect to (y,u) but may have a nonsingular matrix derivative with respect to y. In such a case, one interprets y as the algebraic variable, in that it can locally be solved in terms of (q,u) via the constraint, and the control variable u as "free" to optimize over. We now briefly elaborate on this case.

We take the configuration manifold for the algebraic variables to be $M_a = Y_a \times U \ni (y,u)$, where y is interpreted as the algebraic constraint variable and u is interpreted as the control variable. We will assume that the control space U is compact. The constraint has the form $\phi(q,y,u) = 0$, and we assume that $\partial\phi/\partial y$ is pointwise invertible. We consider the following optimal control problem,

$$\min \int_0^{t_f} L(q,y,u)dt$$

subject to

$$\dot{q} = f(q,y,u),$$

$$0 = \phi(q,y,u),$$

$$q_0 = q(0).$$

We perform an analogous argument to before, except that, in this case, since U may have a boundary, the optimality for the control variable u will either require u to lie on ∂U or will require the stationarity of the adjoined functional with respect to variations in u. In any case, the necessary conditions for optimality can be expressed as

$$\dot{q} = f(q,y,u), \tag{3.11a}$$

$$\dot{p} = -[D_q f(q,y,u)]^* p - [D_q \phi(q,y,u)]^* \lambda - \nabla_q L(q,y,u), \tag{3.11b}$$

$$0 = \phi(q,y,u), \tag{3.11c}$$

$$0 = \nabla_y L(q,y,u) + [D_y f(q,y,u)]^* p + [D_y \phi(q,y,u)]^* \lambda, \tag{3.11d}$$

$$u = \arg\min_{u' \in U} H_L(q,y,u'), \tag{3.11e}$$

$$0 = p(t_f), \tag{3.11f}$$

where H_L is the augmented Hamiltonian $H_L(q,y,u) = L(q,y,u) + \langle p, f(q,y,u)\rangle + \langle \lambda, \phi(q,y,u)\rangle$.

Assuming that u lies in the interior of U, (3.11e) can be expressed as

$$0 = \nabla_u L(q,y,u) + [D_u f(q,y,u)]^* p + [D_u \phi(q,y,u)]^* \lambda,$$

or $D_u H_L(q,y,u) = 0$. We say that an optimal control problem with a DAE constraint forms a regular index 1 system if both $\partial\phi/\partial y$ and the Hessian $D_u^2 H_L$ are pointwise invertible. In this case, whenever u lies on the interior of U, (y,u,λ) can be locally solved as functions of (q,p). Thus, in principle, the resulting Hamiltonian ODE for (q,p) can be integrated to yield extremal trajectories for the optimal control problem. As mentioned before, without additional assumptions on the DAE and cost function, such a trajectory will only generally be an extremum but not necessarily optimal.

Of course, in practice, one cannot generally analytically integrate the resulting ODE nor determine the functions which give (y,u,λ) in terms of (q,p). Thus, the only practical option is to discretize the presymplectic system above to compute approximate extremal trajectories. To integrate such a presymplectic system, one can again use the presymplectic Galerkin Hamiltonian variational integrator construction discussed in Section 3.3.2. Such an integrator would be natural in the following sense. First, as discussed in Section 3.3.2, a presymplectic Galerkin Hamiltonian variational integrator applied to the augmented adjoint DAE system is equivalent to applying a symplectic Galerkin Hamiltonian variational integrator to the underlying Hamiltonian ODE, with the same Runge–Kutta expansions for q_1, Q^i in both methods. Furthermore, as shown in Sanz-Serna [106], utilizing a symplectic integrator to discretize the extremality conditions is equivalent to first discretizing the ODE constraint by a Runge–Kutta method and then enforcing the associated discrete extremality conditions. This also holds in the DAE case.

More precisely, beginning with a regular index 1 optimal control problem, the processes of reduction, extremization, and discretization commute, for suitable choices of these processes, analogous to those used in the naturality result discussed in Section 3.3.2. The proof is similar to the naturality result discussed in Section 3.3.2, where the arrow given by forming the adjoint is replaced by extremization. In essence, these are the same, since the extremization condition is given by the adjoint system, so we will just elaborate briefly. We already know how to extremize the continuous optimal control problem, with either a DAE constraint or an ODE constraint after reduction, which results in an adjoint system. We also already know how to discretize the resulting adjoint system after discretization, using a (pre)symplectic partitioned Runge–Kutta method. Furthermore, at any step, reduction is just defined to be solving the continuous or discrete constraints for y in terms of (q,u). Thus, the only major difference compared to the previous naturality result is defining the discretization of the optimal control problem and subsequently, how to extremize the discrete optimal control problem. For the regular index 1 optimal control problem,

$$\begin{aligned} &\min \int_0^{t_f} L(q,y,u)dt \\ &\text{subject to} \\ &\qquad \dot{q} = f(q,y,u), \\ &\qquad 0 = \phi(q,y,u), \\ &\qquad q_0 = q(0), \end{aligned}$$

its discretization is obtained by replacing the constraints with a Runge–Kutta discretization and replacing the cost function with its quadrature approximation, using the same quadrature weights as those in the Runge–Kutta discretization. This can be written as

$$\begin{aligned} &\min \Delta t \sum_i b_i L(Q^i,Y^i,U^i) \\ &\text{subject to} \\ &\qquad V^i = f(Q^i,Y^i,U^i), \\ &\qquad 0 = \phi(Q^i,Y^i,U^i), \end{aligned}$$

where $Q^i = q_0 + \Delta t \sum_j a_{ij} V^j$, which implicitly encodes $q(0) = q_0$. One can then extremize this discrete system, which is given by the discrete Euler–Lagrange equations for the discrete action

$$\mathbb{S} = \Delta t \sum_i b_i \Big(\langle P^i, V^i - f(Q^i, Y^i, U^i) \rangle - \langle \Lambda^i, \phi(Q^i, Y^i, U^i) \rangle - L(Q^i, Y^i, U^i) \Big).$$

That is, we enforce the discrete constraints by adding to the discrete Lagrangian the appropriate Lagrange multiplier terms paired with the constraints, where we weighted the Lagrange multipliers P^i, Λ^i by $\Delta t b_i$ just as convention, in order to interpret them as the appropriate variables, as discussed in Appendix 3.6.2. Enforcing extremality of this action recovers a partitioned Runge–Kutta method applied to the adjoint system corresponding to extremizing the continuous optimal control problem, as discussed in Appendix 3.6.2, where the Runge–Kutta coefficients for the momenta are the symplectic adjoint of the original Runge–Kutta coefficients. Alternatively, starting from the original continuous optimal control problem, one could first reduce the DAE constraint to an ODE constraint using the invertibility of $D_y \phi$ to give

$$\begin{aligned} &\min \int_0^{t_f} L(q, y(q,u), u)\, dt \\ &\text{subject to} \\ &\qquad \dot{q} = f(q, y(q,u), u), \\ &\qquad q_0 = q(0). \end{aligned}$$

One can then discretize this using the same Runge–Kutta method as before, where the cost function is replaced with a quadrature approximation, and then extremize using Lagrange multipliers. Alternatively, one can extremize the continuous problem to yield an adjoint system and then apply a partitioned Runge–Kutta method to that system, where the momenta Runge–Kutta coefficients are again the symplectic adjoint of the original Runge–Kutta coefficients. Having defined all of these processes, a direct computation yields that all of the processes commute, analogous to the computation in Appendix 3.6.2.

3.3.4 Numerical Example

For our numerical example, we consider the planar pendulum. Although one can formulate this system as an ODE in the angular variable θ, we instead work with this system in Cartesian coordinates xy where this system is formulated as a DAE, as an academic example of the theory presented in this paper. We will derive the adjoint DAE system associated to the planar pendulum DAE, and subsequently, perform a numerical test demonstrating the presymplecticity of a presymplectic Galerkin Hamiltonian variational integrator applied to this system.

Consider a pendulum of mass $m > 0$ and length $L > 0$ confined to the xy plane, where gravity acts in the vertical y direction, with acceleration $-g < 0$. This is described by the system

$$\begin{aligned} m\ddot{x} &= \rho x, \\ m\ddot{y} &= \rho y - mg, \\ x^2 + y^2 &= L^2. \end{aligned}$$

This system can be derived from the Lagrangian

$$L = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) - mg(y - L) + \frac{1}{2}\rho(x^2 + y^2 - L^2),$$

where the first term is the kinetic energy, the second term is (minus) the potential energy, and the third term enforces the constraint $x^2 + y^2 = L^2$ where ρ is interpreted as a Lagrange multiplier.

If we restrict to the region $y < 0$, the above system can be expressed as a semi-explicit index 1 DAE of the form

$$\dot{x} = v_x, \tag{3.12a}$$

$$\dot{v}_x = \rho x/m, \tag{3.12b}$$

$$0 = x^2 + y^2 - L^2, \tag{3.12c}$$

$$0 = v_x x + v_y y, \tag{3.12d}$$

$$0 = m(v_x^2 + v_y^2) - mgy + L^2\rho. \tag{3.12e}$$

In terms of the notation of Section 3.2.3, we have $(x, v_x) \in M_d = (-1,1) \times \mathbb{R}$ and $(y, v_y, \rho) \in M_a = \mathbb{R}_- \times \mathbb{R} \times \mathbb{R}$. Letting $q = (x, v_x)$ denote the coordinates for the dynamical variables and $u = (y, v_y, \rho)$ denote the coordinates for the algebraic variables, this system can be expressed in the form (2.11a)-(2.11b), where

$$f(q,u) = \begin{pmatrix} v_x \\ \\ \rho x/m \end{pmatrix},$$

$$\phi(q,u) = \begin{pmatrix} x^2 + y^2 - L^2 \\ \\ v_x x + v_y y \\ \\ m(v_x^2 + v_y^2) - mgy + L^2\rho \end{pmatrix}.$$

We regard ϕ as a section of the constraint bundle Φ given by the trivial vector bundle $(M_d \times M_a) \times \mathbb{R}^3 \to M_d \times M_a$. Coordinatize $\overline{T^*M_d}$ by (q,u,p) where $p = (p_x, p_{v_x})$ are the momenta dual to $q = (x, v_x)$ and coordinatize Φ^* by (q,u,λ) where $\lambda = (\lambda_1, \lambda_2, \lambda_3)$ are the coordinates of the fibers dual to the constraint bundle fibers. The Hamiltonian $H : \overline{T^*M_d} \oplus \Phi^* \to \mathbb{R}$ is then given by

$$H(q,u,p,\lambda) = \langle p, f(q,u)\rangle + \langle \lambda, \phi(q,u)\rangle$$
$$= (p_x \ p_{v_x}) \begin{pmatrix} v_x \\ \\ \rho x \end{pmatrix} + (\lambda_1 \ \lambda_2 \ \lambda_3) \begin{pmatrix} x^2+y^2-L^2 \\ \\ v_x x + v_y y \\ \\ m(v_x^2+v_y^2) - mgy + L^2\rho \end{pmatrix}.$$

The presymplectic form Ω_0 on $\overline{T^*M_d} \oplus \Phi^*$ is given by

$$\Omega_0 = dq \wedge dp = dx \wedge dp_x + dv_x \wedge dp_{v_x}.$$

To obtain an expression for the adjoint DAE system (2.13a)-(2.13d), we compute the derivative matrices of f and ϕ.

$$D_q f(q,u) = \begin{pmatrix} 0 & 1 \\ \\ \rho/m & 0 \end{pmatrix},$$

$$D_u f(q,u) = \begin{pmatrix} 0 & 0 & 0 \\ \\ 0 & 0 & x/m \end{pmatrix},$$

$$D_q \phi(q,u) = \begin{pmatrix} 2x & 0 \\ \\ v_x & x \\ \\ 0 & 2mv_x \end{pmatrix},$$

$$D_u \phi(q,u) = \begin{pmatrix} 2y & 0 & 0 \\ \\ v_y & y & 0 \\ \\ -mg & 2mv_y & L^2 \end{pmatrix}.$$

Note that $\det(D_u \phi(q,u)) = 2L^2 y^2 \neq 0$ for $(q,u) \in M_d \times M_a$ and hence, the system is an index 1 DAE as previously claimed.

The adjoint DAE system (2.13a)-(2.13d) for the planar pendulum is then given by

$$\frac{d}{dt}\begin{pmatrix} x \\ v_x \end{pmatrix} = \begin{pmatrix} v_x \\ \rho x/m \end{pmatrix}, \tag{3.13a}$$

$$\frac{d}{dt}\begin{pmatrix} p_x \\ p_{v_x} \end{pmatrix} = -\begin{pmatrix} 0 & 1 \\ \rho/m & 0 \end{pmatrix}^T \begin{pmatrix} p_x \\ p_{v_x} \end{pmatrix} - \begin{pmatrix} 2x & 0 \\ v_x & x \\ 0 & 2mv_x \end{pmatrix}^T \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \end{pmatrix}, \tag{3.13b}$$

$$0 = \begin{pmatrix} x^2+y^2-L^2 \\ v_x x + v_y y \\ m(v_x^2+v_y^2) - mgy + L^2\rho \end{pmatrix}, \tag{3.13c}$$

$$0 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & x/m \end{pmatrix}^T \begin{pmatrix} p_x \\ p_{v_x} \end{pmatrix} + \begin{pmatrix} 2y & 0 & 0 \\ v_y & y & 0 \\ -mg & 2mv_y & L^2 \end{pmatrix}^T \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \end{pmatrix}. \tag{3.13d}$$

We will apply a presymplectic Galerkin Hamiltonian variational integrator (3.7a)-(3.7f) to the above system. We choose a first-order Runge–Kutta method, with Runge–Kutta coefficients $a = 1, b = 1, c = 1$ and hence, $\tilde{a} = 0$. Thus, the internal stages for the position and momenta are given by $Q = q_1$ and $P = p_0$. With these choices, the presymplectic Galerkin Hamiltonian variational integrator can be expressed as

$$
\begin{aligned}
q_1 &= q_0 + \Delta t f(q_1, U), \\
p_1 &= p_0 - \Delta t \left([D_q f(q_1, U)]^* p_0 + [D_q \phi(q_1, U)]^* \Lambda \right), \\
0 &= \phi(q_1, U), \\
0 &= [D_u f(q_1, U)]^* p_0 + [D_u \phi(q_1, U)]^* \Lambda.
\end{aligned}
$$

For our example, we set $m = g = L = 1$. Letting $U = (Y, V_y, \mathscr{P})$ and $\Lambda = (\Lambda_1, \Lambda_2, \Lambda_3)$ denote the internal stages corresponding to $u = (y, v_y, \rho)$ and $\lambda = (\lambda_1, \lambda_2, \lambda_3)$, respectively, the above integrator applied to the adjoint DAE system for the planar pendulum (3.13a)-(3.13d), with $m = g = L = 1$, can be expressed as

$$\begin{pmatrix} x_1 \\ (v_x)_1 \end{pmatrix} = \begin{pmatrix} x_0 \\ (v_x)_0 \end{pmatrix} + \Delta t \begin{pmatrix} (v_x)_1 \\ \mathscr{P} x_1 \end{pmatrix},$$

$$\begin{pmatrix} (p_x)_1 \\ (p_{v_x})_1 \end{pmatrix} = \begin{pmatrix} (p_x)_0 \\ (p_{v_x})_0 \end{pmatrix} - \Delta t \left(\begin{pmatrix} 0 & 1 \\ \mathscr{P} & 0 \end{pmatrix}^T \begin{pmatrix} (p_x)_0 \\ (p_{v_x})_0 \end{pmatrix} + \begin{pmatrix} 2x_1 & 0 \\ (v_x)_1 & x_1 \\ 0 & 2(v_x)_1 \end{pmatrix}^T \begin{pmatrix} \Lambda_1 \\ \Lambda_2 \\ \Lambda_3 \end{pmatrix} \right),$$

$$0 = \begin{pmatrix} x_1^2 + Y^2 - 1 \\ (v_x)_1 x_1 + V_y Y \\ (v_x)_1^2 + V_y^2 - Y + \mathscr{P} \end{pmatrix},$$

$$0 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & x_1 \end{pmatrix}^T \begin{pmatrix} (p_x)_0 \\ (p_{v_x})_0 \end{pmatrix} + \begin{pmatrix} 2Y & 0 & 0 \\ V_y & Y & 0 \\ -1 & 2V_y & 1 \end{pmatrix}^T \begin{pmatrix} \Lambda_1 \\ \Lambda_2 \\ \Lambda_3 \end{pmatrix}.$$

We refer to this method as PGHVI–1. We will compare this to the first-order method where the Runge–Kutta coefficients are the same for both q and p, i.e., $a = 1 = \tilde{a}$. This method is given by applying the backward Euler method in both the q and p variables, i.e.,

$$\begin{pmatrix} x_1 \\ (v_x)_1 \end{pmatrix} = \begin{pmatrix} x_0 \\ (v_x)_0 \end{pmatrix} + \Delta t \begin{pmatrix} (v_x)_1 \\ \mathscr{P} x_1 \end{pmatrix},$$

$$\begin{pmatrix} (p_x)_1 \\ (p_{v_x})_1 \end{pmatrix} = \begin{pmatrix} (p_x)_0 \\ (p_{v_x})_0 \end{pmatrix} - \Delta t \left(\begin{pmatrix} 0 & 1 \\ \mathscr{P} & 0 \end{pmatrix}^T \begin{pmatrix} (p_x)_1 \\ (p_{v_x})_1 \end{pmatrix} + \begin{pmatrix} 2x_1 & 0 \\ (v_x)_1 & x_1 \\ 0 & 2(v_x)_1 \end{pmatrix}^T \begin{pmatrix} \Lambda_1 \\ \Lambda_2 \\ \Lambda_3 \end{pmatrix} \right),$$

$$0 = \begin{pmatrix} x_1^2 + Y^2 - 1 \\ (v_x)_1 x_1 + V_y Y \\ (v_x)_1^2 + V_y^2 - Y + \mathscr{P} \end{pmatrix},$$

$$0 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & x_1 \end{pmatrix}^T \begin{pmatrix} (p_x)_1 \\ (p_{v_x})_1 \end{pmatrix} + \begin{pmatrix} 2Y & 0 & 0 \\ V_y & Y & 0 \\ -1 & 2V_y & 1 \end{pmatrix}^T \begin{pmatrix} \Lambda_1 \\ \Lambda_2 \\ \Lambda_3 \end{pmatrix},$$

which we refer to as BE–1.

For our numerical test, we will qualitatively compare the preservation of the presymplectic form $\Omega_0 = dx \wedge dp_x + dv_x \wedge dp_{v_x}$ between the two methods. Since Type II boundary conditions arise in adjoint sensitivity analysis, we place Type II boundary conditions, i.e., by specifying $q_0 = (x_0, (v_x)_0)$ and $p_1 = ((p_x)_1, (p_{v_x})_1)$, and subsequently, numerically solve the resulting system for q_1, p_0, U, Λ. We use various nearby values for the initial position $q_0 = (x_0, (v_x)_0)$ and various nearby values for the final momenta $p_1 = ((p_x)_1, (p_{v_x})_1)$. For a presymplectic integrator applied to a presymplectic system with presymplectic form $dx \wedge dp_x + dv_x \wedge dp_{v_x}$, we expect that the area occupied by the distribution of points $(x_0, (p_x)_0)$ is the same as the area occupied by the distribution of points $(x_1, (p_x)_1)$; similarly, we expect that the area occupied by the distribution of points $((v_x)_0, (p_{v_x})_0)$ is the same as the area occupied by the distribution of points $((v_x)_1, (p_{v_x})_1)$. Since we choose to only solve the system for one timestep, we take a large timestep to highlight the difference between the two methods, $\Delta t = 2$, which corresponds to roughly one-third of the period of the pendulum.

Note that, with Type II boundary conditions, both methods give a map $(q_0, p_1) \mapsto (q_1, p_0)$ which implicitly determines an evolution map $(q_0, p_0) \mapsto (q_1, p_1)$; below, we plot the phase space cross-sections of these implicit evolution maps. The evolution of the (x, p_x) and (v_x, p_{v_x}) distributions by PGHVI–1 is shown in Figure 3.3 and Figure 3.4, respectively. The evolution of the (x, p_x) and (v_x, p_{v_x}) distributions by BE–1 is shown in Figure 3.5 and Figure 3.6, respectively. As can be qualitatively seen from Figures 3.3, 3.4, 3.5, 3.6, the PGHVI–1 method preserves the phase space area in both the (x, p_x) and (v_x, p_{v_x}) cross-sections, whereas the BE–1 method does not.

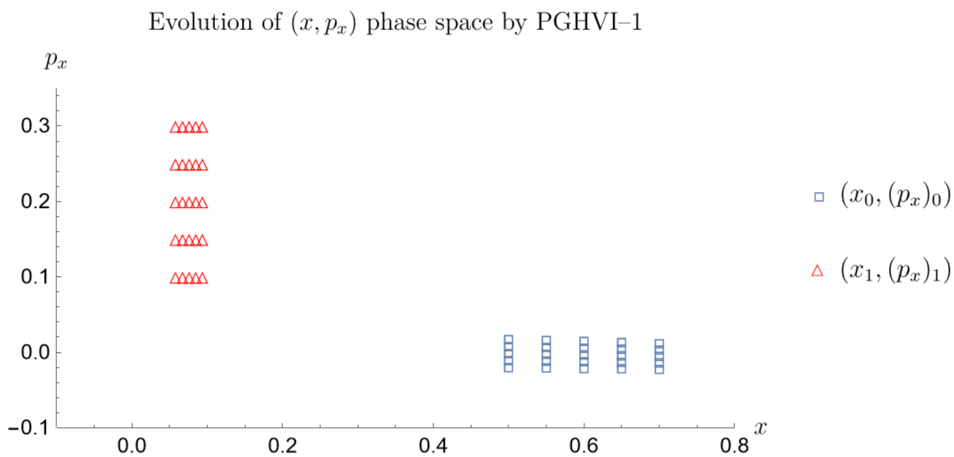


Figure 3.3. (x, p_x) phase space cross-section of PGHVI–1 applied to a distribution of initial conditions q_0 and final momenta p_1

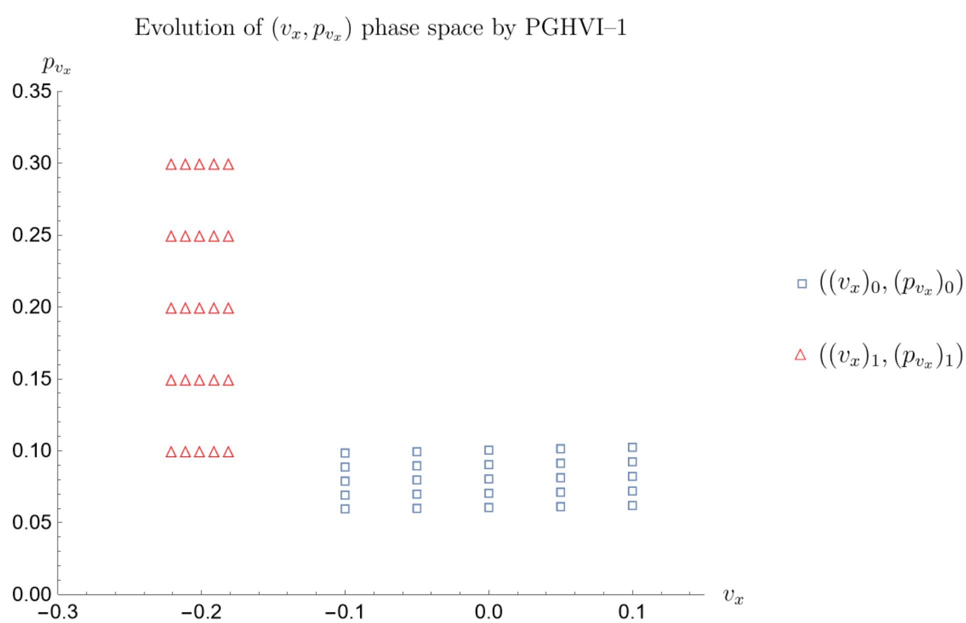


Figure 3.4. (v_x, p_{v_x}) phase space cross-section of PGHVI–1 applied to a distribution of initial conditions q_0 and final momenta p_1

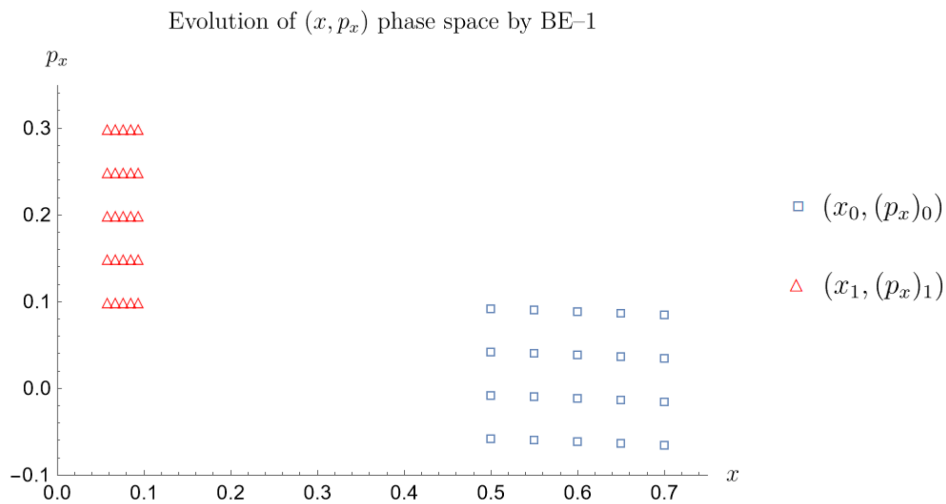


Figure 3.5. (x, p_x) phase space cross-section of BE–1 applied to a distribution of initial conditions q_0 and final momenta p_1

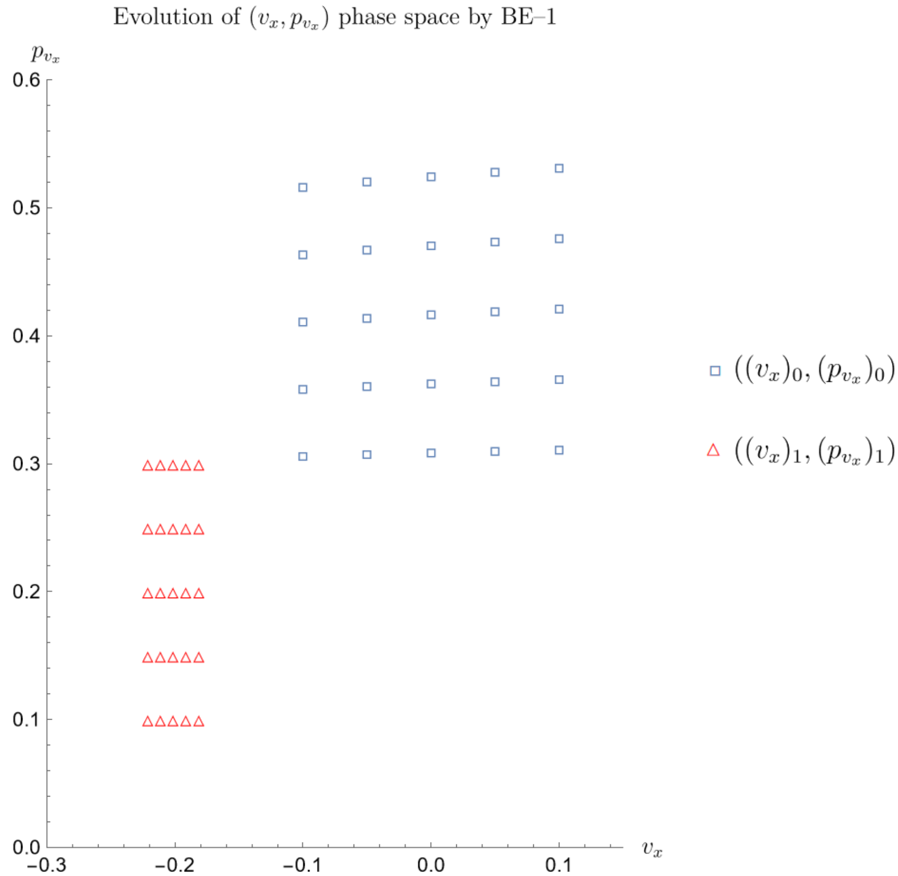


Figure 3.6. (v_x, p_{v_x}) phase space cross-section of BE–1 applied to a distribution of initial conditions q_0 and final momenta p_1

3.4 Conclusion and Future Research Directions

In this paper, we utilized symplectic and presymplectic geometry to study the properties of adjoint systems associated with ODEs and DAEs, respectively. The (pre)symplectic structure of these adjoint systems led us to a geometric characterization of the adjoint variational quadratic conservation law used in adjoint sensitivity analysis. As an application of this geometric characterization, we constructed structure-preserving discretizations of adjoint systems by utilizing (pre)symplectic integrators, which led to natural discrete analogues of the quadratic conservation laws.

A natural research direction is to extend the current framework to adjoint systems for differential equations with nonholonomic constraints, in order to more generally allow for constraints between configuration variables and their derivatives. In this setting, it is reasonable to expect that the geometry of the associated adjoint systems can be described using Dirac structures (see, for example, Yoshimura and Marsden [119, 120]), which generalize the symplectic and presymplectic structures of adjoint ODE and DAE systems, respectively. Structure-preserving discretizations of such systems could then be studied through the lens of discrete Dirac structures (Leok and Ohsawa [75]). These discrete Dirac structures make use of the notion of a retraction (Absil et al. [2]). The tangent and cotangent lifts of a retraction also provide a useful framework for constructing geometric integrators (Barbero-Liñán and Martín de Diego [9]). It would be interesting to synthesize the notion of tangent and cotangent lifts of retraction maps with discrete Dirac structures in order to construct discrete Dirac integrators for adjoint systems with nonholonomic constraints which generalize the presymplectic integrators constructed in Barbero-Liñán and Martín de Diego [10].

Another natural research direction is to extend the current framework to evolutionary partial differential equations (PDEs). There are two possible approaches in this direction. The first is to consider evolutionary PDEs as ODEs evolving on infinite-dimensional spaces, such as Banach or Hilbert manifolds. One can then investigate the geometry of the infinite-dimensional symplectic structure associated with the corresponding adjoint system. In practice, adjoint systems for evolutionary PDEs are often formed after semi-discretization, leading to an ODE on a finite-dimensional space. Understanding the reduction of the infinite-dimensional symplectic structure of the adjoint system to a finite-dimensional symplectic structure under semi-discretization could provide useful insights into structure-preservation. The second approach would be to explore the multisymplectic structure of the adjoint system associated with a PDE. This approach would be insightful for several reasons. First, an adjoint variational quadratic conservation law arising from multisymplecticity would be adapted to spacetime instead of just time. With appropriate spacetime splitting and boundary conditions, such a quadratic conservation law would induce either a temporal or spatial conservation law. As such, one could use the multisymplectic conservation law to determine adjoint sensitivities for a PDE with respect to spatial or temporal directions, which could be useful in practice [79]. Furthermore, the multisymplectic framework would apply equally as well to nonevolutionary (elliptic) PDEs, where there is no interpretation of a PDE as an infinite-dimensional evolutionary ODE. Additionally, adjoint systems for PDEs with constraints could be investigated with multi-Dirac structures (Vankerschaver et al. [115]). In future work, we aim to explore both approaches, relate them once a spacetime splitting has been chosen, and investigate structure-preserving discretizations of such systems by utilizing the multisymplectic variational integrators constructed in Tran and Leok [112].

3.5 Acknowledgements

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3.6 Chapter Appendix

3.6.1 Proofs of Discrete Adjoint Variational Quadratic Conservation Laws

Proof of Proposition 3.3.1.

Proof. We begin by substituting (3.4c) and (3.3a) into the left hand side of (3.5),

$$
\begin{aligned}
\langle p_1, \delta q_1 \rangle = \langle p_0, \delta q_0 \rangle &+ \Delta t \sum_i b_i \langle p_0, Df(Q^i)\delta Q^i \rangle \\
&- \Delta t \sum_i b_i \langle [Df(Q^i)]^* P^i, \delta q_0 \rangle - \Delta t \sum_i b_i \langle dL(Q^i), \delta q_0 \rangle \\
&- \Delta t^2 \sum_{ij} b_i b_j \langle [Df(Q^i)]^* P^i, Df(Q^j)\delta Q^j \rangle - \Delta t^2 \sum_{ij} b_i b_j \langle dL(Q^i), Df(Q^j)\delta Q^j \rangle \\
= \langle p_0, \delta q_0 \rangle &+ \Delta t \sum_i b_i \left\langle P^i + \Delta t \sum_j \tilde{a}_{ij}([Df(Q^j)]^* P^j + dL(Q^j)), Df(Q^i)\delta Q^i \right\rangle \\
&- \Delta t \sum_i b_i \left\langle [Df(Q^i)]^* P^i, \delta Q^i - \Delta t \sum_j a_{ij} Df(Q^j)\delta Q^j \right\rangle - \Delta t \sum_i b_i \langle dL(Q^i), \delta q_0 \rangle \\
&- \Delta t^2 \sum_{ij} b_i b_j \langle [Df(Q^i)]^* P^i, Df(Q^j)\delta Q^j \rangle - \Delta t^2 \sum_{ij} b_i b_j \langle dL(Q^i), Df(Q^j)\delta Q^j \rangle,
\end{aligned}
$$

where, in the last equality, we substituted (3.4d) and (3.3b). We now group and simplify the above expression,

$$
\begin{aligned}
\langle p_1, \delta q_1 \rangle = \langle p_0, \delta q_0 \rangle &+ \Delta t \sum_i b_i \left\langle P^i + \Delta t \sum_j \tilde{a}_{ij} [Df(Q^j)]^* P^j, Df(Q^i) \delta Q^i \right\rangle \\
&- \Delta t \sum_i b_i \left\langle [Df(Q^i)]^* P^i, \delta Q^i - \Delta t \sum_j a_{ij} Df(Q^j) \delta Q^j \right\rangle \\
&- \Delta t^2 \sum_{ij} b_i b_j \langle [Df(Q^i)]^* P^i, Df(Q^j) \delta Q^j \rangle \\
&+ \Delta t \sum_i b_i \left\langle \Delta t \sum_j \tilde{a}_{ij} dL(Q^j), Df(Q^i) \delta Q^i \right\rangle - \Delta t \sum_i b_i \langle dL(Q^i), \delta q_0 \rangle \\
&- \Delta t^2 \sum_{ij} b_i b_j \langle dL(Q^i), Df(Q^j) \delta Q^j \rangle \\
= \langle p_0, \delta q_0 \rangle &+ \Delta t^2 \sum_{ij} \underbrace{(b_j \tilde{a}_{ji} + b_i a_{ij} - b_i b_j)}_{=0} \langle [Df(Q^i)]^* P^i, Df(Q^j) \delta Q^j \rangle \\
&+ \Delta t \sum_i b_i \left\langle \Delta t \sum_j \tilde{a}_{ij} dL(Q^j), Df(Q^i) \delta Q^i \right\rangle - \Delta t \sum_i b_i \langle dL(Q^i), \delta q_0 \rangle \\
&- \Delta t^2 \sum_{ij} b_i b_j \langle dL(Q^i), Df(Q^j) \delta Q^j \rangle \\
= \langle p_0, \delta q_0 \rangle &- \Delta t \sum_i b_i \langle dL(Q^i), \delta q_0 \rangle \\
&- \Delta t^2 \sum_{ij} \underbrace{(b_i b_j - b_j \tilde{a}_{ji})}_{=b_i a_{ij}} \langle dL(Q^i), Df(Q^j) \delta Q^j \rangle \\
= \langle p_0, \delta q_0 \rangle &- \Delta t^2 \sum_i b_i \left\langle dL(Q^i), \frac{\delta q_0}{\Delta t} + \sum_j a_{ij} Df(Q^j) \delta Q^j \right\rangle \\
= \langle p_0, \delta q_0 \rangle &- \Delta t \sum_i b_i \langle dL(Q^i), \delta Q^i \rangle,
\end{aligned}
$$

where, in the last equality, we used (3.3b). □

Proof of Proposition 3.3.2.

Proof. For brevity, we denote

$$D_q f_i \equiv D_q f(Q^i, U^i),$$

$$D_u f_i \equiv D_u f(Q^i, U^i),$$

$$D_q \phi_i \equiv D_q \phi(Q^i, U^i),$$

$$D_u \phi_i \equiv D_u \phi(Q^i, U^i).$$

Starting from $\langle p_1, \delta q_1\rangle$, we substitute the evolution equations (3.7c), (3.7d), (3.8a), (3.8b),

$$\begin{aligned}
\langle p_1, \delta q_1\rangle &= \langle p_0, \delta q_0\rangle \\
&\quad - \Delta t \sum_i b_i \langle [D_q f_i]^* P^i + [D_q \phi_i]^* \Lambda^i, \delta q_0\rangle + \Delta t \sum_i b_i \langle p_0, D_q f_i \delta Q^i + D_u f_i \delta U^i\rangle \\
&\quad - \Delta t^2 \sum_{ij} b_i b_j \langle [D_q f_i]^* P^i + [D_q \phi_i]^* \Lambda^i, D_q f_j \delta Q^j + D_u f_j \delta U^j)\rangle \\
&= \langle p_0, \delta q_0\rangle \\
&\quad - \Delta t \sum_i b_i \left\langle [D_q f_i]^* P^i + [D_q \phi_i]^* \Lambda^i, \delta Q^i - \Delta t \sum_j a_{ij} (D_q f_j \delta Q^j + D_u f_j \delta U^j) \right\rangle \\
&\quad + \Delta t \sum_i b_i \left\langle P^i + \Delta t \sum_j \tilde{a}_{ij} ([D_q f_j]^* P^j + [D_q \phi_j]^* \Lambda^j), D_q f_i \delta Q^i + D_u f_i \delta U^i \right\rangle \\
&\quad - \Delta t^2 \sum_{ij} b_i b_j \langle [D_q f_i]^* P^i + [D_q \phi_i]^* \Lambda^i, D_q f_j \delta Q^j + D_u f_j \delta U^j\rangle \\
&= \langle p_0, \delta q_0\rangle - \Delta t \sum_i b_i \langle [D_q f_i]^* P^i + [D_q \phi_i]^* \Lambda^i, \delta Q^i\rangle \\
&\quad + \Delta t \sum_i b_i \langle P^i, D_q f_i \delta Q^i + D_u f_i \delta U^i\rangle \\
&\quad + \Delta t^2 \sum_{ij} \underbrace{(b_j \tilde{a}_{ji} + b_i a_{ij} - b_i b_j)}_{=0} \langle [D_q f_i]^* P^i + [D_q \phi_i]^* \Lambda^i, D_q f_j \delta Q^j + D_u f_j \delta U^j\rangle \\
&= \langle p_0, \delta q_0\rangle + \Delta t \sum_i b_i \Big(\langle [D_u f_i]^* P^i, \delta U^i\rangle - \langle [D_q \phi_i]^* \Lambda^i, \delta Q^i\rangle \Big) \\
&= \langle p_0, \delta q_0\rangle + \Delta t \sum_i b_i \Big(- \langle [D_u \phi_i]^* \Lambda^i, \delta U^i\rangle - \langle [D_q \phi_i]^* \Lambda^i, \delta Q^i\rangle \Big) \\
&= \langle p_0, \delta q_0\rangle - \Delta t \sum_i b_i \langle \Lambda^i, D_u \phi_i \delta U^i + D_q \phi_i \delta Q^i\rangle \\
&= \langle p_0, \delta q_0\rangle,
\end{aligned}$$

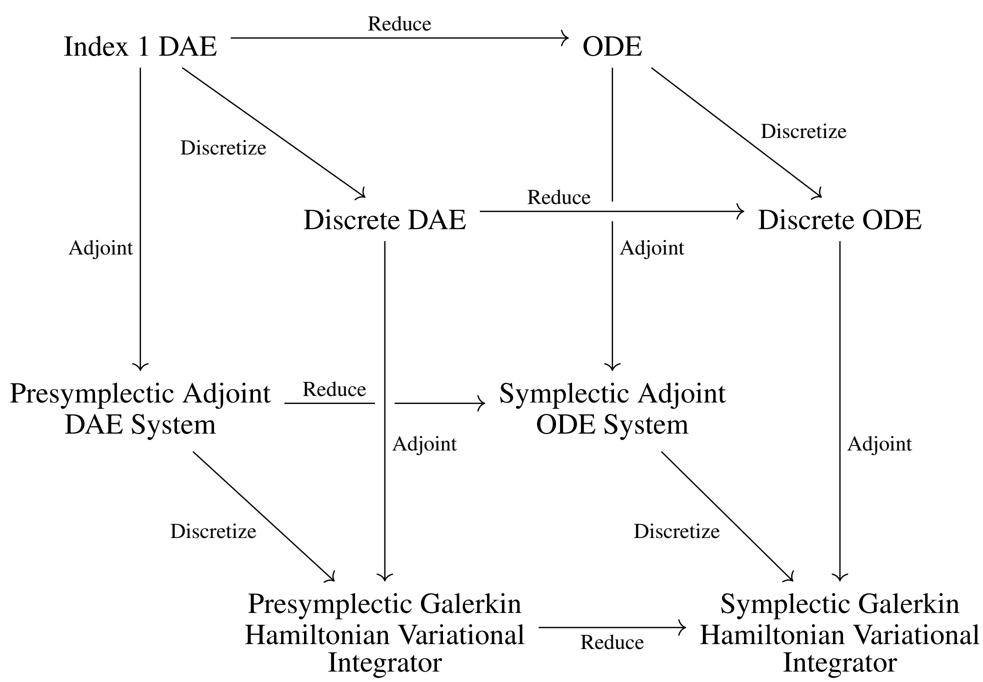
where in the third to last equality, we used the constraint equation (3.7f) and in the last equality, we used the constraint equation (3.8c). □

Proof of Proposition 3.3.3.

Proof. The proof uses computations analogous to those used in the proofs of Propositions 3.3.1 and 3.3.2. In particular, starting from the simplest case of the nonaugmented adjoint ODE system, Proposition 3.3.1 considers the case of augmenting the Hamiltonian, whereas Proposition 3.3.2 considers the case of replacing the ODE with a DAE. The case at hand combines both and the proof involves a combination of both computations. □

3.6.2 Proof of Naturality of Adjoint System Discretization

In this appendix, we prove the statement in Section 3.3.2 that (for suitable choices of) discretization, reduction, and forming the adjoint all commute when applied to an index 1 DAE. The definitions and choices of these processes were made in Section 3.3.2. To prove that the diagram commutes, we prove that each face of the diagram commutes. We again include the relevant diagram which we wish to show commutes below.



Back Face. We have already proved that the back face commutes (i.e., that reduction and forming the adjoint commute when starting with an index 1 DAE), as discussed in Section 3.2.3.

One can then interpret the above diagram as an extension of this result with an extra dimension corresponding to discretization.

Right Face. This was proven in Sanz-Serna [106]. One can then interpret the above diagram as an extension of the result in Sanz-Serna [106] by adding the reduction operation.

Bottom Face. Consider the augmented adjoint DAE system corresponding to the DAE (2.11a)-(2.11b), which we take to have index 1, i.e., $\partial\phi/\partial u$ is pointwise invertible. We consider the augmented case because the nonaugmented case can be obtained by taking $L \equiv 0$. We show that reducing the system first and then applying a symplectic Galerkin Hamiltonian variational integrator is equivalent to applying a presymplectic Galerkin Hamiltonian variational integrator, with the same partitioned Runge–Kutta coefficients, and then reducing.

We start with the former approach. The symplectic adjoint ODE system given by reduction, as discussed in Section 3.2.3, is the Hamiltonian system corresponding to the Hamiltonian

$$H(q',p') = \langle p', f'(q')\rangle + L'(q'),$$

where we have solved $u = u(q')$ and defined $f'(q') \equiv f(q',u(q')), L'(q') \equiv L(q',u(q'))$. Applying the symplectic Galerkin Hamiltonian variational integrator construction yields the integrator

$$q_1 = q_0 + \Delta t \sum_i b_i f'(Q^i) \tag{3.6.1a}$$

$$= q_0 + \Delta t \sum_i b_i f(Q^i, u(Q^i)),$$

$$Q^i = q_0 + \Delta t \sum_j a_{ij} f'(Q^j) \tag{3.6.1b}$$

$$= q_0 + \Delta t \sum_j a_{ij} f(Q^j, u(Q^j)),$$

$$p_1 = p_0 - \Delta t \sum_i b_i([Df'(Q^i)]^* P^i + dL'(Q^i)), \tag{3.6.1c}$$

$$P^i = p_0 - \Delta t \sum_j \tilde{a}_{ij}([Df'(Q^j)]^* P^j + dL'(Q^j)). \tag{3.6.1d}$$

Note that the derivative Df' can be equivalently expressed as

$$Df'(Q^i) = D_1 f(Q^i, u(Q^i)) + D_2 f(Q^i, u(Q^i)) Du(Q^i),$$

where D_i denotes differentiation with respect to the i^{th} argument. We switch to indexing the derivative operator here, so we do not have to make the distinction between total derivatives D_q and partial derivatives ∂_q. Similarly, we can express dL' as follows. First, note that we have been implicitly identifying the row vector dL' with the column vector given by its transpose $\nabla L'$. Thus, dL' in equations (3.6.1c)-(3.6.1d) should really be written as $\nabla L'$. Thus,

$$dL'(Q^i) \cong \nabla L'(Q^i) = \nabla_1 L(Q^i, u(Q^i)) + [Du(Q^i)]^* \nabla_2 L(Q^i, u(Q^i)).$$

Now, we show that the second approach is equivalent to the above system. The starting point is the presymplectic Galerkin Hamiltonian variational integrator, equations (3.9a)-(3.9f). From (3.9e), we can solve for U^i in terms of Q^i as $U^i = u(Q^i)$. Plugging this into (3.9a)-(3.9b) gives precisely (3.6.1a)-(3.6.1b). Thus, we just need to see that, after solving the constraint (3.9f) for Λ^i, the two momenta equations (3.9c)-(3.9d) are equivalent to (3.6.1c)-(3.6.1d). Solving (3.9f) for Λ^i gives

$$\Lambda^i = -([D_2\phi(Q^i, u(Q^i))]^*)^{-1} [D_2 f(Q^i, u(Q^i))]^* P^i - ([D_2\phi(Q^i, u(Q^i))]^*)^{-1} \nabla_2 L(Q^i, u(Q^i)).$$

Multiplying both sides by $[D_1\phi(Q^i, u(Q^i))]^*$ yields

$$\begin{aligned}
[D_1\phi(Q^i, u(Q^i))]^* \Lambda^i &= -[D_1\phi(Q^i, u(Q^i))]^* ([D_u\phi(Q^i, u(Q^i))]^*)^{-1} [D_2 f(Q^i, u(Q^i))]^* P^i \\
&\quad - [D_1\phi(Q^i, u(Q^i))]^* ([\nabla_u\phi(Q^i, u(Q^i))]^*)^{-1} \nabla_2 L(Q^i, u(Q^i)) \\
&= [Du(Q^i)]^* [D_2 f(Q^i, u(Q^i))]^* P^i + [Du(Q^i)]^* \nabla_2 L(Q^i, u(Q^i)) \\
&= [D_2 f(Q^i, u(Q^i)) Du(Q^i)]^* P^i + [Du(Q^i)]^* \nabla_2 L(Q^i, u(Q^i)),
\end{aligned}$$

where in the second equality, we used $D_1\phi(Q^i,u(Q^i)) = -D_2\phi(Q^i,u(Q^i))Du(Q^i)$ from the implicit function theorem. Plugging this expression and $U^i = u(Q^i)$ into (3.9c)-(3.9d) yields (3.6.1c)-(3.6.1d), noting the above expressions for Df', dL'.

Remark 3.6.1. *Note that, in the above, we used the implicit function theorem to obtain the local function $u = u(q)$. This is sufficient to prove that the two processes are the same for a single integration step, assuming that the timestep Δt is sufficiently small and the vector field f and constraint ϕ are sufficiently regular, so that q_0, q_1, and all of the internal stages Q^i are in the neighborhood where the local function is defined. For each subsequent time step, one generally needs a different local function. This does not matter in practice since one works directly with the presymplectic integrator and solves the constraints iteratively.*

Top Face. We want to prove that, starting from an index 1 DAE, the processes of discretization and reduction commute, where the discretization of the ODE and DAE have the same Runge–Kutta coefficients.

We start first with reduction then discretization. Starting from the index 1 DAE $\dot{q} = f(q,u)$, $\phi(q,u) = 0$, we apply the reduction operation, which gives the ODE $\dot{q} = f(q,u(q))$. Applying a Runge–Kutta discretization gives

$$q_1 = q_0 + \Delta t \sum_i b_i f(Q^i,u(Q^i)),$$
$$Q^i = q_0 + \Delta t \sum_j a_{ij} f(Q^j,u(Q^j)).$$

On the other hand, we can discretize the DAE and then reduce. We discretize the DAE $\dot{q} = f(q,u)$, $\phi(q,u) = 0$ by applying a Runge–Kutta discretization with the same coefficients as before,

$$q_1 = q_0 + \Delta t \sum_i b_i f(Q^i, U^i),$$
$$Q^i = q_0 + \Delta t \sum_j a_{ij} f(Q^j, U^j),$$
$$0 = \phi(Q^i, U^i).$$

To reduce this system, we solve the constraint equations $U^i = u(Q^i)$ and substitute these into the two evolution equations, which yields the same system obtained from first reducing and then discretizing.

Front Face. The starting point for this loop is a discrete DAE system, which arises as a Runge–Kutta discretization of an index 1 DAE, i.e., it is given by the discrete system

$$q_1 = q_0 + \Delta t \sum_i b_i f(Q^i, U^i), \tag{3.6.2a}$$
$$Q^i = q_0 + \Delta t \sum_j a_{ij} f(Q^j, U^j), \tag{3.6.2b}$$
$$0 = \phi(Q^i, U^i). \tag{3.6.2c}$$

From here, we wish to show that reducing and forming the discrete adjoint system commute.

First, we recall the notion of a discrete adjoint system. Suppose we are given a generally nonlinear system of equations, $F(x_1) = x_0$, where $x_1 \in V$ is unknown, $x_0 \in W$ is given, and $F: V \to W$ (where V and W are vector spaces). To define the adjoint system, we first consider the variational equations associated with this nonlinear system given by its linearization,

$$DF(x_1)\delta x_1 = \delta x_0,$$

where $DF(x_1)$ is a linear map $V \to W$ and $\delta x_0 \in W$ is given. Suppose that we are interested in computing the quantity $\langle s_1, \delta x_1 \rangle$ for a given vector $s_1 \in V^*$. In the setting of adjoint sensitivity analysis, the quantity $\langle s_1, \delta x_1 \rangle$ is the sensitivity of the terminal cost function. We define the associated adjoint equation as

$$[DF(x_1)]^* s_0 = s_1.$$

For a solution $s_0 \in W^*$ of this system, one has

$$\langle s_1, \delta x_1 \rangle = \langle [DF(x_1)]^* s_0, \delta x_1 \rangle = \langle s_0, DF(x_1)\delta x_1 \rangle = \langle s_0, \delta x_0 \rangle.$$

Thus, to compute $\langle s_1, \delta x_1 \rangle$, one could solve the variational equation for δx_1 and pair it with s_1 which is given, or, alternatively, solve the adjoint equation for s_0 and pair it with δx_0 which is given, since these linear systems are solvable by assumption. We define the adjoint system associated with the equation $F(x_1) = x_0$ as this equation combined with the associated adjoint equation, i.e., as the combined system

$$F(x_1) = x_0,$$
$$[Df(x_1)]^* s_0 = s_1.$$

Following Ibragimov [57], we will utilize an alternative characterization of the adjoint system. We define the discrete adjoint action

$$\mathbb{S}(x_1, s_0) \equiv \langle s_0, F(x_1) \rangle.$$

Then, observe that $\mathbb{S}$ is a generating function for the adjoint system $(x_1, s_0) \mapsto (x_0, s_1)$, in the sense that

$$x_0 = \frac{\delta}{\delta s_0} \mathbb{S}(x_1, s_0) = F(x_1),$$
$$s_1 = \frac{\delta}{\delta x_1} \mathbb{S}(x_1, s_0) = [Df(x_1)]^* s_0.$$

This characterization serves two purposes. First, it will simplify the calculation of the adjoint system for the case at hand. Furthermore, it resembles the process of forming the adjoint at the continuous level: starting from the (discrete or continuous) differential(-algebraic) equation at hand, one forms the (discrete or continuous) adjoint action and applies the variational principle to obtain the adjoint system. To obtain the augmented adjoint system, we add a discrete Lagrangian $\mathbb{L} : V \to \mathbb{R}$ to the action (as a convention, we subtract the discrete Lagrangian). We define the augmented discrete adjoint action to be

$$\mathbb{S}_{\mathbb{L}}(x_1, s_0) \equiv \langle s_0, F(x_1) \rangle - \mathbb{L}(x_1).$$

The map that this generates defines the augmented discrete adjoint system,

$$\begin{aligned} x_0 &= \frac{\delta}{\delta s_0} \mathbb{S}_{\mathbb{L}}(x_1, s_0) = F(x_1), \\ s_1 &= \frac{\delta}{\delta x_1} \mathbb{S}_{\mathbb{L}}(x_1, s_0) = [Df(x_1)]^* s_0 - d\mathbb{L}(x_1). \end{aligned}$$

Observe that this definition of an augmented discrete adjoint system is natural in the sense that,

$$\langle s_1, \delta x_1 \rangle = \langle [Df(x_1)]^* s_0 + d\mathbb{L}(x_1), \delta x_1 \rangle = \langle s_0, x_0 \rangle - \langle dL(x_1), \delta x_1 \rangle,$$

which resembles the continuous analogue of the adjoint sensitivity result for a running cost function.

Now, we use this notion of a discrete adjoint system for the problem at hand. We begin first with reduction and then forming the adjoint system. Applying the reduction operation to the discrete DAE system (3.6.2a)-(3.6.2c), given by solving $\phi(Q^i, U^i) = 0$ for $U^i = u(Q^i)$,

$$q_1 = q_0 + \Delta t \sum_i b_i f(Q^i, u(Q^i)), \tag{3.6.3a}$$

$$Q^i = q_0 + \Delta t \sum_j a_{ij} f(Q^j, u(Q^j)), \tag{3.6.3b}$$

Let us define $Q^i = q_0 + \Delta t \sum_j a_{ij} V^j$. We think of the internal stages Q as functions of the internal stages V, which are the internal stage proxies for $\dot{q}$. Our discrete system (3.6.3a)-(3.6.3b) can then be defined by $x_1 = \{V^i\}_{i=1}^s$, $x_0 = \{0\}_{i=1}^s$, where s is the number of internal stages, and

$$x_0 = F(x_1) \equiv \begin{pmatrix} V^1 - f(Q^i(V), u(Q^i(V))) \\ \vdots \\ V^s - f(Q^s(V), u(Q^s(V))) \end{pmatrix}.$$

Observe that $F = 0$ only gives the internal stage equations (3.6.3b). We do this for simplicity, since we will assume $c_s = 1$ as is typical for a Runge–Kutta discretization of a DAE as previously discussed and hence, equation (3.6.3a) is redundant, since $a_{sj} = b_j$.

We define F and x_1 in terms of V instead of Q because when we form the adjoint action, we pair the components of F with the dual variable s_0. In order to interpret s_0 as representing the momenta internal stages P^i, it should be paired with the proxy for the tangent vector V, instead of Q. We now form the discrete adjoint action. We define the dual variable for the adjoint system to be $s_0 = \{\Delta t b_i P^i\}_{i=1}^s$. The normalization factor $\Delta t b_i$ is used so that the discrete action is the quadrature approximation of the continuous action. This is just a convention, but we would have to reinterpret the components of s_0 if we did not choose this convention. Finally, we define the discrete Lagrangian to be the quadrature approximation of the continuous Lagrangian $L'(q) \equiv L(q, u(q))$, i.e., $\mathbb{L}(x_1) = \Delta t \sum_i b_i L'(Q^i(V))$. This is the natural choice because the discrete sensitivity of a running cost function is $\Delta t \sum_i b_i \langle dL'(Q^i(V)), \delta Q^i(V)\rangle$, which equals $\langle d\mathbb{L}(x_1), \delta x_1\rangle$ with the above choice of $\mathbb{L}$. The augmented discrete adjoint action is then

$$\begin{aligned}\mathbb{S}_{\mathbb{L}}(\{V^i\},\{b_iP^i\}) = \mathbb{S}_{\mathbb{L}}(x_1,s_0) = \langle s_0, F(x_1)\rangle - \mathbb{L}(x_1)\\ = \Delta t \sum_i b_i \Big(\langle P^i, V^i - f(Q^i(V), u(Q^i(V)))\rangle - L'(Q^i(V))\Big).\end{aligned}$$

To define the discrete adjoint system, we have to give s_1, which we take to be $s_1 = \{\Delta t b_i p_1\}_{i=1}^s$, where p_1 is given. Thus, the augmented discrete adjoint system is given by

$$\begin{aligned}0 &= \frac{\delta}{\delta P^k}\mathbb{S}_{\mathbb{L}} = V^k - f(Q^k(V), u(Q^k(V))),\\ \Delta t b_k p_1 &= \frac{\delta}{\delta V^k}\mathbb{S}_{\mathbb{L}}\\ &= \Delta t b_k P^k - \Delta t^2 \sum_i b_i a_{ik}\Big([D_1 f(Q^i(V), u(Q^i(V)))]^* P^i\\ &\qquad + [D_2 f(Q^i(V), u(Q^i(V)))Du(Q^i(V))]^* P^i + dL'(Q^i(V))\Big).\end{aligned}$$

The first set of equations above, combined with the definition of Q in terms of V, gives (3.6.3b). For the second set of equations, we first divide through by $\Delta t b_k$ and rearrange to obtain

$$\begin{aligned}P^k &= p_1 + \Delta t \sum_i \frac{b_i a_{ik}}{b_k}\Big([D_1 f(Q^i(V), u(Q^i(V)))]^* P^i\\ &\qquad + [D_2 f(Q^i(V), u(Q^i(V)))Du(Q^i(V))]^* P^i + dL'(Q^i(V))\Big).\\ &= p_1 + \sum_i (b_i - \tilde{a}_{ki})\Big([D_1 f(Q^i(V), u(Q^i(V)))]^* P^i\\ &\qquad + [D_2 f(Q^i(V), u(Q^i(V)))Du(Q^i(V))]^* P^i + dL'(Q^i(V))\Big).\end{aligned}$$

Note that this is the usual symplectic partitioned Runge–Kutta expansion for the internal stages P^i, expressed in terms of p_1 instead of p_0. Thus, the full adjoint system, combined with the redundant $k = s$ stages, yields a symplectic partitioned Runge–Kutta method.

Now, in the other direction, we first form the adjoint system corresponding to the discrete DAE system and subsequently reduce. We begin by forming the adjoint system. We form the discrete action analogously to before, but now the discrete system (3.6.2a)-(3.6.2c) also has constraints which we must incorporate into F, since we have not yet reduced the system. We take $x_1 = \{\{V^i\},\{U^i\}\}_{i=1}^s$ and $s_0 = \{\{\Delta t b_i P^i\},\{\Delta t b_i \Lambda^i\}\}_{i=1}^s$. We define F as

$$x_0 = F(x_1) \equiv \begin{pmatrix} V^1 - f(Q^i(V),U^i) \\ \vdots \\ V^s - f(Q^s(V),U^i)) \\ -\phi(Q^1(V),U^1) \\ \vdots \\ -\phi(Q^s(V),U^s) \end{pmatrix}.$$

Note again that Q is a function of V as $Q^i = q_0 + \Delta t \sum_j a_{ij} V^j$. It is not a priori a function of U because the condition $V^i = f(Q^i(V),U^i)$ has not yet been enforced. Rather, it is a consequence of the variational principle, which formally matters when one computes the variation of the discrete action. Define the discrete Lagrangian $\mathbb{L}(x_1) = \sum_i b_i L(Q^i(V),U^i)$. We form the augmented discrete adjoint action

$$\begin{aligned} \mathbb{S}_{\mathbb{L}}(\{V^i\},\{b_i P^i\}) &= \mathbb{S}_{\mathbb{L}}(x_1,s_0) = \langle s_0, F(x_1)\rangle - \mathbb{L}(x_1) \\ &= \Delta t \sum_i b_i \Big(\langle P^i, V^i - f(Q^i(V),U^i)\rangle - \langle \Lambda^i, \phi(Q^i,U^i)\rangle - L(Q^i(V),U^i) \Big). \end{aligned}$$

We use this as a generating function to compute the adjoint system as before. The computation is analogous so we will just state the result,

$$
\begin{aligned}
V^k &= f(Q^k(V),U^k),\\
P^k &= p_1 + \Delta t \sum_i (b_i - \tilde{a}_{ki}) \left([D_1 f(Q^i(V),U^i)]^* P^i + [D_1\phi(Q^i(V),U^i)]^*\Lambda^i + D_q L(Q^i(V),U^i)\right),\\
0 &= \phi(Q^i(V),U^i),\\
0 &= [D_2 f(Q^i(V),U^i)]^* P^i + [D_2\phi(Q^i(V),U^i)]^*\Lambda^i + D_2 L(Q^i(V),U^i).
\end{aligned}
$$

Finally, we reduce by solving the last two equations for U^i, Λ^i as functions of $Q^i(V^i)$, P^i. Finally, an implicit function theorem computation analogous to the proof of the bottom face shows that this is the same as the system obtained by first reducing and then forming the discrete adjoint.

Left Face. The proof for the left face is formally similar to the right face, but since we have already computed both directions, we will include it for completeness. Starting from an index 1 DAE, forming the adjoint and then discretizing just give the presymplectic Galerkin Hamiltonian variational integrator (3.9a)-(3.9f). In the other direction, we first discretize the DAE and then take the adjoint which we did in the proof of the front face. Expressed in terms of Q, instead of V, this is

$$
\begin{aligned}
Q^k &= q_0 + \Delta t \sum_j a_{ij} f(Q^j,U^j),\\
P^k &= p_1 + \Delta t \sum_i (b_i - \tilde{a}_{ki}) \left([D_1 f(Q^i,U^i)]^* P^i + [D_1\phi(Q^i,U^i)]^*\Lambda^i + D_q L(Q^i,U^i)\right),\\
0 &= \phi(Q^i,U^i),\\
0 &= [D_2 f(Q^i,U^i)]^* P^i + [D_2\phi(Q^i,U^i)]^*\Lambda^i + D_2 L(Q^i,U^i).
\end{aligned}
$$

Returning to the system given by first forming the adjoint and then discretizing, (3.9a)-(3.9f), one substitutes (3.9c) into (3.9d) to write the internal stages for P^i in terms of p_1, and this gives the above system.

Chapter 4

Type II Hamiltonian Lie Group Variational Integrators with Applications to Geometric Adjoint Sensitivity Analysis

4.1 Introduction

In this paper, we aim to develop Lie group variational integrators from a Type II variational principle with the motivating application of performing intrinsic geometric adjoint sensitivity analysis on Lie groups. Lie Group variational integrators are a class of geometric structure-preserving integrators for integrating Lagrangian or Hamiltonian systems evolving over tangent and cotangent bundles of Lie groups (see [16; 62; 68–70; 81; 86]). Such methods generally have good conservation properties, such as respecting the symplecticity and momentum-preservation of these systems. Adjoint systems provide an efficient method for performing dynamically-constrained optimization and sensitivity analysis. The geometry of these systems has gained interest as it can be described by a Hamiltonian structure. Particularly, the Hamiltonian structure of adjoint systems encode a quadratic conservation law which is the key to adjoint sensitivity analysis [106]. We aim to synthesize these two areas of research, by developing Lie group variational integrators which are applicable to the maximally degenerate Hamiltonian structures found in adjoint systems and hence, develop geometric integrators which respect the quadratic conservation law enjoyed by adjoint systems, making them particularly useful for adjoint sensitivity analysis on Lie groups. We begin with a brief introduction and review of these topics.

4.1.1 Lagrangian and Hamiltonian Variational Integrators

Geometric numerical integration aims to preserve geometric conservation laws under discretization, and this field is surveyed in the monograph by Hairer et al. [51]. Discrete variational mechanics [75; 84] provides a systematic method of constructing symplectic integrators. It is typically approached from a Lagrangian perspective by introducing the *discrete Lagrangian*, $L_d : Q \times Q \to \mathbb{R}$, which is a Type I generating function of a symplectic map and approximates the *exact discrete Lagrangian*, which is constructed from the Lagrangian $L : TQ \to \mathbb{R}$ as

$$L_d^E(q_0, q_1; h) = \operatorname{ext}_{\substack{q \in C^2([0,h],Q) \\ q(0)=q_0, q(h)=q_1}} \int_0^h L(q(t), \dot{q}(t))dt, \tag{4.1.1}$$

which is equivalent to Jacobi's solution of the Hamilton–Jacobi equation. The exact discrete Lagrangian generates the exact discrete-time flow map of a Lagrangian system, but, in general, it cannot be computed explicitly. Instead, this can be approximated by replacing the integral with a quadrature formula, and replacing the space of C^2 curves with a finite-dimensional function space.

Given a finite-dimensional function space $\mathbb{M}^n([0,h]) \subset C^2([0,h], Q)$ and a quadrature formula $\mathscr{G} : C^2([0,h], Q) \to \mathbb{R}$, $\mathscr{G}(f) = h\sum_{j=1}^m b_j f(c_j h) \approx \int_0^h f(t)dt$, the *Galerkin discrete Lagrangian* is

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

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

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

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

$$q_k^1 = q_{k+1}^0, \qquad p_{k+1} = D_2 L_d(q_k^0, q_k^1), \qquad p_k = -D_1 L_d(q_k^0, q_k^1), \tag{4.1.2}$$

where D_i denotes the partial derivative with respect to the i-th argument. Making the identification $q_k = q_k^0 = q_{k-1}^1$, we obtain the *discrete Lagrangian map* and *discrete Hamiltonian map* which are $F_{L_d} : (q_{k-1}, q_k) \mapsto (q_k, q_{k+1})$ and $\tilde{F}_{L_d} : (q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$, respectively. The last two equations of (4.1.2) define the *discrete fiber derivatives*, $\mathbb{F}L_d^{\pm} : Q \times Q \to T^*Q$,

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

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

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

Theorem 4.1.1 (Discrete Noether's theorem (Theorem 1.3.3 of [84]))**.** *If a discrete Lagrangian L_d*

is invariant under the diagonal action of G on $Q \times Q$, then the single unique discrete momentum map, $\mathbf{J}_{L_d} = (\mathbb{F}L_d^{\pm})^* \mathbf{J}$, is invariant under the discrete Lagrangian map F_{L_d}, i.e., $F_{L_d}^* \mathbf{J}_{L_d} = \mathbf{J}_{L_d}$.

Theorem 4.1.2 (Variational error analysis (Theorem 2.3.1 of [84]))**.** *If a discrete Lagrangian L_d approximates the exact discrete Lagrangian L_d^E to order p, i.e., $L_d(q_0, q_1; h) = L_d^E(q_0, q_1; h) + \mathscr{O}(h^{p+1})$, then the discrete Hamiltonian map $\tilde{F}_{L_d}$ is an order p accurate one-step method.*

The bounded energy error of variational integrators can be understood by performing backward error analysis, which then shows that the discrete flow map is approximated with exponential accuracy by the exact flow map of the Hamiltonian vector field of a modified Hamiltonian [11; 111].

Given a degenerate Hamiltonian, where the Legendre transform $\mathbb{F}H : T^*Q \to TQ$, $(q,p) \mapsto (q, \frac{\partial H}{\partial p})$, is noninvertible, there is no equivalent Lagrangian formulation. Thus, a characterization of variational integrators directly in terms of the continuous Hamiltonian is desirable. This is achieved by considering the Type II analogue of Jacobi's solution, given by

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

A computable Galerkin discrete Hamiltonian H_d^+ is obtained by choosing a finite-dimensional function space and a quadrature formula,

$$H_d^+(q_0, p_1) = \operatorname{ext}_{\substack{q\in\mathbb{M}^n([0,h]) \\ q(0)=q_0 \\ (q(c_jh),p(c_jh))\in T^*Q}} \left[p_1 q(t_1) - h \sum_{j=1}^m b_j [p(c_jh)\dot{q}(c_jh) - H(q(c_jh), p(c_jh))] \right].$$

Interestingly, the Galerkin discrete Hamiltonian does not require a choice of a finite-dimensional function space for the curves in the momentum, as the quadrature approximation of the action integral only depend on the momentum values $p(c_jh)$ at the quadrature points, which are determined by the extremization principle. In essence, this is because the action integral does not depend on the time derivative of the momentum $\dot{p}$. As such, both the Galerkin discrete Lagrangian and the Galerkin discrete Hamiltonian depend only on the choice of a finite-dimensional function space for curves in the position, and a quadrature rule. It was shown in Proposition 4.1 of [76] that when the Hamiltonian is hyperregular, and for the same choice of function space and quadrature rule, they induce equivalent numerical methods.

The *Type II discrete Hamilton's phase space variational principle* states that

$$\delta\left\{p_N q_N - \sum_{k=0}^{N-1}\left[p_{k+1}q_{k+1} - H_d^+(q_k, p_{k+1})\right]\right\} = 0,$$

for discrete curves in T^*Q with fixed (q_0, p_N) boundary conditions. This yields the *discrete Hamilton's equations*, which are given by

$$q_{k+1} = D_2 H_d^+(q_k, p_{k+1}), \qquad p_k = D_1 H_d^+(q_k, p_{k+1}). \tag{4.1.3}$$

Given a discrete Hamiltonian H_d^+, we introduce the *discrete fiber derivatives* (or discrete Legendre transforms), $\mathbb{F}^+ H_d^+$,

$$\mathbb{F}^+ H_d^+ : (q_0, p_1) \mapsto (D_2 H_d^+(q_0, p_1), p_1),$$
$$\mathbb{F}^- H_d^+ : (q_0, p_1) \mapsto (q_0, D_1 H_d^+(q_0, p_1)).$$

The discrete Hamiltonian map can be expressed in terms of the discrete fiber derivatives,

$$\tilde{F}_{H_d^+}(q_0, p_0) = \mathbb{F}^+ H_d^+ \circ (\mathbb{F}^- H_d^+)^{-1}(q_0, p_0) = (q_1, p_1),$$

Similar to the Lagrangian case, we have a discrete Noether's theorem and variational error analysis result for Hamiltonian variational integrators.

Theorem 4.1.3 (Discrete Noether's theorem (Theorem 5.3 of [76]))**.** *Given the action Φ on the configuration manifold Q, let Φ^{T^*Q} be the cotangent lifted action on T^*Q. If the generalized discrete Lagrangian $R_d(q_0, q_1, p_1) = p_1 q_1 - H_d^+(q_0, p_1)$ is invariant under the cotangent lifted* *action Φ^{T^*Q}, then the discrete Hamiltonian map $\tilde{F}_{H_d^+}$ preserves the momentum map, i.e., $\tilde{F}^*_{H_d^+}\mathbf{J} = \mathbf{J}$.*

Theorem 4.1.4 (Variational error analysis (Theorem 2.2 of [107]))**.** *If a discrete Hamiltonian H_d^+ approximates the exact discrete Hamiltonian $H_d^{+,E}$ to order p, i.e., $H_d^+(q_0, p_1; h) = H_d^{+,E}(q_0, p_1; h) + \mathscr{O}(h^{p+1})$, then the discrete Hamiltonian map $\tilde{F}_{H_d^+}$ is an order p accurate one-step method.*

It should be noted that there is an analogous theory of discrete Hamiltonian variational integrators based on Type III generating functions $H_d^-(p_0, q_1)$.

Remark 4.1.1. *It should be noted that the current construction of Hamiltonian variational integrators is only valid on vector spaces and local coordinate charts as it involves Type II/Type III generating functions $H_d^+(q_k.p_{k+1})$, $H_d^-(p_k, q_{k+1})$, which depend on the position at one boundary point, and the momentum at the other boundary point. However, this does not make intrinsic sense on a manifold, since one needs the base point in order to specify the corresponding cotangent space. One possible approach to constructing an intrinsic formulation of Hamiltonian variational integrators on general cotangent bundles is to start with discrete Dirac mechanics [75], and consider a generating function $E_d^+(q_k, q_{k+1}, p_{k+1})$, $E_d^-(q_k, p_k, q_{k+1})$, that depends on the position at both boundary points and the momentum at one of the boundary points. This approach can be viewed as a discretization of the generalized energy $E(q, v, p) = \langle p, v\rangle - L(q, v)$, in contrast to the Hamiltonian $H(q, p) = \operatorname{ext}_v \langle p, v\rangle - L(q, v) = \langle p, v\rangle - L(q, v)|_{p=\frac{\partial L}{\partial v}}$.*

As mentioned in the previous remark, an issue with Type II Hamiltonian variational integrators is that they are only valid on vector spaces or on local charts, due to the Type II boundary conditions $q(t_k) = q_k, p(t_{k+1}) = p_{k+1}$, which requires a local trivialization of T^*Q. Furthermore, these methods cannot in general be extended to arbitrary parallelizable manifolds M, i.e., $T^*M \cong M \times V$ for some vector space V, since the isomorphism $T^*M \cong M \times V$ may be neither explicit nor computable. However, for a Lie group G, the trivialization $T^*G \cong G \times \mathfrak{g}^*$ is given simply by left or right translation. Using this trivialization, we will extend the construction of Type II Hamiltonian variational integrators to the setting of Hamiltonian systems on the cotangent bundle of a Lie group.

4.1.2 Lie Group Variational Integrators

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

These ideas were introduced in [68], and applied to a system of extended rigid bodies interacting under their mutual gravitational potential in [69; 70], wherein symmetry reduction to a relative frame is also addressed. The superior computational efficiency of Lie group variational integrators for the full body simulation of systems of extended rigid bodies in the context of astrodynamics was demonstrated in [39].

Lie group variational integrators can be seen as the synthesis of Lie group methods (see, for example, [59]) and variational integrators that serves as the basis for constructing efficient geometric structure-preserving integrators for the dynamics of mechanical systems which evolve on Lie groups.

The basic idea of a Lie group method is to express the solution in terms of an element of the Lie algebra,

$$g(t) = g_0 \exp(\xi(t)),$$

as opposed to a group element, and to use the exponential map and group composition to ensure that the solution remains on the group. The problem reduces to finding an appropriate Lie algebra element $\xi \in \mathfrak{g}$, which is desirable, as the Lie algebra is always linear, even when the Lie group is nonlinear, and interpolants can be easily obtained. We construct an interpolant on the Lie group by using polynomial interpolation at the level of the Lie algebra.

The exponential (or an approximation thereof, such as the Cayley transform, or more generally, the diagonal Padé approximants, for quadratic matrix Lie groups [28]) allows one to approximate a curve on G by a discrete time curve on the Lie algebra. One can combine this with an approximation space for the fibers of $TG \cong G \times \mathfrak{g}$ to obtain a discrete Lagrangian. Enforcing a discrete variational principle then results in a Lie group variational integrator. For more details, see [16; 62; 68–70; 81; 86].

4.1.3 Adjoint Systems and their Geometry

The solution of many nonlinear problems involves successive linearization, and as such variational equations and their adjoints play a critical role in a variety of applications. Adjoint equations are of particular interest when the parameter space has significantly higher dimension than that of the output or objective. In particular, the simulation of adjoint equations arise in sensitivity analysis [25; 26], adaptive mesh refinement [80], uncertainty quantification [118], automatic differentiation [47], superconvergent functional recovery [96], optimal control [102], optimal design [41], optimal estimation [93], and deep learning viewed as an optimal control problem [12].

The study of geometric aspects of adjoint systems arose from the observation that the combination of any system of differential equations and its adjoint equations are described by a formal Lagrangian [57; 58]. This naturally leads to the question of when the formation of adjoints and discretization commutes [110], and prior work on this include the Ross–Fahroo lemma [103], and the observation by Sanz-Serna [106] that the adjoints and discretization commute if and only if the discretization is symplectic.

We will briefly review the geometry of adjoint and variational systems. Let M be a manifold; throughout this paper, we will assume that all manifolds are smooth and finite-dimensional and all maps between them are smooth, unless otherwise stated. Let $\dot{q} = F(q)$ be an ODE on M, specified by a vector field F on M. Then, the adjoint system associated to F is the ODE on T^*M with the coordinate expression

$$\dot{q} = F(q),$$
$$\dot{p} = -[DF(q)]^* p,$$

where DF is the linearization of F. The adjoint system can be viewed as the ODE on T^*M corresponding to the vector field given by the cotangent lift of F. Intrinsically, the adjoint system can be understood as a Hamiltonian system on T^*M relative to the canonical symplectic form on T^*M, with Hamiltonian given by

$$H(q, p) = \langle p, F(q) \rangle.$$

Furthermore, we associate to F the variational system, which is the ODE on TM with coordinate expression

$$\dot{q} = F(q),$$
$$\dot{v} = DF(q)v.$$

The variational system can be viewed as the ODE on TM corresponding to the vector field given by the tangent lift of F.

The importance of the adjoint and variational systems is that they satisfy an adjoint-variational quadratic conservation law: for any solution curves (q, p) of the adjoint system and (q, v) of the variational system, covering the same base curve q, one has

$$\frac{d}{dt} \langle p, v \rangle = 0.$$

This quadratic conservation law is the key to adjoint sensitivity analysis [106]. The interest in studying the geometry of these adjoint and variational systems arises from the fact that this quadratic conservation law can also be interpreted as symplecticity of the Hamiltonian flow of the adjoint system [113].

In [113], we developed Type II variational integrators for adjoint systems for ODEs and DAEs on vector spaces by utilizing their respective symplectic and presymplectic structures. One of the goals of this paper is to extend this construction to the nonlinear setting and in particular, adjoint systems over Lie groups.

4.1.4 Main Contributions

In this paper, we develop a continuous and discrete theory for Type II variational principles on cotangent bundles of Lie groups, which gives an intrinsic meaning to Hamiltonian systems with fixed initial position g_0 and fixed terminal momenta p_1 boundary conditions, in contrast to traditional variational principles for Lie group variational integrators which assume fixed initial and final positions. The motivation for developing Type II variational principles is that the corresponding Type II boundary conditions arise in adjoint sensitivity analysis, which is the motivating application of this paper. Traditionally, such Type II variational principles are only globally defined on vector spaces, or locally defined on charts on a general manifold; however, for Lie groups, left-trivialization allows us to define such a Type II variational principle globally on the cotangent bundle of a Lie group. Specifically, in Section 4.2, we develop a novel Type II variational principle for Hamiltonian systems on cotangent bundles of Lie groups by introducing a d'Alembert variational principle. This is a novel variational principle since typically, variational principles are given by a stationarity condition for the action corresponding to fixed initial and terminal positions, g_0 and g_1; however, in our setting, since the final position g_1 is not fixed, virtual work can be deposited into the system by varying g_1. This is accounted for in our variational principle by demanding that the action is stationary only modulo this virtual work term arising from g_1 boundary variations. Subsequently, we discretize the variational principle to develop structure-preserving numerical methods for such systems. We prove that such methods are symplectic and also momentum-preserving. We also develop a discrete reduction theory for left-invariant systems, and show that the discrete reduction theory can be interpreted as momentum preservation associated to left-invariance.

In Section 4.3, we apply the continuous and discrete theory developed in Section 4.2 to the particular case of adjoint Hamiltonian systems on Lie groups. In the continuous setting, we introduce the adjoint and variational equations associated to an ODE on a Lie group, and prove global existence and uniqueness results for these equations. In the discrete setting, we show how our variational integrators can be used to perform intrinsic structure-preserving adjoint sensitivity analysis on Lie groups. In particular, we show how initial condition sensitivities and parameter sensitivities of cost functions can be computed exactly within this framework. Finally, we conclude with two numerical examples, which utilizes this geometric adjoint sensitivity analysis to solve an initial condition optimization problem and an optimal control problem on $SO(3)$.

4.2 Hamiltonian Variational Integrators on Cotangent Bundles of Lie Groups

In this paper, we aim to construct and analyze geometric integration methods for Hamiltonian dynamics on the cotangent bundle T^*G of a Lie group G, subject to Type II boundary conditions $g(0) = g_0, p(T) = p_1$. Throughout, our our motivating class of examples is adjoint systems.

Example 4.2.1 (Adjoint Systems on Lie Groups)**.** *Consider an ODE on a Lie group G given by $\dot{g} = f(g)$, specified by a vector field F on G. We associate to F the adjoint Hamiltonian $H : T^*G \to \mathbb{R}$, given by*

$$H(g, p) = \langle p, F(q) \rangle.$$

We refer to the Hamiltonian system $i_{X_H}\Omega = dH$, relative to the canonical symplectic form Ω on

T^*G, as the adjoint system associated to the ODE $\dot{g} = F(g)$. The motivation for considering Type II boundary conditions arises from the fact that, viewing the ODE on G as flowing forward in time, the momenta p can be interpreted as flowing backward in time, which backpropagates sensitivity information back to the initial time. We will describe this in more detail in Section 4.3.

We also provide as another motivating example the class of mechanical systems on T^*G. Although we will not be particularly concerned with this class of examples in this paper, it is worthwhile pointing out the distinctions between these two classes of examples (see Remark 4.2.1).

Example 4.2.2 (Mechanical Systems on TG)**.** *We consider a mechanical system on a Lie group G described by a Lagrangian $L : TG \to \mathbb{R}$. By left-trivialization of the tangent bundle,*

$$TG \ni (g, \dot{g}) \mapsto (g, \xi) = (g, g^{-1}\dot{g}) \in G \times \mathfrak{g},$$

the Euler–Lagrange equations for $l(g, \xi) \equiv L(g, g\xi)$ can be expressed as

$$\begin{aligned} \frac{d}{dt}\frac{\delta l}{\delta \xi} &= ad^*_\xi \frac{\delta l}{\delta \xi} + d_g l, \\ \frac{d}{dt} g &= g\xi. \end{aligned}$$

Assuming that the Lagrangian is hyperregular, i.e., $\mathbb{F}L : TG \to T^*G$ is a diffeomorphism, the system can be equivalently described as a Hamiltonian system on T^*G; or by left-trivialization, it can be equivalently described as a Hamiltonian system on $G \times \mathfrak{g}^* \ni (g, \mu)$ given by

$$\begin{aligned} \frac{d}{dt}\mu &= ad^*_\xi \mu + g\frac{\delta l}{\delta g}, \\ \frac{d}{dt} g &= \xi, \\ \mu &= \frac{\delta l}{\delta \xi}. \end{aligned}$$

For more details on this class of examples, see [16; 17; 62].

Remark 4.2.1. *It is interesting to note that these two classes of examples, Example 4.2.1 and Example 4.2.2, are at the opposing ends of the spectrum of regularity and degeneracy for Hamiltonian systems.*

Recall that a Hamiltonian is said to be regular if the Hessian of the Hamiltonian $D_p^2 H(q,p)$ *is invertible for all* $(q,p) \in T^*G$ *and degenerate otherwise. If the Hamiltonian is regular, then the (inverse) Legendre transform* $\mathbb{F}H : T^*G \to TG$ *is a local diffeomorphism.*

On the one hand, systems of the form described in Example 4.2.2 are regular and furthermore, they are maximally regular (or hyperregular) in the sense that $\mathbb{F}H : T^*G \to TG$ *is a global diffeomorphism.*

On the other hand, adjoint systems of the form described in Example 4.2.1 are maximally degenerate, in the sense that the Hessian $D_p^2 H(q,p)$ *is the zero matrix. While this appears to be a deficiency of such systems, we will see that this is a key property of these systems, arising from the fact that these systems are lifts of differential equations on the base space* G*.*

Because adjoint systems are degenerate, they do not admit an equivalent Lagrangian description. As such, we aim to construct integrators for Hamiltonian systems on T^*G *without assuming that they arise from a Lagrangian system.*

4.2.1 A Type II Variational Principle for Hamiltonian Systems on Cotangent Bundles of Lie Groups

A common approach to constructing geometric integrators for Lagrangian and Hamiltonian systems is to restrict the variational principle, from which these systems arise, to some appropriate finite-dimensional space of possible trajectories, and solve the approximate problem on this restricted space. We thus aim to construct integrators for Hamiltonian systems on T^*G by first formulating a variational principle for these systems in the continuous setting and subsequently restricting to a discrete variational principle.

To develop a variational principle for Hamiltonian systems on T^*G, we first consider the boundary conditions that we wish to place on the system. Note that fixed endpoint conditions on the basespace $g(0) = g_0, g(T) = g_1$ are generally incompatible with systems of the form Example 4.2.1, since adjoint systems on T^*G cover first-order ODEs on G and thus, one cannot freely specify both $g(0)$ and $g(T)$. As such, we instead consider Type II boundary conditions of the form $g(0) = g_0, p(T) = p_1$. For general Hamiltonian systems on the cotangent bundle of a manifold, the issue with these boundary conditions is that one cannot intrinsically specify a covector $p(T) = p_1$ without specifying the basepoint $q(T) = q_1$. This is not an issue for adjoint systems in particular, since the time-T flow of the underlying ODE on G determines the basepoint where p_1 is specified. However, since we would like our theory to apply to general Hamiltonian systems on T^*G, we do not want to restrict to adjoint systems in particular. Fortunately, we can make sense of Type II boundary conditions, since T^*G is trivializable by left-translation.

Let $\mathfrak{g} = T_eG$ denote the Lie algebra of G and $\mathfrak{g}^* = T_e^*G$ be its dual. We will denote the duality pairing between $v \in T_gG$ and $p \in T_g^*G$ as $\langle p, v\rangle$, where the base point is understood in context. Let $L_g : G \to G$ denote left-translation by g, $L_g(x) = gx$. Left-translation induces maps on the tangent bundle and cotangent bundle of G by pushforward and pullback, respectively, which we denote as

$$T_xL_g : T_xG \to T_{gx}G,$$

$$T_x^*L_g : T_{gx}^*G \to T_x^*G.$$

For $v_g \in T_gG, p_g \in T_g^*G$, we will denote their left-translations to their respective fibers over the identity as simply

$$g^{-1}v_g \equiv T_gL_{g^{-1}}(v_g) \in \mathfrak{g},$$

$$g^*p_g \equiv T_e^*L_g(p_g) \in \mathfrak{g}^*.$$

This notation is suggestive, since in the case that G is a matrix Lie group, the left-translation of a tangent vector to the fiber over the identity acts by matrix multiplication by the inverse of g and the left-translation of a covector to the fiber over the identity acts by matrix multiplication by the adjoint of g.

A useful fact is that the pairing $\langle p_g, v_g\rangle$ is preserved under left-translation,

$$\begin{aligned}\langle g^* \cdot p_g, g^{-1} \cdot v_g\rangle &= \langle T_e^* L_g(p_g), T_g L_{g^{-1}}(v_g)\rangle \\ &= \langle p_g, T_e L_g \circ T_g L_{g^{-1}}(v_g)\rangle \\ &= \langle p_g, T_g(L_g \circ L_{g^{-1}})(v_g)\rangle \\ &= \langle p_g, v_g\rangle.\end{aligned}$$

By left-translation on the cotangent bundle, we get the left-trivialization $T^*G \cong G \times \mathfrak{g}^*$. With this trivialization, we can make sense of Type II boundary conditions $g(0) = g_0 \in G, \mu(T) = \mu_1 \in \mathfrak{g}^*$, with coordinates (g, μ) on $G \times \mathfrak{g}^*$.

What remains is to construct a variational principle. Recall that the action for a Hamiltonian system on T^*G is given by

$$S[g, p] = \int_0^T \Big(\langle p, \dot{g}\rangle - H(g, p)\Big) dt,$$

where $H : T^*G \to \mathbb{R}$. By left-translation, with $\mu = g^* \cdot p$, we define the left-trivialized Hamiltonian $h : G \times \mathfrak{g}^* \to \mathbb{R}$ as

$$h(g, \mu) \equiv H(g, g^{*-1} \cdot \mu) = H(g, p).$$

The action can then be expressed as

$$\begin{aligned}S[g,p] &= \int_0^T \Big(\langle p,\dot{g}\rangle - H(g,p)\Big)dt \\ &= \int_0^T \Big(\langle g^*\cdot p, g^{-1}\cdot\dot{g}\rangle - H(g,p)\Big)dt \\ &= \int_0^T \Big(\langle \mu, g^{-1}\cdot\dot{g}\rangle - h(g,\mu)\Big)dt =: s[g,\mu];\end{aligned}$$

we refer to $s[g,\mu]$ as the left-trivialized action.

Now, we prescribe boundary conditions $g(0) = g_0 \in G$, $\mu(T) = \mu_1 \in \mathfrak{g}^*$. Given a curve $(g(t), p(t))$ on T^*G, by left-translation, the terminal momenta condition $\mu(T) = \mu_1$ on $\mathfrak{g}^*$ corresponds to $p(T) = g(T)^{*-1}\cdot\mu_1 \in T^*_{g(T)}G$. To state a variational principle, we observe that by left-translation, we can prescribe a boundary condition on $p(T)$ (equivalently, on $\mu(T)$) but we cannot fix the terminal point $g(T)$. As such, a variation δg can always introduce virtual work on the system by varying the terminal point $g(T)$; the virtual work done by varying the terminal point is given by $\langle p(T), \delta g(T)\rangle$, or equivalently, $\langle \mu(T), \eta(T)\rangle$ where we defined the left-trivialization of the variation $\eta = g^{-1}\cdot\delta g$. Thus, we cannot demand the the action S (equivalently, s) is stationary since one can always introduce virtual work as described above; however, we can demand that it is stationary modulo the virtual work that is introduced into the system by varying the terminal point $g(T)$. Thus, we impose the variational principle

$$\delta S[g,p] = \langle p(T), \delta g(T)\rangle,$$

or equivalently, by left translation

$$\delta s[g,\mu] = \langle \mu(T), \eta(T)\rangle,$$

where the variations fix $g(0)$ and $p(T)$ (equivalently, $\mu(T)$). We refer to this variational principle as the Type II d'Alembert variational principle, due to its similarity to the d'Alembert variational principle which utilizes virtual work to derive forced Lagrangian or Hamiltonian systems [84].

Theorem 4.2.1 (Type II d'Alembert Variational Principle)**.** *The following are equivalent*

(i) *The Type II d'Alembert variational principle*

$$\delta S[g,p] = \langle p(T), \delta g(T) \rangle,$$

on T^*G is satisfied, where the variations of the action $\delta g, \delta p$ satisfy $\delta g(0) = 0, \delta p(T) = 0$, corresponding to boundary conditions $g(0) = g_0, p(T) = g(T)^{*-1} \cdot \mu_1$.

(ii) *Hamilton's equations hold in canonical coordinates on T^*G, with the above Type II boundary conditions,*

$$\dot{g} = D_p H(g,p), \tag{4.2.1a}$$

$$\dot{p} = -D_g H(g,p), \tag{4.2.1b}$$

$$g(0) = g_0, \tag{4.2.1c}$$

$$p(T) = g(T)^{*-1} \cdot \mu_1. \tag{4.2.1d}$$

(iii) *The Type II d'Alembert variational principle*

$$\delta s[g,\mu] = \langle \mu(T), \eta(T) \rangle$$

on $G \times \mathfrak{g}^*$ is satisfied, where the variation δg is left-trivialized as $\eta = g^{-1} \cdot \delta g$ and the variation δp is left-trivialized as $\delta\mu = g^* \cdot \delta p$, with $\delta\eta(0) = 0, \delta\mu(T) = 0$, corresponding to boundary conditions $g(0) = g_0, \mu(T) = \mu_1$.

(iv) *The Lie–Poisson equations hold on* $G \times \mathfrak{g}^*$*, with the above Type II boundary conditions,*

$$\dot{g} = g \cdot D_\mu h(g,\mu), \tag{4.2.2a}$$

$$\dot{\mu} = -g^* \cdot D_g h(g,\mu) + \operatorname{ad}^*_{D_\mu h(g,\mu)} \mu, \tag{4.2.2b}$$

$$g(0) = g_0, \tag{4.2.2c}$$

$$\mu(T) = \mu_1. \tag{4.2.2d}$$

Remark 4.2.2. *Above, we denote by* $D_g H, D_p H, D_g h, D_\mu h$ *the functional derivatives satisfying*

$$dH(g,p)\cdot(\delta g,\delta p) = \langle D_g H(g,p), \delta g\rangle + \langle \delta p, D_p H(g,p)\rangle,$$
$$dh(g,\mu)\cdot(\delta g,\delta \mu) = \langle D_g h(g,\mu), \delta g\rangle + \langle \delta \mu, D_\mu h(g,\mu)\rangle.$$

Proof. To see that (i) and (ii) are equivalent, compute the variation of S,

$$\begin{aligned}\delta S[g,p] &= \int_0^T \Big(\langle \delta p, \dot{g}\rangle + \Big\langle p, \frac{d}{dt}\delta g \Big\rangle - \langle D_g H, \delta g\rangle - \langle \delta p, D_p H\rangle \Big) dt \\ &= \int_0^T \Big(\langle \delta p, \dot{g} - D_p H\rangle + \langle -\dot{p} - D_g H, \delta g\rangle \Big) dt + \langle p, \delta g\rangle \Big|_0^T.\end{aligned}$$

If (ii) holds, the integrand above vanishes by the equations of motion; furthermore, $\delta g(0) = 0$. Thus, the above expression reduces to

$$\delta S[g,p] = \langle p(T), \delta g(T)\rangle,$$

i.e., (i) holds. Conversely, if (i) holds, we have

$$0 = \delta S[g,p] - \langle p(T), \delta g(T)\rangle = \int_0^T \Big(\langle \delta p, \dot{g} - D_p H\rangle + \langle -\dot{p} - D_g H, \delta g\rangle \Big) dt.$$

Then, by the fundamental lemma of the calculus of variations, (ii) holds.

To see that (iii) is equivalent to (iv), compute the variation of s. For simplicity, we denote the left-translation of $\dot{g}$ by $\xi = g^{-1}\cdot\dot{g}$ and similarly $\eta = g^{-1}\cdot\delta g$.

$$\begin{aligned}
\delta s[g,\mu] &= \int_0^T \Big(\langle \delta\mu, g^{-1}\cdot\dot{g}\rangle + \Big\langle \mu, g^{-1}\frac{d}{dt}\delta g - g^{-1}\cdot\delta g g^{-1}\cdot\dot{g} \Big\rangle - \langle \delta\mu, D_\mu h\rangle - \langle D_g h, \delta g\rangle \Big) dt \\
&= \int_0^T \Big(\langle \delta\mu, g^{-1}\cdot\dot{g} - D_\mu h\rangle + \langle \mu, \dot{\eta} + \mathrm{ad}_\xi \eta\rangle - \langle g^*\cdot D_g h, \eta\rangle \Big) dt \\
&= \int_0^T \Big(\langle \delta\mu, g^{-1}\cdot\dot{g} - D_\mu h\rangle + \langle -\dot{\mu} + \mathrm{ad}^*_\xi \mu - g^*\cdot D_g h, \eta\rangle \Big) dt + \langle \mu, \eta\rangle\Big|_0^T.
\end{aligned}$$

If (iv) holds, the integrand above vanishes by the equations of motion, noting that $\xi = g^{-1}\cdot\dot{g} = D_\mu h$; furthermore, $\eta(0) = 0$. Thus, the above expression reduces to

$$\delta s[g,\mu] = \langle \mu(T), \eta(T)\rangle,$$

i.e., (iii) holds. Conversely, if (iii) holds, we have

$$0 = \delta s[g,\mu] - \langle \mu(T), \eta(T)\rangle = \int_0^T \Big(\langle \delta\mu, g^{-1}\cdot\dot{g} - D_\mu h\rangle + \langle -\dot{\mu} + \mathrm{ad}^*_\xi \mu - g^*\cdot D_g h, \eta\rangle \Big) dt.$$

Then, by the fundamental lemma of the calculus of variations, (iv) holds. Finally, (i) and (iii) are equivalent by left-translation, since $\langle p(T), \delta g(T)\rangle = \langle \mu(T), \eta(T)\rangle$ and $S[g,p] = s[g,\mu]$. □

Remark 4.2.3. *Note that one can also modify the above variational principle to include external forces by adding the virtual work done by the external force. Given a left-trivialized external force $f : [0,T] \to \mathfrak{g}^*$, one can modify the above variational principle to*

$$\delta s[g,\mu] = \langle \mu(T), \eta(T)\rangle + \int_0^T \langle f, \eta\rangle dt,$$

or equivalently,

$$\delta S[g,p] = \langle p(T), \delta g(T)\rangle + \int_0^T \langle g^{*-1}\cdot f, \delta g\rangle dt.$$

This modifies the momenta equations (4.2.2b) *on* $G \times \mathfrak{g}$ *to include the external force,*

$$\dot{\mu} = -g^* \cdot D_g h(g,\mu) + \mathrm{ad}^*_{D_\mu h(g,\mu)}\mu + f,$$

or equivalently, modifies the momenta equation (4.2.1b) *on* T^*G *to be*

$$\dot{p} = -D_g H(g,p) + g^{*-1} \cdot f.$$

4.2.2 Discrete Hamiltonian Variational Integrators on Cotangent Bundles of Lie Groups

In this section, we develop a discrete counterpart to the continuous Type II variational principle on cotangent bundles of Lie groups developed in the previous section.

Consider the action

$$s[g,\mu] = \int_0^T \Big(\langle \mu, g^{-1} \cdot \dot{g}\rangle - h(g,\mu)\Big)dt.$$

We will construct discrete Hamiltonian variational integrators for the Lie–Poisson system (4.2.2a)-(4.2.2d) by discretizing the Type II d'Alembert variational principle (Theorem 4.2.1).

Partition $[0,T]$ into $\cup_{k=0}^{N-1}[t_k,t_{k+1}]$ where

$$0 = t_0 < t_1 < \cdots < t_{N-1} < t_N = T,$$

with uniformly spaced intervals $t_{k+1} - t_k = \Delta t = T/N$. To discretize the variational principle, we need a sequence of points $\{g_k \in G\}_{k=0}^{N-1}$ which interpolates a curve $g(t) \in G$. A simple way to do this is to utilize a retraction to relate a curve on G to a curve on $\mathfrak{g}$. Let τ be a retraction $\tau : \mathfrak{g} \to G$, which is a C^2-diffeomorphism about the origin such that $\tau(0) = e$. Let $d\tau_\xi : \mathfrak{g} \to \mathfrak{g}$ denote the right-trivialized tangent map of τ and $d\tau_\xi^{-1}$ its inverse (for a definition, see [17]). Using the retraction, we can approximate the velocity $g^{-1}\cdot\dot{g}\in\mathfrak{g}$ by

$$\xi_{k+1}=\tau^{-1}(g_k^{-1}g_{k+1})/\Delta t. \tag{4.2.3}$$

This defines the desired interpolated curve $\{g_k\}$ on G through elements $\{\xi_k\}$ on $\mathfrak{g}$ via $g_{k+1}=g_k\tau(\Delta t\xi_{k+1})$. We approximate the action as

$$s_d[\{g_k\},\{m_k\}]=\sum_{k=0}^{N-1}\Delta t\Big(\langle m_{k+1},\xi_{k+1}\rangle-h(g_k,m_{k+1})\Big),$$

where again $\{\xi_k\}$ and $\{g_k\}$ are related by (4.2.3). Note that, by (4.2.3), the variations in ξ are related to the variations of g; this is explicitly given by ([62])

$$\delta\xi_{k+1}=\delta\tau^{-1}(g_k^{-1}g_{k+1})/\Delta t=d\tau^{-1}_{\Delta t\xi_{k+1}}(-g_k^{-1}\delta g_k+\mathrm{Ad}_{\tau(\Delta t\xi_{k+1})}g_{k+1}^{-1}\delta g_{k+1})/\Delta t. \tag{4.2.4}$$

We now derive a variational integrator from a discrete approximation of the Type II d'Alembert variational principle.

Theorem 4.2.2 (Discrete Type II d'Alembert Variational Principle)**.** *The following are equivalent*

(i) *The discrete Type II d'Alembert variational principle holds*

$$\delta s_d[\{g_k\},\{m_k\}]=\langle(d\tau^{-1}_{-\Delta t\xi_N})^*m_N,g_N^{-1}\delta g_N\rangle,$$

subject to variations $\delta g_k,\delta m_k$ satisfying $\delta g_0=0,\delta m_N=0$, corresponding to Type II boundary conditions which prescribe $g_0=g(0),m_N=m(T)$.

(ii) *The discrete Lie–Poisson equations hold*

$$(d\tau^{-1}_{\Delta t\xi_{k+1}})^* m_{k+1} - \mathrm{Ad}^*_{\tau(\Delta t\xi_k)}(d\tau^{-1}_{\Delta t\xi_k})^* m_k = -\Delta t g_k^* \cdot D_g h(g_k, m_{k+1}), \tag{4.2.5a}$$

$$\xi_{k+1} = D_\mu h(g_k, m_{k+1}), \tag{4.2.5b}$$

$$g_{k+1} = g_k \tau(\Delta t \xi_{k+1}), \tag{4.2.5c}$$

with the above boundary conditions.

Proof. Compute the variation of s_d,

$$\delta s_d = \underbrace{\sum_{k=0}^{N-1} \Delta t \Big[\langle \delta m_{k+1}, \xi_{k+1}\rangle - \langle \delta m_{k+1}, D_\mu h(g_k, m_{k+1})\rangle\Big]}_{\equiv(a)} + \underbrace{\sum_{k=0}^{N-1} \Delta t \Big[\langle m_{k+1}, \delta\xi_{k+1}\rangle - \langle D_g h(g_k, m_{k+1}), \delta g_k\rangle\Big]}_{\equiv(b)}.$$

We will simplify the expressions (a) and (b) individually.

For (a), note that the $k = N-1$ term vanishes since $\delta m_N = 0$. Thus, the sum runs 0 to $N-2$. We re-index $k \to k-1$ so that (a) becomes

$$\text{(a)} = \sum_{k=1}^{N-1} \Delta t \Big[\langle \delta m_k, \xi_k - D_\mu h(g_{k-1}, m_k)\rangle\Big].$$

For (b), we rewrite the variation in ξ in terms of the variation of g,

$$\begin{aligned}
\text{(b)} &= \sum_{k=0}^{N-1} \Delta t \Big[\langle m_{k+1}, d\tau^{-1}_{\Delta t\xi_{k+1}}(-g_k^{-1}\delta g_k + \mathrm{Ad}_{\tau(\Delta t\xi_{k+1})} g_{k+1}^{-1}\delta g_{k+1})/\Delta t\rangle - \langle D_g h(g_k, m_{k+1}), \delta g_k\rangle\Big] \\
&= \sum_{k=0}^{N-1} \Delta t \Big[\langle -(g_k^{-1})^*(d\tau^{-1}_{\Delta t\xi_{k+1}})^* m_{k+1}/\Delta t - D_g h(g_k, m_{k+1}), \delta g_k\rangle\Big] \\
&\quad + \sum_{k=0}^{N-1} \Delta t \langle (g_{k+1}^{-1})^* \mathrm{Ad}^*_{\tau(\Delta t\xi_{k+1})}(d\tau^{-1}_{\Delta t\xi_{k+1}})^* m_{k+1}/\Delta t, \delta g_{k+1}\rangle.
\end{aligned}$$

In the first sum above, note that the $k = 0$ vanishes since $\delta g_0 = 0$. In the second sum above, we explicitly write the $k = N-1$ term and re-index the resulting sum $k \to k-1$. This gives

$$\begin{aligned}
\text{(b)} = \sum_{k=1}^{N-1} \Delta t \Big[\langle -(g_k^{-1})^* (d\tau^{-1}_{\Delta t \xi_{k+1}})^* m_{k+1}/\Delta t - D_g h(g_k, m_{k+1}), \delta g_k \rangle \Big] \\
+ \sum_{k=1}^{N-1} \Delta t \langle (g_k^{-1})^* \mathrm{Ad}^*_{\tau(\Delta t \xi_k)} (d\tau^{-1}_{\Delta t_{\xi_k}})^* m_k/\Delta t, \delta g_k \rangle \\
+ \Delta t \langle (g_N^{-1})^* \mathrm{Ad}^*_{\tau(\Delta t \xi_N)} (d\tau^{-1}_{\Delta t \xi_N})^* m_N/\Delta t, \delta g_N \rangle.
\end{aligned}$$

Note that, since $\mathrm{Ad}^*_{\tau(\Delta t \xi_N)} (d\tau^{-1}_{\Delta t \xi_N})^* = (d\tau^{-1}_{-\Delta t \xi_N})^*$ [17], the last term equals

$$\langle (d\tau^{-1}_{-\Delta t \xi_N})^* m_N, g_N^{-1} \delta g_N \rangle,$$

which is precisely the virtual work term in the discrete Type II d'Alembert variational principle. Putting everything together, we have

$$\begin{aligned}
&\delta s_d[\{g_k\}, \{m_k\}] - \langle (d\tau^{-1}_{-\Delta t \xi_N})^* m_N, g_N^{-1} \delta g_N \rangle \\
&\quad = \sum_{k=1}^{N-1} \Delta t \Big[\langle \delta m_k, \xi_k - D_\mu h(g_{k-1}, m_k) \rangle \\
&\qquad + \langle -(g_k^{-1})^* (d\tau^{-1}_{\Delta t \xi_{k+1}})^* m_{k+1}/\Delta t - D_g h(g_k, m_{k+1}) \\
&\qquad + (g_k^{-1})^* \mathrm{Ad}^*_{\tau(\Delta t \xi_k)} (d\tau^{-1}_{\Delta t_{\xi_k}})^* m_k/\Delta t, \delta g_k \rangle \Big].
\end{aligned}$$

Clearly, if the discrete Lie–Poisson equations hold, then the above vanishes, i.e., the discrete Type II d'Alembert variational principle holds, $\delta s_d[\{g_k\}, \{m_k\}] = \langle (d\tau^{-1}_{-\Delta t \xi_N})^* m_N, g_N^{-1} \delta g_N \rangle$. Conversely, if the discrete Type II d'Alembert variational principle holds, the above vanishes, which gives

$$0 = \sum_{k=1}^{N-1} \Delta t \Big[\langle \delta m_k, \xi_k - D_\mu h(g_{k-1}, m_k) \rangle$$
$$+ \langle -(g_k^{-1})^* (d\tau^{-1}_{\Delta t \xi_{k+1}})^* m_{k+1}/\Delta t - D_g h(g_k, m_{k+1})$$
$$+ (g_k^{-1})^* \mathrm{Ad}^*_{\tau(\Delta t \xi_k)} (d\tau^{-1}_{\Delta t_{\xi_k}})^* m_k/\Delta t, \delta g_k \rangle \Big].$$

Since the variations δm_k and δg_k are arbitrary and independent for $k = 1, \ldots, N-1$, this gives the discrete Lie–Poisson equations (4.2.5a)-(4.2.5c). □

Note that this integrator is similar to (and in some cases, the same as) various variational Lie group integrators in the literature, but there are some important distinctions.

For example, in [17], variational integrators for dynamics on TG are derived through a discrete Hamilton–Pontryagin principle. This can be related to our integrator, given that the Hamiltonian arises from a regular Lagrangian. In particular, if one is given a regular left-trivialized Lagrangian $l(g, \xi)$, from which $h(g, \mu)$ arises via the Legendre transform, then we can invert (4.2.5b) to obtain $m_{k+1} = D_\xi l(g_k, \xi_{k+1})$ and we have the relation $\partial l/\partial g = -\partial h/\partial g$. Substituting these into the equations (4.2.5a)-(4.2.5c) produces equation (4.19) of [17]. Of course, this equivalence does not hold when the Hamiltonian is not regular. In particular, note that the Legendre transform with respect to the Hamiltonian, equation (4.2.5b), appears in the discrete Lie–Poisson equations derived from the Hamiltonian side, as opposed to the Legendre transform with respect to the Lagrangian. Thus, our method is applicable to degenerate Hamiltonian systems, such as adjoint systems, which we will discuss further in Section 4.3.

As previously noted, an important distinction with the above integrator is that it is defined and derived from a variational principle entirely on the Hamiltonian side; this is particularly important when the Hamiltonian is not regular, as in the case of adjoint systems. Furthermore, the variational integrators in the literature make use of fixed endpoint boundary conditions, $\delta g_0 = 0 = \delta g_N$, in the variational principle ([17; 62; 81; 86]). As previously discussed, these boundary conditions are incompatible with adjoint systems. By utilizing a discrete Type II d'Alembert variational principle, we were able to derive an integrator on the Hamiltonian side which does not assume that the Hamiltonian is regular, nor assume fixed endpoint boundary conditions. Thus, as we will see in Section 4.3, we will be able to apply our integrator to adjoint systems to develop a structure-preserving integrator which preserves the quadratic adjoint sensitivity conservation law.

It is also interesting to note the virtual work term arising at the terminal point in the discrete variational principle,

$$\langle (d\tau^{-1}_{-\Delta t \xi_N})^* m_N, g_N^{-1}\delta g_N\rangle$$

is different than what one might expect from the continuous variational principle, $\langle \mu_N, g_N^{-1}\delta g_N\rangle$. This is due to the fact that the retraction relates the dynamics on G to dynamics on $\mathfrak{g}$, and so the pairing $\langle \mu, g^{-1}\dot{g}\rangle$ compared to the pairing $\langle m_k, \xi_k\rangle$ should not be identified, but rather, are related by a coordinate change. In fact, the coordinate change is given by the cotangent lift of τ^{-1}, which is precisely $(d\tau^{-1}_{-\Delta t \xi_N})^*$. As we will see below, this also induces a coordinate change in the expression for the symplectic form, which is the exterior derivative of the one-form corresponding to the above boundary term; the expression for the one-form and its exterior derivative is also derived in [17] through a discrete Hamilton–Pontryagin principle.

Reduction for Left-invariant Hamiltonians

A particularly important class of Hamiltonians are the left-invariant Hamiltonians, which are functions $H : T^*G \to \mathbb{R}$ that are invariant under the cotangent lift of left-multiplication by any $x \in G$, i.e.,

$$H \circ T^*L_x = H \text{ for all } x \in G.$$

In terms of our notation, that is

$$H(xg, x^{*-1}p) = H(g,p) \text{ for all } x \in G,\ (g,p) \in T^*G.$$

For such left-invariant Hamiltonians, the dynamics on T^*G reduce to dynamics on $\mathfrak{g}^*$ [82].

Given a left-invariant Hamiltonian H, we define the reduced Hamiltonian $\tilde{H} : \mathfrak{g}^* \to \mathbb{R}$ by

$$\tilde{H}(\mu) = H(e,\mu).$$

Then, equation (4.2.2b) for $\dot{\mu}$ reduces to

$$\dot{\mu} = \mathrm{ad}^*_{D_\mu \tilde{H}(\mu)} \mu, \tag{4.2.6}$$

where we used that

$$\tilde{H}(\mu) = H(e,\mu) = H(g, g^{*-1}\mu) = h(g,\mu)$$

and hence also, $D_g h(g,\mu) = 0$. Thus, as can be seen from equation (4.2.6), the momentum equation decouples from the dynamics on G: (4.2.6) can be solved independently and subsequently, (4.2.2a) can be used to reconstruct the dynamics on G. Hence, for a left-invariant system, the full dynamics on T^*G is completely encoded by the reduced dynamics on $\mathfrak{g}^*$.

Now, we develop a discrete analogue of the Type II variational principle in the left-invariant setting. Define the reduced discrete action

$$\tilde{s}_d[\{g_k\},\{m_k\}] = \sum_{k=0}^{N-1} \Delta t \Big(\langle m_{k+1}, \xi_{k+1} \rangle - \tilde{H}(m_{k+1}) \Big).$$

Theorem 4.2.3 (Discrete Type II d'Alembert Reduced Variational Principle)**.** *Let $H : T^*G \to \mathbb{R}$ be left-invariant and let $h, \tilde{H}, s_d, \tilde{s}_d$ be defined as above. The following are equivalent*

(i) *The discrete Type II d'Alembert variational principle holds*

$$\delta s_d[\{g_k\},\{m_k\}] = \langle (d\tau^{-1}_{-\Delta t \xi_N})^* m_N, g_N^{-1} \delta g_N \rangle,$$

subject to variations $\delta g_k, \delta m_k$ satisfying $\delta g_0 = 0, \delta m_N = 0$, corresponding to Type II *boundary conditions which prescribe* $g_0 = g(0), m_N = m(T)$.

(ii) *The discrete Lie–Poisson equations hold*

$$
\begin{aligned}
(d\tau^{-1}_{\Delta t\xi_{k+1}})^* m_{k+1} - \mathrm{Ad}^*_{\tau(\Delta t\xi_k)}(d\tau^{-1}_{\Delta t\xi_k})^* m_k &= -\Delta t g_k^* \cdot D_g h(g_k, m_{k+1}), \\
\xi_{k+1} &= D_\mu h(g_k, m_{k+1}), \\
g_{k+1} &= g_k \tau(\Delta t \xi_{k+1}),
\end{aligned}
$$

with the above boundary conditions.

(iii) *The discrete reduced Type II d'Alembert variational principle holds*

$$
\delta \tilde{s}_d[\{g_k\}, \{m_k\}] = \langle (d\tau^{-1}_{-\Delta t\xi_N})^* m_N, g_N^{-1}\delta g_N \rangle,
$$

subject to variations $\delta g_k, \delta m_k$ *satisfying* $\delta g_0 = 0, \delta m_N = 0$*, corresponding to Type II boundary conditions which prescribe* $g_0 = g(0), m_N = m(T)$.

(iv) *The discrete reduced Lie–Poisson equations hold*

$$
(d\tau^{-1}_{\Delta t\xi_{k+1}})^* m_{k+1} - \mathrm{Ad}^*_{\tau(\Delta t\xi_k)}(d\tau^{-1}_{\Delta t\xi_k})^* m_k = 0, \tag{4.2.7a}
$$

$$
\xi_{k+1} = D_\mu \tilde{H}(m_{k+1}), \tag{4.2.7b}
$$

$$
g_{k+1} = g_k \tau(\Delta t \xi_{k+1}), \tag{4.2.7c}
$$

with the above boundary conditions.

Proof. We already know that (i) is equivalent to (ii) by Theorem 4.2.2. Furthermore, (i) is clearly equivalent to (iii), since $s_d = \tilde{s}_d$. To see this, it suffices to show that $h(g, m_{k+1}) = \tilde{H}(m_{k+1})$. By the definition of h, we have

$$
h(g, m_{k+1}) = H(g, g^{*-1} m_{k+1}) = H(e, m_{k+1}) = \tilde{H}(m_{k+1}),
$$

where in the second equality, we used left-invariance of H.

Finally, we show that (ii) is equivalent to (iv). Clearly (4.2.5c) is the same as (4.2.7c). Since $\tilde{H}(m_{k+1}) = H(g_k, m_{k+1})$, we have that

$$D_\mu h(g_k, m_{k+1}) = D_\mu \tilde{H}(m_{k+1}),$$

so that (4.2.5b) is equivalent to (4.2.7b). Finally, we have

$$D_g h(g_k, m_{k+1}) = D_g \tilde{H}(m_{k+1}) = 0,$$

so that (4.2.5a) is equivalent to (4.2.7a). $\square$

In practice, many Hamiltonian systems on T^*G arise from left-invariant Hamiltonians. The practical importance of the reduced formulation is that the dynamics on T^*G (or, equivalently, on $G \times \mathfrak{g}^*$) can be reduced to dynamics on $\mathfrak{g}^*$. To see this, note that we can eliminate $\{\xi_k\}$ in equation (4.2.7a) by using equation (4.2.7b) to obtain

$$(d\tau^{-1}_{\Delta t D_\mu \tilde{H}(m_{k+1})})^* m_{k+1} - \mathrm{Ad}^*_{\tau(\Delta t D_\mu \tilde{H}(m_k))} (d\tau^{-1}_{\Delta t D_\mu \tilde{H}(m_k)})^* m_k = 0,$$

which only involves $\{m_k\}$. In the literature, this is often presented as a discrete coadjoint flow (see, for example, [81; 86]), which we can see by making the definition $\mu_k = (d\tau^{-1}_{\Delta t D_\mu \tilde{H}(m_k)})^* m_k$, so that the above becomes

$$\mu_{k+1} = \mathrm{Ad}^*_{\tau(\Delta t D_\mu \tilde{H}(m_k))} \mu_k. \tag{4.2.8}$$

In the following section, we will derive symplecticity and momentum conservation of the discrete Lie–Poisson equations (4.2.5a)-(4.2.5c). Subsequently, we will derive the discrete reduced Lie–Poisson equation (4.2.8) from a different perspective, by viewing it as a consequence of momentum conservation associated to the left-invariance symmetry.

Discrete Conservation Properties

In this section, we will show that the integrator (4.2.5a)-(4.2.5c) is both symplectic and momentum-preserving. Such symplectic-momentum schemes also enjoy long-term energy stability [84].

Discrete Symplecticity. We now show that the integrator (4.2.5a)-(4.2.5c) is symplectic. In essence, symplecticity of the integrator follows from the fact that the integrator was derived from a discrete variational principle, but we will show it explicitly. We perform the computation explicitly for two reasons. First, the proof of symplecticity for variational integrators is traditionally derived from the boundary term in the variational principle [84] or through the use of a generating function [76]. However, in our case, we utilize a modified d'Alembert Type II variational principle which involves a virtual work term. Thus, we cannot appeal directly to the previous methods. Furthermore, the setup for the proof will introduce the concept of variational equations which will be useful for discussing adjoint systems in Section 4.3; additionally, the computation for symplecticity will be similar to the computation for the quadratic conservation law for discrete adjoint systems.

From the boundary term arising from the variation of the discrete action s_d, we see that the discrete canonical form has the expression

$$\Theta_k = \langle (d\tau^{-1}_{-\Delta t \xi_k})^* m_k, g_k^{-1} dg_k \rangle, \tag{4.2.9}$$

whose action on a vector $\delta_k = \delta m_k \partial/\partial m_k + \delta g_k \partial/\partial g_k$ is given by

$$\Theta_k \cdot \delta_k = \langle (d\tau^{-1}_{-\Delta t \xi_k})^* m_k, g_k^{-1} \delta g_k \rangle.$$

Then, the corresponding discrete symplectic form $\Omega_k \equiv d\Theta_k$ has the expression

$$\Omega_k = \langle (d\tau^{-1}_{-\Delta t \xi_k})^* dm_k \wedge g_k^{-1} dg_k \rangle. \tag{4.2.10}$$

Its action on vectors $\delta_k^i = \delta m_k^i \partial/\partial m_k + \delta g_k^i \partial/\partial g_k$ is given by

$$\Omega_k \cdot (\delta_k^1, \delta_k^2) = \langle (d\tau_{-\Delta t \xi_k}^{-1})^* \delta m_k^1, g_k^{-1} \delta g_k^2 \rangle - \langle (d\tau_{-\Delta t \xi_k}^{-1})^* \delta m_k^2, g_k^{-1} \delta g_k^1 \rangle.$$

Symplecticity of the integrator (4.2.5a)-(4.2.5c) is the statement that $\Omega_{k+1} = \Omega_k$ when the discrete Lie–Poisson equations (4.2.5a)-(4.2.5c) hold, where the symplectic forms are evaluated on first variations of the discrete Lie–Poisson equations, i.e., variations whose flow preserves solutions of the discrete Lie–Poisson equations. Equivalently, such first variations are those which preserve (4.2.5a)-(4.2.5c) to linear order. By linearizing these equations, we obtain

$$\begin{aligned}
(d\tau_{\Delta t \xi_{k+1}}^{-1})^* dm_{k+1} - \mathrm{Ad}^*_{\tau(\Delta t \xi_k)} (d\tau_{\Delta t \xi_k}^{-1})^* dm_k & \qquad (4.2.11a)\\
= -\Delta t g_k^* \cdot D^2_{\mu g} h(g_k, m_{k+1}) dm_{k+1} + \text{variation in } g_k, &\\
d\xi_{k+1} = D^2_{g\mu} h(g_k, m_{k+1}) dg_k + \text{variation in } m_{k+1}, & \qquad (4.2.11b)\\
0 = d(g_{k+1} - g_k \tau(\Delta t \xi_{k+1})). & \qquad (4.2.11c)
\end{aligned}$$

In equation (4.2.11a) above, we omitted the terms involving the variation of (4.2.5a) with respect to g_k. Similarly, in equation (4.2.11b), we omitted the terms involving the variation of (4.2.5b) with respect to m_{k+1}. This is because it is difficult to express the former explicitly but we will write them as follows. Observe that equation (4.2.5a) and (4.2.5b) can respectively be expressed as

$$\frac{\delta}{\delta \eta_k} (\Delta t^{-1} s_d) = 0,$$
$$\frac{\delta}{\delta m_{k+1}} (\Delta t^{-1} s_d) = 0,$$

where $\eta_k = g_k^{-1} \delta g_k$, and the variations in g and ξ are related by the identity (4.2.4). Additionally, the variational derivatives are defined by

$$\delta s_d = \sum_k \left[\left\langle \delta m_{k+1}, \frac{\delta}{\delta m_{k+1}} s_d \right\rangle + \left\langle \frac{\delta}{\delta \eta_k} s_d, \eta_k \right\rangle \right].$$

Thus, the omitted variations in (4.2.11a), (4.2.11b) have the expressions,

$$\frac{\delta^2(\Delta t^{-1} s_d)}{\delta^2 \eta_k} g_k^{-1} dg_k,$$
$$\frac{\delta^2(\Delta t^{-1} s_d)}{\delta^2 m_{k+1}} dm_{k+1},$$

respectively. Additionally, we will combine (4.2.11b)-(4.2.11c). Analogous to the identity (4.2.4), (4.2.11c) can be expressed as

$$d\xi_{k+1} = d\tau^{-1}_{\Delta t \xi_{k+1}} (-g_k^{-1} dg_k + \mathrm{Ad}_{\tau(\Delta t \xi_{k+1})} g_{k+1}^{-1} dg_{k+1})/\Delta t.$$

Thus, we can combine (4.2.11b)-(4.2.11c) to yield

$$d\tau^{-1}_{\Delta t \xi_{k+1}} (-g_k^{-1} dg_k + \mathrm{Ad}_{\tau(\Delta t \xi_{k+1})} g_{k+1}^{-1} dg_{k+1})/\Delta t = D^2_{g\mu} h(g_k, m_{k+1}) dg_k + \frac{\delta^2(\Delta t^{-1} s_d)}{\delta^2 m_{k+1}} dm_{k+1}.$$

We will additionally multiply both sides by Δt and act on both sides by $d\tau_{\Delta t \xi_{k+1}}$. Thus, we have the equations for the first variations of the discrete Lie–Poisson equations,

$$\begin{aligned}(d\tau^{-1}_{\Delta t \xi_{k+1}})^* dm_{k+1} - \mathrm{Ad}^*_{\tau(\Delta t \xi_k)} (d\tau^{-1}_{\Delta t \xi_k})^* dm_k \\ = -\Delta t g_k^* \cdot D^2_{\mu g} h(g_k, m_{k+1}) dm_{k+1} + \frac{\delta^2(\Delta t^{-1} s_d))}{\delta^2 \eta_k} g_k^{-1} dg_k, \end{aligned} \tag{4.2.12a}$$

$$\begin{aligned}-g_k^{-1} dg_k + \mathrm{Ad}_{\tau(\Delta t \xi_{k+1})} g_{k+1}^{-1} dg_{k+1} \\ = \Delta t d\tau_{\Delta t \xi_{k+1}} D^2_{g\mu} h(g_k, m_{k+1}) dg_k + \Delta t d\tau_{\Delta t \xi_{k+1}} \frac{\delta^2(\Delta t^{-1} s_d)}{\delta^2 m_{k+1}} dm_{k+1}. \end{aligned} \tag{4.2.12b}$$

Remark 4.2.4. *In the subsequent proof of symplecticity of the discrete Lie–Poisson equations,* *some notation and manipulations for the computations will be useful.*

First, note that although for notational simplicity we will work at the level of differential forms, we will always implicitly understand that the differential forms will be evaluated on vectors. Because of this, we can manipulate expressions involving differential forms and the duality pairing with a wedge product $\langle \cdot \wedge \cdot \rangle$ *as we would an expression of the ordinary duality pairing. For example, given the expression for* $\Omega_k \cdot (\delta_k^1, \delta_k^2)$ *above, we can manipulate the expression as follows*

$$\Omega_k = \langle (d\tau^{-1}_{-\Delta t \xi_k})^* dm_k \wedge g_k^{-1} dg_k \rangle = \langle dm_k \wedge d\tau^{-1}_{-\Delta t \xi_k} g_k^{-1} dg_k \rangle,$$

i.e., we can move $(d\tau^{-1}_{-\Delta t \xi_k})^*$ *across the duality pairing by taking the adjoint, because we can do so in the expression* $\Omega_k \cdot (\delta_k^1, \delta_k^2)$*, when the differential form is evaluated on vectors.*

Furthermore, for some parts of the subsequent computation, it will be useful to used indexed coordinates. Let g_k^A*,* $A = 1, \ldots, \dim(G)$ *be coordinates for* g_k *on* G *and let* m_{kA} *be coordinates for* m_k *on* $\mathfrak{g}^*$*. Then, for example, a typical duality pairing* $\langle m_k, g_k^{-1} \delta g_k \rangle$ *can be expressed as*

$$\langle m_k, g_k^{-1} \delta g_k \rangle = m_{kA} (g_k^{-1} \delta g_k)^A,$$

where we are using the Einstein summation convention that repeated indices, one raised and one lowered, are implicitly summed over. Similarly, an expression involving differential forms paired with the duality pairing and wedge product, such as $\langle dm_k \wedge g_k^{-1} dg_k \rangle$*, can be expressed as*

$$\langle dm_k \wedge g_k^{-1} dg_k \rangle = dm_{kA} \wedge (g_k^{-1} \delta g_k)^A = dm_{kA} \wedge (g_k^{-1})^A_B \delta g_k^B = (g_k^{-1})^A_B dm_{kA} \wedge \delta g_k^B.$$

In the last equality above, we used bilinearity of the wedge product and the fact that the quantity $(g_k^{-1})^A_B$*, for each index* A, B*, is simply a number. In particular, indexed coordinates will be useful* *for quantities involving the second variations of s_d above, which can be expressed as*

$$\left(\frac{\delta^2 s_d}{\delta^2 \eta_k} g_k^{-1} dg_k\right)_A = \frac{\delta^2 s_d}{\delta \eta^A \delta \eta^B} (g_k^{-1} dg_k)^B,$$
$$\left(\frac{\delta^2 s_d}{\delta^2 m_{k+1}} dm_{k+1}\right)^A = \frac{\delta^2 s_d}{\delta m_{(k+1)A} \delta m_{(k+1)B}} dm_{(k+1)B}.$$

Similarly, the derivatives of the Hamiltonian in indexed coordinates become partial derivatives, e.g.,

$$(D_g h(g_k, m_{k+1}))_A = \frac{\partial}{\partial g_k^A} h(g_k, m_{k+1}).$$

We are now ready to prove the integrator (4.2.5a)-(4.2.5c) is symplectic.

Theorem 4.2.4. *The integrator* (4.2.5a)-(4.2.5c) *is symplectic, i.e., the symplectic form is preserved,*

$$\Omega_{k+1} = \Omega_k,$$

subject to first variations of the discrete Lie–Poisson equations. We will prove this by computing expressions for Ω_{k+1} and Ω_k separately and subsequently showing that their expressions are equivalent.

Proof. We will start with computing an expression for

$$\Omega_{k+1} = \langle (d\tau^{-1}_{-\Delta t \xi_{k+1}})^* dm_{k+1} \wedge g_{k+1}^{-1} dg_{k+1} \rangle.$$

Using the identity $\mathrm{Ad}^*_{\tau(\Delta t \xi_j)}(d\tau^{-1}_{\Delta t \xi_j})^* = (d\tau^{-1}_{-\Delta t \xi_j})^*$ and subsequently, equation (4.2.12a), we have

$$\begin{aligned}
\Omega_{k+1} &= \langle \mathrm{Ad}^*_{\tau(\Delta t \xi_{k+1})}(d\tau^{-1}_{\Delta t \xi_{k+1}})^* dm_{k+1} \wedge g^{-1}_{k+1} dg_{k+1} \rangle \\
&= \langle (d\tau^{-1}_{\Delta t \xi_{k+1}})^* dm_{k+1} \wedge \mathrm{Ad}_{\tau(\Delta t \xi_{k+1})} g^{-1}_{k+1} dg_{k+1} \rangle \\
&= \langle \mathrm{Ad}^*_{\tau(\Delta t \xi_k)}(d\tau^{-1}_{\Delta t \xi_k})^* dm_k \wedge \mathrm{Ad}_{\tau(\Delta t \xi_{k+1})} g^{-1}_{k+1} dg_{k+1} \rangle \\
&\quad - \Delta t \langle g_k^* D^2_{\mu g} h(g_k, m_{k+1}) dm_{k+1} \wedge \mathrm{Ad}_{\tau(\Delta t \xi_{k+1})} g^{-1}_{k+1} dg_{k+1} \rangle \\
&\quad + \left\langle \frac{\delta^2(\Delta t^{-1} s_d)}{\delta \eta_k^2} g_k^{-1} dg_k \wedge \mathrm{Ad}_{\tau(\Delta t \xi_{k+1})} g^{-1}_{k+1} dg_{k+1} \right\rangle .
\end{aligned}$$

Using equation (4.2.12b) in the third term above, this becomes

$$\begin{aligned}
\Omega_{k+1} = &\langle \mathrm{Ad}^*_{\tau(\Delta t \xi_k)}(d\tau^{-1}_{\Delta t \xi_k})^* dm_k \wedge \mathrm{Ad}_{\tau(\Delta t \xi_{k+1})} g^{-1}_{k+1} dg_{k+1} \rangle \\
& - \Delta t \langle g_k^* D^2_{\mu g} h(g_k, m_{k+1}) dm_{k+1} \wedge \mathrm{Ad}_{\tau(\Delta t \xi_{k+1})} g^{-1}_{k+1} dg_{k+1} \rangle \\
& + \left\langle \frac{\delta^2(\Delta t^{-1} s_d)}{\delta^2 \eta_k} g_k^{-1} dg_k \wedge g_k^{-1} dg_k \right\rangle \\
& + \Delta t \left\langle \frac{\delta^2(\Delta t^{-1} s_d)}{\delta^2 \eta_k} g_k^{-1} dg_k \wedge d\tau_{\Delta t \xi_{k+1}} D^2_{g\mu} h(g_k, m_{k+1}) dg_k \right\rangle \\
& + \Delta t \left\langle \frac{\delta^2(\Delta t^{-1} s_d)}{\delta^2 \eta_k} g_k^{-1} dg_k \wedge d\tau_{\Delta t \xi_{k+1}} \frac{\delta^2(\Delta t^{-1} s_d)}{\delta^2 m_{k+1}} dm_{k+1} \right\rangle .
\end{aligned}$$

The third term above vanishes by the symmetry of the second variation and the asymmetry of the wedge product. To see this, in coordinates, the third term above can be expressed as

$$\Delta t^{-1} \left\langle \frac{\delta^2 s_d}{\delta^2 \eta_k} g_k^{-1} dg_k \wedge g_k^{-1} dg_k \right\rangle = \Delta t^{-1} \frac{\delta^2 s_d}{\delta \eta_k^A \delta \eta_k^B} (g_k^{-1} dg_k)^A \wedge (g_k^{-1} dg_k)^B .$$

The second variation of s_d above is symmetric under the interchange $A \leftrightarrow B$ while the wedge product above is antisymmetric under the interchange $A \leftrightarrow B$; hence, this term vanishes. Thus, we have the expression

$$\Omega_{k+1} = \underbrace{\langle \mathrm{Ad}^*_{\tau(\Delta t \xi_k)} (d\tau^{-1}_{\Delta t \xi_k})^* dm_k \wedge \mathrm{Ad}_{\tau(\Delta t \xi_{k+1})} g^{-1}_{k+1} dg_{k+1} \rangle}_{\equiv (a1)}$$
$$\underbrace{-\Delta t \langle g^*_k D^2_{\mu g} h(g_k, m_{k+1}) dm_{k+1} \wedge \mathrm{Ad}_{\tau(\Delta t \xi_{k+1})} g^{-1}_{k+1} dg_{k+1} \rangle}_{\equiv (a2)}$$
$$\underbrace{+\Delta t \left\langle \frac{\delta^2 (\Delta t^{-1} s_d)}{\delta^2 \eta_k} g_k^{-1} dg_k \wedge d\tau_{\Delta t \xi_{k+1}} D^2_{g\mu} h(g_k, m_{k+1}) dg_k \right\rangle}_{\equiv (a3)}$$
$$\underbrace{+\Delta t \left\langle \frac{\delta^2 (\Delta t^{-1} s_d)}{\delta^2 \eta_k} g_k^{-1} dg_k \wedge d\tau_{\Delta t \xi_{k+1}} \frac{\delta^2 (\Delta t^{-1} s_d)}{\delta^2 m_{k+1}} dm_{k+1} \right\rangle}_{\equiv (a4)}..$$

Now, we will determine an expression for

$$\Omega_k = \langle (d\tau^{-1}_{-\Delta t \xi_k})^* dm_k \wedge g_k^{-1} dg_k \rangle.$$

Using equation (4.2.12b), we have

$$\begin{aligned}
\Omega_k &= \langle (d\tau^{-1}_{-\Delta t \xi_k})^* dm_k \wedge g_k^{-1} dg_k \rangle \\
&= \langle (d\tau^{-1}_{-\Delta t \xi_k})^* dm_k \wedge \mathrm{Ad}_{\tau(\Delta t \xi_{k+1})} g^{-1}_{k+1} dg_{k+1} \rangle \\
&\quad - \Delta t \langle (d\tau^{-1}_{-\Delta t \xi_k})^* dm_k \wedge d\tau_{\Delta t \xi_{k+1}} D^2_{g\mu} h(g_k, m_{k+1}) dg_k \rangle \\
&\quad - \Delta t \left\langle (d\tau^{-1}_{-\Delta t \xi_k})^* dm_k \wedge d\tau_{\Delta t \xi_{k+1}} \frac{\delta^2 (\Delta t^{-1} s_d)}{\delta^2 m_{k+1}} dm_{k+1} \right\rangle.
\end{aligned}$$

Using equation (4.2.12a) in the third term above, this becomes

$$
\begin{aligned}
\Omega_k &= \langle (d\tau^{-1}_{-\Delta t \xi_k})^* dm_k \wedge g_k^{-1} dg_k \rangle \\
&= \langle (d\tau^{-1}_{-\Delta t \xi_k})^* dm_k \wedge \mathrm{Ad}_{\tau(\Delta t \xi_{k+1})} g_{k+1}^{-1} dg_{k+1} \rangle \\
&\quad - \Delta t \langle (d\tau^{-1}_{-\Delta t \xi_k})^* dm_k \wedge d\tau_{\Delta t \xi_{k+1}} D^2_{g\mu} h(g_k, m_{k+1}) dg_k \rangle \\
&\quad - \Delta t \left\langle (d\tau^{-1}_{\Delta t \xi_{k+1}})^* dm_{k+1} \wedge d\tau_{\Delta t \xi_{k+1}} \frac{\delta^2(\Delta t^{-1} s_d)}{\delta^2 m_{k+1}} dm_{k+1} \right\rangle \\
&\quad - \Delta t^2 \left\langle g_k^* D^2_{\mu g} h(g_k, m_{k+1}) dm_{k+1} \wedge d\tau_{\Delta t \xi_{k+1}} \frac{\delta^2(\Delta t^{-1} s_d)}{\delta^2 m_{k+1}} dm_{k+1} \right\rangle \\
&\quad - \Delta t \left\langle \frac{\delta^2(\Delta t^{-1} s_d)}{\delta^2 \eta_k} g_k^{-1} dg_k \wedge d\tau_{\Delta t \xi_{k+1}} \frac{\delta^2(\Delta t^{-1} s_d)}{\delta^2 m_{k+1}} dm_{k+1} \right\rangle .
\end{aligned}
$$

The third term above can be expressed as

$$
-\left\langle (d\tau^{-1}_{\Delta t \xi_{k+1}})^* dm_{k+1} \wedge d\tau_{\Delta t \xi_{k+1}} \frac{\delta^2 s_d}{\delta^2 m_{k+1}} dm_{k+1} \right\rangle = -\left\langle dm_{k+1} \wedge \frac{\delta^2 s_d}{\delta^2 m_{k+1}} dm_{k+1} \right\rangle .
$$

By applying an analogous symmetry and antisymmetry argument to the term in Ω_{k+1}, this term vanishes. Thus, we have the expression

$$
\begin{aligned}
\Omega_k = &\underbrace{\langle (d\tau^{-1}_{-\Delta t \xi_k})^* dm_k \wedge \mathrm{Ad}_{\tau(\Delta t \xi_{k+1})} g_{k+1}^{-1} dg_{k+1} \rangle}_{\equiv (\mathrm{b1})} \\
&\underbrace{- \Delta t \langle (d\tau^{-1}_{-\Delta t \xi_k})^* dm_k \wedge d\tau_{\Delta t \xi_{k+1}} D^2_{g\mu} h(g_k, m_{k+1}) dg_k \rangle}_{\equiv (\mathrm{b2})} \\
&\underbrace{- \Delta t^2 \left\langle g_k^* D^2_{\mu g} h(g_k, m_{k+1}) dm_{k+1} \wedge d\tau_{\Delta t \xi_{k+1}} \frac{\delta^2(\Delta t^{-1} s_d)}{\delta^2 m_{k+1}} dm_{k+1} \right\rangle}_{\equiv (\mathrm{b3})} \\
&\underbrace{- \Delta t \left\langle \frac{\delta^2(\Delta t^{-1} s_d)}{\delta^2 \eta_k} g_k^{-1} dg_k \wedge d\tau_{\Delta t \xi_{k+1}} \frac{\delta^2(\Delta t^{-1} s_d)}{\delta^2 m_{k+1}} dm_{k+1} \right\rangle}_{\equiv (\mathrm{b4})} .
\end{aligned}
$$

Comparing the expressions for Ω_{k+1} and Ω_k above, we see that $(\mathrm{a1}) = (\mathrm{b1})$ (using the identity

$\mathrm{Ad}^*_{\tau(\Delta t\xi_j)}(d\tau^{-1}_{\Delta t\xi_j})^* = (d\tau^{-1}_{-\Delta t\xi_j})^*$); additionally, we see that (a4) = (b4). Thus, we have left to show that (a2) + (a3) = (b2) + (b3). Equivalently, we have to show that (a2) − (b3) = (b2) − (a3). We will compute both sides of this expression.

Starting with the left hand side, we have

$$\begin{aligned}
(\text{a2}) - (\text{b3}) &= -\Delta t\langle g_k^* D^2_{\mu g} h(g_k, m_{k+1}) dm_{k+1} \wedge \mathrm{Ad}_{\tau(\Delta t\xi_{k+1})} g_{k+1}^{-1} dg_{k+1}\rangle \\
&\quad + \Delta t^2 \left\langle g_k^* D^2_{\mu g} h(g_k, m_{k+1}) dm_{k+1} \wedge d\tau_{\Delta t\xi_{k+1}} \frac{\delta^2(\Delta t^{-1} s_d)}{\delta^2 m_{k+1}} dm_{k+1} \right\rangle \\
&= -\Delta t \Big\langle g_k^* D^2_{\mu g} h(g_k, m_{k+1}) dm_{k+1} \\
&\qquad \wedge \left(\mathrm{Ad}_{\tau(\Delta t\xi_{k+1})} g_{k+1}^{-1} dg_{k+1} - \Delta t d\tau_{\Delta t\xi_{k+1}} \frac{\delta^2(\Delta t^{-1} s_d)}{\delta^2 m_{k+1}} dm_{k+1} \right) \Big\rangle \\
&= -\Delta t \left\langle g_k^* D^2_{\mu g} h(g_k, m_{k+1}) dm_{k+1} \wedge \left(g_k^{-1} dg_k + \Delta t d\tau_{\Delta t\xi_{k+1}} D^2_{g\mu} h(g_k, m_{k+1}) dg_k \right) \right\rangle,
\end{aligned}$$

where in the last equality, we used (4.2.12b). We split this expression into two terms

$$\begin{aligned}
(\text{a2}) - (\text{b3}) = &\underbrace{-\Delta t \left\langle g_k^* D^2_{\mu g} h(g_k, m_{k+1}) dm_{k+1} \wedge g_k^{-1} dg_k \right\rangle}_{\equiv(\text{x1})} \\
&\underbrace{-\Delta t^2 \left\langle g_k^* D^2_{\mu g} h(g_k, m_{k+1}) dm_{k+1} \wedge d\tau_{\Delta t\xi_{k+1}} D^2_{g\mu} h(g_k, m_{k+1}) dg_k \right\rangle}_{\equiv(\text{x2})}.
\end{aligned}$$

For the right hand side, we have

$$\begin{aligned}
(\text{b2}) - (\text{a3}) &= -\Delta t\langle (d\tau^{-1}_{-\Delta t\xi_k})^* dm_k \wedge d\tau_{\Delta t\xi_{k+1}} D^2_{g\mu} h(g_k, m_{k+1}) dg_k\rangle \\
&\quad - \Delta t \left\langle \frac{\delta^2 s_k}{\delta^2 \eta_k} g_k^{-1} dg_k \wedge d\tau_{\Delta t\xi_{k+1}} D^2_{g\mu} h(g_k, m_{k+1}) dg_k \right\rangle \\
&= -\Delta t \left\langle \left((d\tau^{-1}_{-\Delta t\xi_k})^* dm_k + \frac{\delta^2(\Delta t^{-1} s_d)}{\delta^2 \eta_k} g_k^{-1} dg_k \right) \wedge d\tau_{\Delta t\xi_{k+1}} D^2_{g\mu} h(g_k, m_{k+1}) dg_k \right\rangle \\
&= -\Delta t \Big\langle \left((d\tau^{-1}_{\Delta t\xi_{k+1}})^* dm_{k+1} + \Delta t g_k^* D^2_{\mu g} h(g_k, m_{k+1}) dm_{k+1} \right) \\
&\qquad \wedge d\tau_{\Delta t\xi_{k+1}} D^2_{g\mu} h(g_k, m_{k+1}) dg_k \Big\rangle
\end{aligned}$$

We split this expression into two terms

$$(\mathrm{b2}) - (\mathrm{a3}) = \underbrace{-\Delta t \left\langle (d\tau^{-1}_{\Delta t \xi_{k+1}})^* dm_{k+1} \wedge d\tau_{\Delta t \xi_{k+1}} D^2_{g\mu} h(g_k, m_{k+1}) dg_k \right\rangle}_{\equiv(\mathrm{y1})}$$
$$\underbrace{-\Delta t^2 \left\langle g_k^* D^2_{\mu g} h(g_k, m_{k+1}) dm_{k+1} \wedge d\tau_{\Delta t \xi_{k+1}} D^2_{g\mu} h(g_k, m_{k+1}) dg_k \right\rangle}_{\equiv(\mathrm{y2})}.$$

Clearly, (x2) = (y2). Furthermore, we express (y1) as

$$\begin{aligned}
(\mathrm{y1}) &= -\Delta t \left\langle (d\tau^{-1}_{\Delta t \xi_{k+1}})^* dm_{k+1} \wedge d\tau_{\Delta t \xi_{k+1}} D^2_{g\mu} h(g_k, m_{k+1}) dg_k \right\rangle \\
&= -\Delta t \left\langle dm_{k+1} \wedge D^2_{g\mu} h(g_k, m_{k+1}) dg_k \right\rangle \\
&= -\Delta t \, dm_{(k+1)A} \wedge \frac{\partial^2}{\partial g^B \partial \mu_A} h(g_k, m_{k+1}) dg_k^B \\
&= -\Delta t \frac{\partial^2}{\partial g^B \partial \mu_A} h(g_k, m_{k+1}) dm_{(k+1)A} \wedge dg_k^B.
\end{aligned}$$

We express (x1) as

$$\begin{aligned}
(\mathrm{x1}) &= -\Delta t \left\langle g_k^* D^2_{\mu g} h(g_k, m_{k+1}) dm_{k+1} \wedge g_k^{-1} dg_k \right\rangle \\
&= -\Delta t \left\langle D^2_{\mu g} h(g_k, m_{k+1}) dm_{k+1} \wedge dg_k \right\rangle \\
&= -\Delta t \frac{\partial^2}{\partial g^B \partial \mu_A} h(g_k, m_{k+1}) dm_{(k+1)A} \wedge dg_k^B.
\end{aligned}$$

Thus, (x1) = (y1) and so we have shown (a2) − (b3) = (b2) − (a3). Thus, $\Omega_{k+1} = \Omega_k$ as claimed. □

Discrete Noether's Theorem. We will now show that the integrator (4.2.5a)-(4.2.5c) preserves the momentum map associated with a symmetry of the discrete action.

Let $\{g_k^\varepsilon, m_k^\varepsilon\}$ be a one-parameter family of discrete time curves with $g_k^0 = g_k$ and $m_k^0 = m_k$.

Let

$$\delta g_k = \frac{d}{d\varepsilon} g_k^\varepsilon \Big|_{\varepsilon=0},$$
$$\delta m_k = \frac{d}{d\varepsilon} m_k^\varepsilon \Big|_{\varepsilon=0},$$

denote the variations associated to the one-parameter family of discrete time curves. Furthermore, let $s_k = \langle m_{k+1}, \xi_{k+1} \rangle - h(g_k, m_{k+1})$ denote the k^{th} discrete action density. Then, we have the following momentum preservation property of (4.2.5a)-(4.2.5c).

Theorem 4.2.5 (Discrete Noether's Theorem)**.** *Suppose that* (4.2.5a)-(4.2.5c) *hold and furthermore, suppose that the k^{th} discrete action density is invariant under the above variations,*

$$\delta s_k = 0.$$

Then, for any time indices $I < J$,

$$\Theta_I \cdot \delta g_I = \Theta_J \cdot \delta g_J, \tag{4.2.13}$$

where Θ_k is the discrete canonical form (4.2.9)*.*

Proof. Define the IJ-partial discrete action sum as

$$s_d^{IJ} \equiv \sum_{k=I}^{J-1} \Delta t s_k.$$

By assumption, $\delta s_d^{IJ} = 0$ subject to the above variations. We compute the variation explicitly

$$
\begin{aligned}
0 = \delta s_d^{IJ} &= \sum_{k=I}^{J-1} \Delta t \delta s_k \\
&= \sum_{k=I}^{J-1} \Delta t \langle \delta m_{k+1}, \xi_{k+1} - D_\mu h(g_k, m_{k+1}) \rangle \\
&\quad + \sum_{k=I}^{J-1} \Big[\langle m_{k+1}, \delta \xi_{k+1} \rangle - \langle D_g h(g_k, m_{k+1}), \delta g_k \rangle \Big].
\end{aligned}
$$

The first sum above vanishes by (4.2.5b). Analogous to the proof of Theorem 4.2.2, we rewrite the second sum by rewriting the variations $\{\delta\xi_k\}$ in terms of $\{\delta g_k\}$. This gives

$$
\begin{aligned}
0 &= \delta s_d^{IJ} \\
&= \sum_{k=I}^{J-1} \Delta t \langle -(g_k^{-1})^* (d\tau^{-1}_{\Delta t \xi_{k+1}})^* m_{k+1}/\Delta t - D_g h(g_k, m_{k+1}), \delta g_k \rangle \\
&\quad + \sum_{k=I}^{J-1} \Delta t \langle (g_{k+1})^* \mathrm{Ad}^*_{\tau(\Delta t \xi_{k+1})} (d\tau^{-1}_{\Delta t \xi_{k+1}})^* m_{k+1}/\Delta t, \delta g_{k+1} \rangle.
\end{aligned}
$$

We explicitly write the $k = I$ term in the first sum above and the $k = J-1$ term in the second sum, and subsequently, reindex the second sum from $k \to k-1$. This gives

$$
\begin{aligned}
0 &= \delta s_d^{IJ} \\
&= \Delta t \langle -(g_I^{-1})^* (d\tau^{-1}_{\Delta t \xi_{I+1}})^* m_{I+1}/\Delta t - D_g h(g_I, m_{I+1}), \delta g_I \rangle \\
&\quad + \Delta t \langle (g_J)^* \mathrm{Ad}^*_{\tau(\Delta t \xi_J)} (d\tau^{-1}_{\Delta t \xi_J})^* m_J/\Delta t, \delta g_J \rangle + \\
&\quad + \sum_{k=I+1}^{J-1} \Delta t \Big[\langle -(g_k^{-1})^* (d\tau^{-1}_{\Delta t \xi_{k+1}})^* m_{k+1}/\Delta t - D_g h(g_k, m_{k+1}) \\
&\qquad\qquad + (g_k)^* \mathrm{Ad}^*_{\tau(\Delta t \xi_k)} (d\tau^{-1}_{\Delta t \xi_k})^* m_k/\Delta t, \delta g_k \rangle \Big].
\end{aligned}
$$

The summation above vanishes by (4.2.5a). Additionally, we rewrite the first term above using (4.2.5a) and we rewrite the second term above using the identity $\mathrm{Ad}^*_{\tau(\Delta t \xi_J)} (d\tau^{-1}_{\Delta t \xi_J})^* = (d\tau^{-1}_{-\Delta t \xi_J})^*$.

Hence,

$$
\begin{aligned}
0 &= \delta s_d^{IJ} \\
&= -\langle (d\tau^{-1}_{-\Delta t \xi_I})^* m_I, g_I^{-1} \delta g_I \rangle + \langle (d\tau^{-1}_{-\Delta t \xi_J})^* m_J, g_J^{-1} \delta g_J \rangle \\
&= -\Theta_I \cdot \delta g_I + \Theta_J \cdot \delta g_J. \qquad \square
\end{aligned}
$$

As an application of Theorem 4.2.5, we will re-derive the discrete reduced Lie–Poisson equation (4.2.8), interpreted as momentum conservation associated to left-invariance symmetry. Let H be a left-invariant Hamiltonian, let X be a right-invariant vector field on G with $X(e) = \chi \in \mathfrak{g}$, and let φ_ε denote the time-ε flow of X. We choose X to be a right-invariant vector field, since its flow is given by left translations

$$
\varphi_\varepsilon(g) = e^{\varepsilon\chi} g.
$$

We define a one-parameter family of discrete time curves $\{g_k^\varepsilon, m_k^\varepsilon\}$ as

$$
\begin{aligned}
g_k^\varepsilon &= \varphi_\varepsilon(g_k) = e^{\varepsilon\chi} g, \\
m_k^\varepsilon &= m_k,
\end{aligned}
$$

i.e., the one-parameter family of discrete time curves is defined by flowing g_k by φ_ε, whereas m_k^ε remains constant with ε. To see why we defined m_k^ε this way, recall that the left-trivialized momenta m_k corresponds to a momenta $p_k = (g_k)^{*-1} m_k$ or equivalently, $m_k = g_k^* p_k$. For a given $x \in G$, the point (g_k, p_k) transforms under the cotangent lift of left-multiplication by x as $(g_k, p_k) \mapsto (x g_k, x^{*-1} p_k)$. Thus, m_k transforms as

$$
m_k = g_k^* p_k \mapsto (x g_k)^* x^{*-1} p_k = g_k^* x^* x^{*-1} p_k = g_k^* p_k = m_k,
$$

i.e., m_k is invariant under this transformation; thus, we define m_k^ε to be constant in ε. Additionally, observe that the variations associated to this one-parameter family of discrete time curves can be expressed as

$$\delta g_k = \frac{d}{d\varepsilon}\Big|_0 g_k^\varepsilon = \frac{d}{d\varepsilon}\Big|_0 \varphi_\varepsilon(g_k) = X(g_k),$$
$$\delta m_k = \frac{d}{d\varepsilon}\Big|_0 m_k^\varepsilon = \frac{d}{d\varepsilon}\Big|_0 m_k = 0.$$

Now, we will verify the assumption of Theorem 4.2.5. The k^{th} discrete action density is

$$s_k = \langle m_{k+1}, \xi_{k+1}\rangle - h(g_k, m_{k+1}) = \langle m_{k+1}, \xi_{k+1}\rangle - \tilde{H}(m_{k+1}),$$

where in the second equality, we used that $h(g_k, m_{k+1}) = \tilde{H}(m_{k+1})$ for a left-invariant Hamiltonian (see Section 4.2.2). As stated above, $m_j^\varepsilon = m_j$ is invariant under this transformation. Furthermore, since $\xi_j = \tau^{-1}(g_k^{-1} g_{k+1})/\Delta t$, the corresponding transformation for ξ_j is given by

$$\begin{aligned}\xi_j^\varepsilon &= \tau^{-1}((g_k^\varepsilon)^{-1} g_{k+1}^\varepsilon)/\Delta = \tau^{-1}((e^{\varepsilon\chi} g_k)^{-1} e^{\varepsilon\chi} g_{k+1})/\Delta t \\ &= \tau^{-1}(g_k^{-1}(e^{\varepsilon\chi})^{-1} e^{\varepsilon\chi} g_{k+1})/\Delta = \tau^{-1}(g_k^{-1} g_{k+1})/\Delta t = \xi_j,\end{aligned}$$

i.e., ξ_j is also invariant under this transformation. Hence, s_k is invariant under the above variation, so Theorem 4.2.5 applies. We thus have $\Theta_{k+1}\cdot\delta g_{k+1} = \Theta_k \cdot \delta g_k$, i.e.,

$$\langle (d\tau^{-1}_{-\Delta t \xi_{k+1}})^* m_{k+1}, g_{k+1}^{-1}\delta g_{k+1}\rangle = \langle (d\tau^{-1}_{-\Delta t \xi_k})^* m_k, g_k^{-1}\delta g_k\rangle.$$

Equivalently, this can be expressed as

$$\Longrightarrow \langle g_{k+1}^{*-1}(d\tau^{-1}_{-\Delta t \xi_{k+1}})^* m_{k+1}, \delta g_{k+1}\rangle = \langle g_k^{*-1}(d\tau^{-1}_{-\Delta t \xi_k})^* m_k, \delta g_k\rangle,$$
$$\Longrightarrow \langle g_{k+1}^{*-1}(d\tau^{-1}_{-\Delta t \xi_{k+1}})^* m_{k+1} g_{k+1}^*, \delta g_{k+1} g_{k+1}^{-1}\rangle = \langle g_k^{*-1}(d\tau^{-1}_{-\Delta t \xi_k})^* m_k g_k^*, \delta g_k g_k^{-1}\rangle.$$

Now, observe that since X is right-invariant,

$$\delta g_j g_j^{-1} = X(g_j)g_j^{-1} = X(g_j g_j^{-1}) = X(e) = \chi.$$

Hence, we have

$$\langle g_{k+1}^{*-1}(d\tau^{-1}_{-\Delta t\xi_{k+1}})^* m_{k+1} g_{k+1}^*, \chi\rangle = \langle g_k^{*-1}(d\tau^{-1}_{-\Delta t\xi_k})^* m_k g_k^*, \chi\rangle.$$

In particular, $\chi \in \mathfrak{g}$ was arbitrary, so we have

$$g_{k+1}^{*-1}(d\tau^{-1}_{-\Delta t\xi_{k+1}})^* m_{k+1} g_{k+1}^* = g_k^{*-1}(d\tau^{-1}_{-\Delta t\xi_k})^* m_k g_k^*.$$

Multiplying on the left by g_k^* and on the right by g_k^{*-1} gives

$$\mathrm{Ad}^*_{g_k}\mathrm{Ad}^*_{g_{k+1}^{-1}}(d\tau^{-1}_{-\Delta t\xi_{k+1}})^* m_{k+1} = (d\tau^{-1}_{-\Delta t\xi_k})^* m_k.$$

Since for any $x, y \in G$, $\mathrm{Ad}_x\mathrm{Ad}_y = \mathrm{Ad}_{xy}$ and $\mathrm{Ad}_{x^{-1}} = \mathrm{Ad}_x^{-1}$, we have

$$\mathrm{Ad}^*_{g_k}\mathrm{Ad}^*_{g_{k+1}^{-1}} = \mathrm{Ad}^*_{g_{k+1}^{-1}g_k} = \mathrm{Ad}^*_{(g_k^{-1}g_{k+1})^{-1}} = \mathrm{Ad}^*_{\tau(\Delta t\xi_{k+1})^{-1}} = \mathrm{Ad}^{*-1}_{\tau(\Delta t\xi_{k+1})}.$$

Using this in the equation above yields

$$\mathrm{Ad}^{*-1}_{\tau(\Delta t\xi_{k+1})}(d\tau^{-1}_{-\Delta t\xi_{k+1}})^* m_{k+1} = (d\tau^{-1}_{-\Delta t\xi_k})^* m_k.$$

From the identity $\mathrm{Ad}^*_{\tau(\Delta t\xi_j)}(d\tau^{-1}_{\Delta t\xi_j})^* = (d\tau^{-1}_{-\Delta t\xi_j})^*$, we can rewrite the left and right hand sides as

$$(d\tau^{-1}_{-\Delta t\xi_{k+1}})^* m_{k+1} = \mathrm{Ad}^*_{\tau(\Delta t\xi_k)}(d\tau^{-1}_{\Delta t\xi_k})^* m_k,$$

which is precisely the discrete reduced Lie–Poisson equation (4.2.7a).

4.3 Adjoint Systems on Lie Groups

The aim of this section is to develop the geometric theory of adjoint sensitivity analysis on Lie groups, in both the continuous and discrete settings. We thus focus on the case where the Hamiltonian system on T^*G is an adjoint system, as introduced in Example 4.2.1.

Let F be a vector field on G and consider the differential equation $\dot{g} = F(g)$. We define the adjoint Hamiltonian associated to F as

$$\begin{aligned} H &: T^*G \to \mathbb{R}, \\ (g,p) &\mapsto H(g,p) \equiv \langle p, F(g) \rangle. \end{aligned}$$

In canonical coordinates (g,p) on T^*G, the adjoint system (4.2.1a)-(4.2.1b) has the form

$$\begin{aligned} \dot{g} &= F(g), \\ \dot{p} &= -[DF(g)]^* p. \end{aligned}$$

We begin by computing the Lie–Poisson equations (4.2.2a)-(4.2.2b) for this particular class of adjoint Hamiltonian systems. We denote by f the left-trivialization of F,

$$\begin{aligned} f &: G \to \mathfrak{g}, \\ g &\mapsto f(g) \equiv g^{-1} \cdot F(g). \end{aligned}$$

Then, the left-trivialized Hamiltonian $h : G \times \mathfrak{g}^* \to \mathbb{R}$ has the form

$$h(g,\mu) = \langle \mu, f(g) \rangle.$$

Computing the functional derivatives of h yields

$$D_\mu h(g,\mu) = f(g),$$
$$D_g h(g,\mu) = [Df(g)]^* \mu.$$

In particular, the Lie–Poisson system (4.2.2a)-(4.2.2b) for the adjoint Hamiltonian has the form

$$\dot{g} = F(g), \tag{4.3.1a}$$
$$\dot{\mu} = -g^* \cdot [Df(g)]^* \mu + \mathrm{ad}^*_{f(g)} \mu. \tag{4.3.1b}$$

We now address the question of existence and uniqueness for solutions of the Type II system (4.2.2a)-(4.2.2d). For general Hamiltonians on T^*G, this is a complicated question which is dependent on the particular Hamiltonian. In particular, since the system has Type II boundary conditions $g(0) = g_0, \mu(T) = \mu_1$, even a local solution theory cannot be stated generally, as opposed to systems with initial-value conditions $g(0) = g_0, \mu(0) = \mu_0$. A simple way to see this is that we can think of a Hamiltonian system on $G \times \mathfrak{g}^*$ with Type II boundary conditions as a fixed-time, free-position-endpoint, fixed-fiber-endpoint shooting control problem: given $g(0) = g_0 \in G$ and $T > 0$, find $\mu(0) = \mu_0$ such that $\mu(T) = \mu_1$ subject to the Hamiltonian dynamics. This is in general a tricky problem that is dependent on the Hamiltonian under consideration.

However, for adjoint systems in particular, we can provide a global solution theory which utilizes the fact that the adjoint system covers an ODE on G; assuming the ODE on G behaves nicely, we will have unique solutions for the adjoint system on T^*G. We make this more precise in the following proposition.

Proposition 4.3.1 (Global Existence and Uniqueness of Solutions to Adjoint Systems on T^*G)**.** *Let $T > 0, g_0 \in G, \mu_1 \in \mathfrak{g}^*$. Let F be a complete vector on field on G, i.e., it generates a global flow $\Phi_F : \mathbb{R} \times G \to G$.*

Then, there exists a unique curve $(g,\mu):[0,T]\to G\times\mathfrak{g}^*$ *satisfying the Lie–Poisson system with Type II boundary conditions* (4.2.2a)-(4.2.2d)*, where h is the left-trivialized adjoint Hamiltonian associated to F.*

Furthermore, there exists a unique curve $(g,p):[0,T]\to T^*G$ *satisfying Hamilton's equations with Type II boundary conditions* (4.2.1a)-(4.2.1d)*, where H is the adjoint Hamiltonian associated to F.*

Proof. By the fundamental theorem on flows [67], there exists a unique curve $g:\mathbb{R}\to G$ satisfying $\dot{g}=F(g)$ and $g(0)=g_0$, given by the flow of F on g_0, $g(t)=\Phi_F(t,g_0)$. In particular, g is a smooth function of t, since F is smooth. Recall that we assume all maps and manifolds are smooth, unless otherwise stated.

Now, with this curve $g(t)$ fixed, we substitute this into the differential equation for μ (4.2.2b), to obtain

$$\dot{\mu}=-g(t)^*\cdot[Df(g(t))]^*\mu+\mathrm{ad}^*_{f(g(t))}\mu.$$

In particular, this equation has the form of a time-dependent linear differential equation on $\mathfrak{g}^*$,

$$\dot{\mu}=L(t)\mu,$$

where we define the time-dependent linear operator $L:\mathbb{R}\to\mathrm{End}(\mathfrak{g}^*)$ by

$$L(t)=-g(t)^*\cdot[Df(g(t))]^*+\mathrm{ad}^*_{f(g(t))}. \tag{4.3.2}$$

Since g is a smooth function of t, L is a smooth, and in particular continuous, function of t. Hence, by the standard solution theory for linear differential equations, there exists a unique curve $\mu:[0,T]\to\mathfrak{g}^*$ satisfying $\dot{\mu}=L(t)\mu$ and $\mu(T)=\mu_1$.

For the second statement of the proposition, note that solution curves $(g,p):[0,T]\to T^*G$ of (4.2.1a)-(4.2.1d) are in one-to-one correspondence with solution curves $(g,\mu):[0,T]\to G\times\mathfrak{g}^*$

of (4.2.2a)-(4.2.2d) via left-translation. □

By the above proposition, we know that there exists a unique solution to the adjoint system on T^*G with Type II boundary conditions, under the assumption that F is complete. For Lie groups, there are two particularly important cases where this assumption is satisfied.

Corollary 4.3.1. *If G is a compact Lie group, then the above proposition holds for any vector field F on G.*

If F is a left-invariant vector field on a (not necessarily compact) Lie group G, then the above proposition holds.

Proof. The first statement follows from the fact that any vector field on a compact manifold is complete. The second statement follows from the fact that any left-invariant vector field on a Lie group is complete. See [67]. □

The Variational System. An important property of adjoint systems is that they satisfy a quadratic conservation law, which is at the heart of the method of adjoint sensitivity analysis [106].

To state this conservation law, we introduce the variational equation associated to an ODE $\dot{g} = F(g)$ on a Lie group G, which is defined to be the linearization of the ODE,

$$\frac{d}{dt}\delta g = DF(g)\delta g.$$

We refer to the combined system

$$\frac{d}{dt}g = F(g), \tag{4.3.3a}$$

$$\frac{d}{dt}\delta g = DF(g)\delta g, \tag{4.3.3b}$$

as the variational system, which is interpreted as an ODE on TG.

As with the adjoint system, it will be useful to left-trivialize this system, which will give an ODE on $G\times\mathfrak{g}$. As before, let $f(g)=g^{-1}\cdot F(g)$ be the left-trivialization of F. Let $\eta=g^{-1}\cdot\delta g$ and let $\xi=g^{-1}\cdot\dot{g}$. As is well-known (see, for example, [82]), we have the relation

$$\dot{\eta}=\delta\xi-[\xi,\eta].$$

In particular, since $\xi=g^{-1}\cdot\dot{g}=f(g)$, we have $\delta\xi=Df(g)\delta g=Df(g)g\cdot\eta$, so that the above relation becomes

$$\dot{\eta}=Df(g)g\cdot\eta-[f(g),\eta],$$

which we refer to as the left-trivialized variational equation. We refer to the combined system

$$\dot{g}=F(g), \tag{4.3.4a}$$

$$\dot{\eta}=Df(g)g\cdot\eta-\mathrm{ad}_{f(g)}\eta, \tag{4.3.4b}$$

as the left-trivialized variational system on $G\times\mathfrak{g}$. Analogous to the existence and uniqueness result for adjoint systems, Proposition 4.3.1, we have the following result.

Proposition 4.3.2 (Global Existence and Uniqueness of Solutions to Variational Systems on TG)**.** *Let $T>0, g_0\in G, \eta_0\in\mathfrak{g}$. Let F be a complete vector on field on G, i.e., it generates a global flow $\Phi_F:\mathbb{R}\times G\to G$.*

Then, there exists a unique curve $(g,\eta):[0,T]\to G\times\mathfrak{g}$ satisfying the left-trivialized variational system (4.3.4a)-(4.3.4b) *with initial conditions $g(0)=g_0,\eta(0)=\eta_0$.*

Furthermore, there exists a unique curve $(g,\delta g):[0,T]\to TG$ satisfying the variational system (4.3.3a)-(4.3.3b) *with initial conditions $g(0)=g_0,\delta g(0)=g_0\cdot\eta_0$.*

Proof. The proof is almost identical to the proof of Proposition 4.3.1, noting that once the solution curve $g(t)$ of $\dot{g}=F(g),g(0)=g_0$ is fixed, the variational equation can be expressed as a time-dependent linear equation on $\mathfrak{g}$,

$$\dot{\eta} = M(t)\eta,$$

where the time-dependent linear operator $M : \mathbb{R} \to \mathrm{End}(\mathfrak{g})$ is smooth. In fact, it is easily verified that $M(t) = -L(t)^*$, where L is the time-dependent linear operator (4.3.2) defined in the proof of Proposition 4.3.1.

Furthermore, by left-translation, solutions to the left-trivialized variational system and the variational system, with the above respective initial conditions, are in one-to-one correspondence.

□

We can now state the quadratic conservation law enjoyed by solutions of the adjoint and variational systems.

Theorem 4.3.1. *Let (g, μ) be a solution curve of the left-trivialized adjoint system and let (g, η) be a solution curve of the left-trivialized variational system, both covering the same base curve g. Let (g, p) and $(g, \delta g)$ be the respective solution curves for the adjoint system and variational system obtained by left-translation. Then,*

$$\frac{d}{dt}\langle \mu(t), \eta(t) \rangle = 0, \tag{4.3.5a}$$

$$\frac{d}{dt}\langle p(t), \delta q(t) \rangle = 0. \tag{4.3.5b}$$

Proof. Note that it suffices to prove either (4.3.5a) or (4.3.5b), since left-translation preserves the duality pairing,

$$\langle \mu(t), \eta(t) \rangle = \langle g(t)^{-1} \cdot p(t), g(t) \cdot \delta q(t) \rangle = \langle p(t), \delta g(t) \rangle.$$

We will prove (4.3.5a). Compute

$$\begin{aligned}
&\frac{d}{dt}\langle \mu(t), \eta(t)\rangle \\
&\quad = \langle \dot{\mu}(t), \eta(t)\rangle + \langle \mu(t), \dot{\eta}(t)\rangle \\
&\quad = \langle -g(t)^* \cdot [Df(g(t))]^* \mu(t) + \mathrm{ad}^*_{f(g(t))}\mu(t), \eta(t)\rangle \\
&\qquad + \langle \mu(t), Df(g(t))g(t)\cdot \eta(t) - \mathrm{ad}_{f(g(t))}\eta(t)\rangle \\
&\quad = -\langle \mu(t), Df(g(t))g(t)\cdot \eta(t)\rangle + \langle \mu(t), Df(g(t))g(t)\cdot \eta(t)\rangle \\
&\qquad + \langle \mu(t), \mathrm{ad}_{f(g(t))}\eta(t)\rangle - \langle \mu(t), \mathrm{ad}_{f(g(t))}\eta(t)\rangle \\
&\quad = 0.
\end{aligned}$$

□

In particular, we have the following corollary of Propositions 4.3.1 and 4.3.2 and Theorem 4.3.1.

Corollary 4.3.2. *Let $T > 0, g_0 \in G, \mu_1 \in \mathfrak{g}^*, \eta_0 \in \mathfrak{g}$. Let F be a complete vector field on G. Then, the solution curves of the adjoint and variational systems from Propositions 4.3.1 and 4.3.2 satisfy the quadratic conservation law*

$$\langle \mu(0), \eta_0\rangle = \langle \mu_1, \eta(T)\rangle.$$

As we will see in Section 4.3.3, this conservation law will be the basis for adjoint sensitivity analysis on Lie groups.

4.3.1 Reduction of Adjoint Systems for Left-invariant Vector Fields

In practice, many interesting mechanical systems arise from the flow of left-invariant vector fields on Lie groups. As such, we will consider adjoint systems in the particular case where the vector field is left-invariant. First, we will show that left-invariant vector fields are in one-to-one correspondence with left-invariant adjoint Hamiltonians. Subsequently, we will state the adjoint equations in this particular case.

Proposition 4.3.3. *Let F be a vector field on G. Then the adjoint Hamiltonian $H(g,p) = \langle p, F(g)\rangle$ associated to F is left-invariant if and only if F is left-invariant.*

Proof. Assume that F is left-invariant, i.e., $F(xg) = xF(g)$ for all $x,g \in G$. Then, for any $x,g \in G, p \in T_g^*G$,

$$H(xg, x^{*-1}p) = \langle x^{*-1}p, F(xg)\rangle = \langle x^{*-1}p, xF(g)\rangle = \langle x^* x^{*-1}p, F(g)\rangle = \langle p, F(g)\rangle = H(g,p),$$

i.e., H is left-invariant.

Conversely, assume that H is left-invariant, i.e., $H(g,p) = H(xg, x^{*-1}p)$ for all $x,g \in G, p \in T_g^*G$. Then, for any $x,g \in G, p \in T_g^*G$,

$$\langle p, F(g)\rangle = H(g,p) = H(xg, x^{*-1}p) = \langle x^{*-1}p, F(xg)\rangle = \langle p, x^{-1}F(xg)\rangle.$$

Since $p \in T_g^*G$ is arbitrary, we have for all $x,g \in G$,

$$F(g) = x^{-1}F(xg),$$

i.e., $xF(g) = F(xg)$, so F is left-invariant. □

Since a left-invariant vector field corresponds to a left-invariant adjoint Hamiltonian, the reduction theory discussed in Section 4.2.2 applies. Thus, the adjoint equation for the momenta μ, from equation (4.2.6), is given by

$$\dot{\mu} = \mathrm{ad}^*_{F(e)}\mu,$$

since $\tilde{H}(\mu) = H(e,\mu) = \langle \mu, F(e)\rangle$ and hence, $D_\mu \tilde{H}(\mu) = F(e)$.

4.3.2 Type II Variational Discretization of Adjoint Systems

In this section, we apply the Type II variational integrators developed in Section 4.2.2 to the particular case of adjoint systems. We will show explicitly that these integrators preserve the adjoint-variational quadratic conservation law which is key to adjoint sensitivity analysis, and thus, these methods are geometric structure-preserving methods for adjoint sensitivity analysis on Lie groups.

Consider the variational integrators that we derived in Section 4.2.2, applied to the adjoint system (4.3.1a)-(4.3.1b). Substituting $h(g,\mu) = \langle \mu, f(g) \rangle$ into the discrete Lie–Poisson equations (4.2.5a)-(4.2.5c), we have the discrete Lie–Poisson adjoint equations

$$(d\tau^{-1}_{\Delta t \xi_{k+1}})^* m_{k+1} - \mathrm{Ad}^*_{\tau(\Delta t \xi_k)} (d\tau^{-1}_{\Delta t \xi_k})^* m_k = -\Delta t g_k^* [Df(g_k)]^* m_{k+1}, \tag{4.3.6a}$$

$$\xi_{k+1} = f(g_k) \tag{4.3.6b}$$

$$g_{k+1} = g_k \tau(\Delta t \xi_{k+1}) = g_k \tau(\Delta t f(g_k)). \tag{4.3.6c}$$

In order to derive a discrete analogue of the adjoint conservation law, we consider the discrete variational equation, which is a discretization of the continuous variational equation (4.3.4b). To derive the discrete variational equation, note that as mentioned in Section 4.2.2, the variation of equation (4.3.6c) can be expressed

$$\delta \xi_{k+1} = d\tau^{-1}_{\Delta t \xi_{k+1}} (-g_k^{-1} \delta g_k + \mathrm{Ad}_{\tau(\Delta t \xi_{k+1})} g_{k+1}^{-1} \delta g_{k+1}) / \Delta t.$$

Furthermore, by taking the variation of equation (4.3.6b), we have

$$\delta \xi_{k+1} = Df(g_k) \delta g_k.$$

Combining these two equations yields

$$Df(g_k)\delta g_k = d\tau^{-1}_{\Delta t\xi_{k+1}}(-g_k^{-1}\delta g_k + \mathrm{Ad}_{\tau(\Delta t\xi_{k+1})}g_{k+1}^{-1}\delta g_{k+1})/\Delta t.$$

Defining the left-trivialized variation $\eta_k = g_k^{-1}\delta g_k$, the above can be expressed as

$$\Delta t\, d\tau_{\Delta t\xi_{k+1}}Df(g_k)g_k\eta_k = -\eta_k + \mathrm{Ad}_{\tau(\Delta t\xi_{k+1})}\eta_{k+1}, \tag{4.3.7}$$

which we refer to as the discrete variational equation.

Theorem 4.3.2. *The discrete Lie–Poisson adjoint equations and the discrete variational equation satisfy the following quadratic conservation law,*

$$\langle (d\tau^{-1}_{-\Delta t\xi_{k+1}})^* m_{k+1}, \eta_{k+1}\rangle = \langle (d\tau^{-1}_{-\Delta t\xi_k})^* m_k, \eta_k\rangle. \tag{4.3.8}$$

Proof. Recall the identity $\mathrm{Ad}^*_{\tau(\Delta t\xi_j)}(d\tau^{-1}_{\Delta t\xi_j})^* = (d\tau^{-1}_{-\Delta t\xi_j})^*$. Starting from the left hand side of equation (4.3.8), we compute

$$\begin{aligned}\langle (d\tau^{-1}_{-\Delta t\xi_{k+1}})^* m_{k+1}, \eta_{k+1}\rangle &= \langle \mathrm{Ad}^*_{\tau(\Delta t\xi_{k+1})}(d\tau^{-1}_{\Delta t\xi_{k+1}})^* m_{k+1}, \eta_{k+1}\rangle \\ &= \langle (d\tau^{-1}_{\Delta t\xi_{k+1}})^* m_{k+1}, \mathrm{Ad}_{\tau(\Delta t\xi_{k+1})}\eta_{k+1}\rangle.\end{aligned}$$

Substituting (4.3.6a) and (4.3.7) yields

$$\begin{aligned}&\langle (d\tau^{-1}_{-\Delta t\xi_{k+1}})^* m_{k+1}, \eta_{k+1}\rangle \\ &\qquad = \langle (d\tau^{-1}_{\Delta t\xi_{k+1}})^* m_{k+1}, \mathrm{Ad}_{\tau(\Delta t\xi_{k+1})}\eta_{k+1}\rangle \\ &\qquad = \langle (d\tau^{-1}_{-\Delta t\xi_k})^* m_k - \Delta t\, g_k^*[Df(g_k)]^* m_{k+1}, \eta_k + \Delta t\, d\tau_{\Delta t\xi_{k+1}}Df(g_k)g_k\eta_k\rangle \\ &\qquad = \langle (d\tau^{-1}_{-\Delta t\xi_k})^* m_k, \eta_k\rangle + \Delta t\langle (d\tau^{-1}_{-\Delta t\xi_k})^* m_k, d\tau_{\Delta t\xi_{k+1}}Df(g_k)g_k\eta_k\rangle \\ &\qquad\quad - \Delta t\langle g_k^*[Df(g_k)]^* m_{k+1}, \eta_k\rangle - \Delta t^2\langle g_k^*[Df(g_k)]^* m_{k+1}, d\tau_{\Delta t\xi_{k+1}}Df(g_k)g_k\eta_k\rangle.\end{aligned}$$

Substitute (4.3.6a) into the second term above,

$$
\begin{aligned}
&\langle (d\tau^{-1}_{-\Delta t \xi_{k+1}})^* m_{k+1}, \eta_{k+1} \rangle \\
&\quad = \langle (d\tau^{-1}_{-\Delta t \xi_k})^* m_k, \eta_k \rangle + \Delta t \langle (d\tau^{-1}_{\Delta t \xi_{k+1}})^* m_{k+1} + \Delta t g_k^* [Df(g_k)]^* m_{k+1}, d\tau_{\Delta t \xi_{k+1}} Df(g_k) g_k \eta_k \rangle \\
&\qquad - \Delta t \langle g_k^* [Df(g_k)]^* m_{k+1}, \eta_k \rangle - \Delta t^2 \langle g_k^* [Df(g_k)]^* m_{k+1}, d\tau_{\Delta t \xi_{k+1}} Df(g_k) g_k \eta_k \rangle \\
&\quad = \langle (d\tau^{-1}_{-\Delta t \xi_k})^* m_k, \eta_k \rangle + \Delta t \langle (d\tau^{-1}_{\Delta t \xi_{k+1}})^* m_{k+1}, d\tau_{\Delta t \xi_{k+1}} Df(g_k) g_k \eta_k \rangle \\
&\qquad + \Delta t^2 \langle g_k^* \cancel{[Df(g_k)]^* m_{k+1}, d\tau_{\Delta t \xi_{k+1}}} Df(g_k) g_k \eta_k \rangle \\
&\qquad - \Delta t \langle g_k^* [Df(g_k)]^* m_{k+1}, \eta_k \rangle - \Delta t^2 \langle g_k^* \cancel{[Df(g_k)]^* m_{k+1}, d\tau_{\Delta t \xi_{k+1}}} Df(g_k) g_k \eta_k \rangle \\
&\quad = \langle (d\tau^{-1}_{-\Delta t \xi_k})^* m_k, \eta_k \rangle + \Delta t \langle m_{k+1}, (d\tau^{-1}_{\Delta t \xi_{k+1}}) d\tau_{\Delta t \xi_{k+1}} Df(g_k) g_k \eta_k \rangle \\
&\qquad - \Delta t \langle g_k^* [Df(g_k)]^* m_{k+1}, \eta_k \rangle \\
&\quad = \langle (d\tau^{-1}_{-\Delta t \xi_k})^* m_k, \eta_k \rangle + \Delta t \langle m_{k+1}, Df(g_k) g_k \eta_k \rangle - \Delta t \langle g_k^* [Df(g_k)]^* m_{k+1}, \eta_k \rangle \\
&\quad = \langle (d\tau^{-1}_{-\Delta t \xi_k})^* m_k, \eta_k \rangle. \qquad \square
\end{aligned}
$$

4.3.3 Adjoint Sensitivity Analysis on Lie Groups

In this section, we utilize the discrete methods for adjoint systems on Lie groups developed in the previous sections to address the following two types of optimization problems: an initial condition optimization problem,

$$
\begin{aligned}
&\min_{g_0 \in G} C(g(T)), \\
&\text{such that } \dot{g}(t) = F(g(t)),\ t \in (0, T), \\
&g(0) = g_0,
\end{aligned}
\tag{4.3.9}
$$

and an optimal control problem,

$$\min_{u\in U} C(g(T)), \tag{4.3.10}$$
$$\text{such that } \dot{g}(t) = F(g(t),u),\ t \in (0,T),$$
$$g(0) = g_0,$$

where in (4.3.10), we have introduced a parameter-dependent vector field F.

Initial Condition Sensitivity. We begin with problem (4.3.9). We refer to $C : G \to \mathbb{R}$ as the terminal cost function. Thus, the problem (4.3.9) is to find an initial condition $g_0 \in G$ which minimizes the cost function at the terminal-value $g(T)$, subject to the dynamics of the ODE $\dot{g} = F(g)$.

For gradient-based algorithms, one needs the derivative of the terminal cost function $C(g(T))$ with respect to the initial condition g_0; we refer to this derivative as the *initial condition sensitivity*. One cannot generally compute an expression for the sensitivity analytically, since such an expression would require knowing $g(T)$ explicitly as a function of g_0.

However, the adjoint system pulls back derivatives with respect to $g(T)$ into derivatives with respect to $g(0)$ [106]. In other words, the derivative of $C(g(T))$ with respect to g_0 can be computed by setting the terminal momenta to be $p(T) = dC(g(T))$ and evolving backwards in time to find the desired derivative $p(0)$. One cannot generally compute the curves $g(t)$ and $p(t)$ exactly, so we instead use the method (4.3.6a)-(4.3.6c) to approximately solve the ODE and its adjoint. By Theorem 4.3.2, the property that the adjoint system pulls back derivatives with respect to $g(T)$ to derivatives with respect to $g(0)$ is preserved by the method, so it exactly gives the desired derivative.

More specifically, to obtain the initial condition sensitivity, recall the quadratic conservation law

$$\langle (d\tau^{-1}_{-\Delta t\xi_N})^* m_N, g_N^{-1}\delta g_N\rangle = \langle (d\tau^{-1}_{-\Delta t\xi_0})^* m_0, g_0^{-1}\delta g_0\rangle.$$

We set $(d\tau^{-1}_{-\Delta t\xi_N})^* m_N = d_L C(g(T))$, where d_L denotes the left-trivialized derivative, $d_L C(g(T)) \equiv g_N^{-*} dC(g(T))$. This gives $m_N = (d\tau_{-\Delta t\xi_N})^* d_L C(g(T))$. Subsequently, evolve the momenta backward in time using (4.3.6a) to obtain m_0. Finally, the left-trivialized derivative of $C(g(T))$ with respect to g_0 is given by $(d\tau^{-1}_{-\Delta t\xi_0})^* m_0$. This is summarized in the following algorithm.

Algorithm 1. Left-Trivialized Initial Condition Sensitivity

Input: g_{init}
Initialize: $g_0 \leftarrow g_{\text{init}}, \{g_k\}_{k=1}^N, \{m_k\}_0^N$
Output: Left-Trivialized Derivative of $C(g(T))$ with respect to g_0
for k=1,...,N **do**
  $g_k \leftarrow g_{k-1}\tau(\Delta t f(g_{k-1}))$
end for
$m_N \leftarrow (d\tau_{-\Delta t f(g_N)})^* d_L C(g_N)$
for k=1,...,N **do**
  $m_{N-k} \leftarrow$ Solve $m : (d\tau^{-1}_{\Delta t\xi_{k+1}})^* m_{N-k+1} - \text{Ad}^*_{\tau(\Delta t\xi_k)}(d\tau^{-1}_{\Delta t\xi_k})^* m = -\Delta t g_k^* [Df(g_k)]^* m_{N-k+1},$
end for
Return $(d\tau^{-1}_{-\Delta t f(g_0)})^* m_0$

This can be combined with a line-search algorithm to solve the optimization problem (4.3.9). More precisely, fixing an inner product on $\mathfrak{g}$, such as the Frobenius inner product

$$(A,B)_F \equiv \text{Tr}(A^* B),$$

we can identity $\mathfrak{g}^*$ with $\mathfrak{g}$ and hence, identify the output of Algorithm 1 with the left-trivialized gradient of $C(g(T))$ with respect to g_0, $\nabla_{g_0} C(g(T))$, which is an element of $\mathfrak{g}$. With this identification, the initial condition can be updated as $g_0 \leftarrow g_0 \tau(-\gamma \nabla_{g_0} C(g(T)))$, for some line-search step size γ.

Remark 4.3.1. *The preceding discussion of adjoint sensitivity analysis for terminal cost functions can be easily adapted to a cost function consisting of both a terminal cost and a running cost,*

$$C(g(T)) + \int_0^T L(g(t))dt.$$

This is done by augmenting the adjoint Hamiltonian with the running cost Lagrangian L, i.e., by using the augmented adjoint Hamiltonian

$$H_L(g,p) \equiv H(g,p) + L(g) = \langle p, F(g) \rangle + L(g).$$

The only modification is an additional term in the momentum equation (4.3.6a) *corresponding to the derivative of L. For more details, see [113].*

The significance of this approach is that it is intrinsic; at any iteration in the line-search algorithm, the iterate g_0 is valued in G, to numerical precision. Furthermore, while this is also true of projection-based optimization algorithms, such methods generally no longer preserve the adjoint-variational quadratic conservation law and hence, may not capture the appropriate descent direction.

Parameter Sensitivity. We now consider problem (4.3.10). The problem (4.3.10) is to find a parameter $u \in U$ which minimizes the terminal cost function $C(g(T))$, subject to the dynamics of the parameter-dependent ODE $\dot{g} = F(g,u)$ with $g(0) = g_0$ fixed. We assume that F is continuously differentiable with respect to u.

For a gradient-based algorithm, we will need the derivative of the terminal cost function $C(g(T))$ with respect to the parameter u; we refer to this derivative as the *parameter sensitivity*.

We begin with a discussion of how the parameter sensitivity is obtained from the adjoint system in the continuous setting, since the derivation will be analogous in the discrete setting. Define the parameter-dependent action as

$$S[g,p;u] \equiv \int_0^T \langle p, \dot{g} - F(g,u) \rangle dt.$$

Consider the augmented cost function, given by subtracting the parameter-dependent action from the terminal cost function,

$$\begin{aligned} J &\equiv C(g(T)) - S[g,p;u] \\ &= C(g(T)) - \int_0^T \langle p, \dot{g} - F(g,u)\rangle dt. \end{aligned}$$

By left-trivialization, this is equivalent to

$$J = C(g(T)) - \int_0^T \langle \mu, \xi - f(g,u)\rangle dt, \tag{4.3.11}$$

where $\xi = g^{-1}\dot{g}$ and f is the left-trivialization of F. Observe that since the integral of (4.3.11) vanishes when $\dot{g} = f(g,u)$, we have that the derivative of J with respect to u equals the derivative of C with respect to u, subject to the variational equations, where the variation $\delta_u g$ is given by the variation of g induced by varying u. Thus,

$$\frac{d}{du}C(g(T)) = \frac{d}{du}J.$$

Proposition 4.3.4. *The (continuous) parameter sensitivity is given by*

$$\frac{d}{du}C(g(T)) = \frac{d}{du}J = \int_0^T \langle \mu, \frac{\partial}{\partial u} f(g,u)\rangle dt,$$

where μ is chosen to satisfy the adjoint equation $-\dot{\mu} + ad_\xi^* \mu - g^*[D_g f(g,u)]^* \mu = 0$ and the terminal condition $\mu(T) = g^{-*} dC(g(T))$.

Proof. We compute dJ/du explicitly,

$$\frac{d}{du}J(g(T)) = \langle dC(g(T)), \delta_u g(T)\rangle - \int_0^T \Big[\langle \mu, \delta_u \xi - [D_g f(g,u)] g \eta_u\rangle - \langle \mu, \frac{\partial}{\partial u} f(g,u)\rangle\Big] dt,$$

where we introduced the left-trivialized variation $\eta_u = g^{-1}\delta_u g$ and we have decomposed the total derivative of f with respect to u into its implicit dependence on u through g as well as its explicit dependence on u, i.e.,

$$\frac{d}{du}f(g,u) = [D_g f(g,u)]\delta_u g + \frac{\partial}{\partial u} f(g,u).$$

Using the relation $\dot{\eta}_u = \delta_u \xi - \mathrm{ad}_\xi \eta_u$, this becomes

$$\begin{aligned}
&\frac{d}{du}J(g(T)) \\
&\quad = \langle dC(g(T)), \delta_u g(T)\rangle - \int_0^T \Big[\langle \mu, \dot{\eta}_u + \mathrm{ad}_\xi \eta_u - [D_g f(g,u)]g\eta_u\rangle - \langle \mu, \frac{\partial}{\partial u} f(g,u)\rangle\Big] dt \\
&\quad = \langle dC(g(T)), \delta_u g(T)\rangle - \langle \mu, \eta_u\rangle\Big|_0^T \\
&\qquad - \int_0^T \Big[\langle -\dot{\mu} + \mathrm{ad}_\xi^* \mu - g^*[D_g f(g,u)]^*\mu, \eta_u\rangle - \langle \mu, \frac{\partial}{\partial u} f(g,u)\rangle\Big] dt,
\end{aligned}$$

where we integrated the $\langle \mu, \dot{\eta}_u\rangle$ term by parts. Now, the first pairing in the integral vanishes if μ satisfies the adjoint equation. Furthermore, $\eta_u(0) = 0$ since the initial condition for problem (4.3.10) is fixed. Hence, we have

$$\frac{d}{du}J(g(T)) = \langle dC(g(T)), \delta_u g(T)\rangle - \langle \mu(T), \eta_u(T)\rangle + \int_0^T \langle \mu, \frac{\partial}{\partial u} f(g,u)\rangle dt.$$

If we choose the terminal condition $\mu(T) = g^{-*}dC(g(T))$, the first two terms on the right hand side cancel, which gives the expression for the desired parameter sensitivity

$$\frac{d}{du}C(g(T)) = \frac{d}{du}J(g(T)) = \int_0^T \langle \mu, \frac{\partial}{\partial u} f(g,u)\rangle dt,$$

where μ is chosen to satisfy the adjoint equation $-\dot{\mu} + \mathrm{ad}_\xi^* \mu - g^*[D_g f(g,u)]^*\mu = 0$ and the terminal condition $\mu(T) = g^{-*}dC(g(T))$. □

From here, the generalization to the discrete setting is straightforward. In analogy with the continuous case, we define the parameter-dependent left-trivialized discrete action

$$s_d[\{g_k\},\{m_k\};u] = \Delta t \sum_{k=0}^{N-1} \Big(\langle m_{k+1}, \xi_{k+1} \rangle - h(g_k, m_{k+1} l; u) \Big),$$

and form the discrete augmented cost function by subtracting the discrete action from the terminal cost, i.e.,

$$\begin{aligned} J_d &\equiv C(g_N) - s_d[\{g_k\},\{m_k\};u] \\ &= C(g_N) - \Delta t \sum_{j=0}^{N-1} \langle m_{j+1}, \xi_{j+1} - f(g_j,u) \rangle. \end{aligned}$$

We then have an analogous result to determine the parameter sensitivity by computing the derivative dJ_d/du.

Proposition 4.3.5. *The (discrete) parameter sensitivity is given by*

$$\frac{d}{du} C(g_N) = \Delta t \sum_{j=0}^{N-1} \langle m_j, \frac{\partial}{\partial u} f(g_j,u) \rangle,$$

where m_j is chosen to satisfy the discrete Lie–Poisson adjoint equation (4.3.6a) *and the terminal condition $m_N = (d\tau_{-\Delta t \xi_N})^* d_L C(g_N)$.*

Proof. Analogous to the continuous setting, we have

$$\frac{d}{du} C(g_N) = \frac{d}{du} J_d.$$

Now, we calculate dJ_d/du explicitly,

$$\frac{d}{du} J_d = \langle dC(g_N), \delta_u g_N \rangle - \Delta t \sum_{j=0}^{N-1} \langle m_{j+1}, \delta_u \xi_{j+1} - D_g f(g_j,u) \delta_u g_j - \frac{\partial f}{\partial u}(g_j,u) \rangle.$$

Using the identity $\delta_u \xi_{j+1} = d\tau^{-1}_{\Delta t \xi_{j+1}} (-g_k^{-1} \delta_u g_k + \mathrm{Ad}_{\tau(\Delta t \xi_{j+1})} g_{j+1}^{-1} \delta_u g_{j+1})/\Delta t$, the above can be expressed as

$$\frac{d}{du}J_d = \langle dC(g_N), \delta_u g_N\rangle - \Delta t \sum_{j=0}^{N-1} \Big[\Delta t^{-1}\langle (d\tau^{-1}_{\Delta t\xi_{j+1}})^* m_{j+1}, -g_j^{-1}\delta_u g_j\rangle$$
$$+ \Delta t^{-1}\langle \mathrm{Ad}^*_{\tau(\Delta t\xi_{j+1})}(d\tau^{-1}_{\Delta t\xi_{j+1}})^* m_{j+1}, g_{j+1}^{-1}\delta_u g_{j+1}\rangle$$
$$- \langle g_j^*[D_g f(g_j,u)]^* m_{j+1}, g_j^{-1}\delta_u g_j\rangle - \langle m_{j+1}, \frac{\partial f}{\partial u}(g_j,u)\rangle\Big].$$

Now, we reindex $j \to j-1$ the second pairing inside the square brackets above; the sum for this term now runs from 1 to N. However, we explicitly write out the $j = N$ term and note that we can include the $j = 0$ term in the sum since $\delta_u g_0 = 0$, as the initial condition g_0 is fixed under the variation. Hence, we have

$$\frac{d}{du}J_d = \langle dC(g_N), \delta_u g_N\rangle - \langle (d\tau^{-1}_{-\Delta t\xi_N})^* m_N, g_N^{-1}\delta_u g_N\rangle$$
$$- \Delta t \sum_{j=0}^{N-1} \Big[\Delta t^{-1}\langle (d\tau^{-1}_{\Delta t\xi_{j+1}})^* m_{j+1}, -g_j^{-1}\delta_u g_j\rangle$$
$$+ \Delta t^{-1}\langle \mathrm{Ad}^*_{\tau(\Delta t\xi_j)}(d\tau^{-1}_{\Delta t\xi_j})^* m_j, g_j^{-1}\delta_u g_j\rangle$$
$$- \langle g_j^*[D_g f(g_j,u)]^* m_{j+1}, g_j^{-1}\delta_u g_j\rangle - \langle m_{j+1}, \frac{\partial f}{\partial u}(g_j,u)\rangle\Big].$$

The first two terms above vanish if we set the terminal condition $(d\tau^{-1}_{-\Delta t\xi_N})^* m_N = g_N^{-*} dC(g_N)$, i.e., $m_N = (d\tau_{-\Delta t\xi_N})^* d_L C(g_N)$. Furthermore, the first three terms in the square brackets vanish if m_j satisfies the discrete Lie–Poisson adjoint equation (4.3.6a). Hence, we have the parameter sensitivity

$$\frac{d}{du}C(g_N) = \frac{d}{du}J_d = \Delta t \sum_{j=0}^{N-1} \langle m_{j+1}, \frac{\partial f}{\partial u}(g_j,u)\rangle. \qquad \square$$

Thus, assuming that we can calculate $\partial f/\partial u$ (which is generally known since we know how the parameter-dependent vector field varies with u), we can calculate the sensitivity $dC(g_N)/du$. This is summarized in the following algorithm.

This can be combined with a line-search algorithm to solve the optimization problem

Algorithm 2. Parameter Sensitivity

Input: g_{init}
Initialize: $g_0 \leftarrow g_{\text{init}}, \{g_k\}_{k=1}^N, \{m_k\}_0^N$
Output: Derivative of $C(g(T))$ with respect to u
for k=1,...,N **do**
  $g_k \leftarrow g_{k-1}\tau(\Delta t f(g_{k-1}))$
end for
$m_N \leftarrow (d\tau_{-\Delta t f(g_N)})^* d_L C(g_N)$
for k=1,...,N **do**
  $m_{N-k} \leftarrow$ Solve m : $(d\tau^{-1}_{\Delta t \xi_{k+1}})^* m_{N-k+1} - \text{Ad}^*_{\tau(\Delta t \xi_k)}(d\tau^{-1}_{\Delta t \xi_k})^* m = -\Delta t g_k^* [D_g f(g_k,u)]^* m_{N-k+1}$,
end for
Return $\Delta t \sum_{j=0}^{N-1} \langle m_{j+1}, \frac{\partial}{\partial u} f(g_j,u)\rangle$

(4.3.10). Note that U could be a vector space, in which case a standard line-search algorithm could be used, or U could be a manifold, in which case a line-search algorithm on manifolds could be used (see, for example, [2]).

Numerical Examples

As examples of adjoint sensitivity analysis on Lie groups, we will solve an example of each of the problems (4.3.9) and (4.3.10).

Initial Condition Sensitivity Example. Fixing $g_{\text{target}} \in G$, find $g_0 \in G$ such that $g(T) = g_{\text{target}}$ subject to the initial-value problem $\dot{g} = F(g), g(0) = g_0$.

Using the Frobenius inner product $(\cdot,\cdot)_F$ and its induced norm $\|\cdot\|_F$, this can be cast as an optimization problem of the form (4.3.9),

$$\min_{g_0 \in G} C(g(T)) \equiv \frac{1}{2}\|g(T) - g_{\text{target}}\|_F^2,$$

$$\text{such that } \dot{g}(t) = F(g(t)),\ t \in (0,T),$$

$$g(0) = g_0.$$

This optimization problem is clearly equivalent to the above shooting problem because C is minimized at the unique minimizer $g(T) = g_{\text{target}}$, since $C(g_{\text{target}}) = 0$ and $C(g) > 0$ for any

$g \neq g_{\text{target}}$ by nondegeneracy of the norm. We choose this simple problem because the analytic answer is known: g_0 should simply be chosen to be the reverse time-T flow of g_{target} under F.

For our numerical example, we take $G = \text{SO}(3)$, $F(g) = gX$ with

$$X = \begin{pmatrix} 0 & -1 & 1 \\ 1 & 0 & 2 \\ -1 & -2 & 0 \end{pmatrix} \in \mathfrak{g}, \; g_{\text{target}} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \in G,$$

and some initial iterate

$$g_0 = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \in G.$$

The left-trivialized gradient can be computed to be $\nabla_{g(T)} C(g(T)) = g(T)^T g_1 - g_1^T g(T)$ [71] which is identified with the left-trivialized derivative through the inner product. This allows us to initialize the terminal momenta m_N as described in the previous section. Subsequently, we solve the optimization problem using Algorithm 1 and a line-search method. For simplicity, since this example is just to provide a demonstration of the theory laid out in the paper, we will use a fixed line-search step size $\gamma = 0.1$, although in practice one would likely use a more sophisticated method such as Armijo backtracking. We take $T = 1$ with $\Delta t = 0.01$. Finally, for the retraction, we use the Cayley transform and its derivatives given by

$$\tau(\xi) = \text{cay}(\xi) \equiv (I_{3\times 3} + \frac{1}{2}\xi)(I_{3\times 3} - \frac{1}{2}\xi)^{-1},$$
$$d\tau_\xi(x) = (I_{3\times 3} - \xi/2)^{-1} x (I_{3\times 3} + \xi/2)^{-1},$$
$$d\tau_\xi^{-1}(x) = (I_{3\times 3} - \xi/2) x (I_{3\times 3} + \xi/2).$$

The cost function $C(g(T))$ over 50 iterations is shown in Figure 4.1. The $SO(3)$ manifold error of each iteration of g_0 is shown in Figure 4.2, where the manifold error is defined as

$$\text{Error}(g) \equiv \frac{1}{2}\|g^T g - \text{Id}_{3\times 3}\|_F^2;$$

as can be seen in the figure, each iterate lies on $SO(3)$ to machine precision.

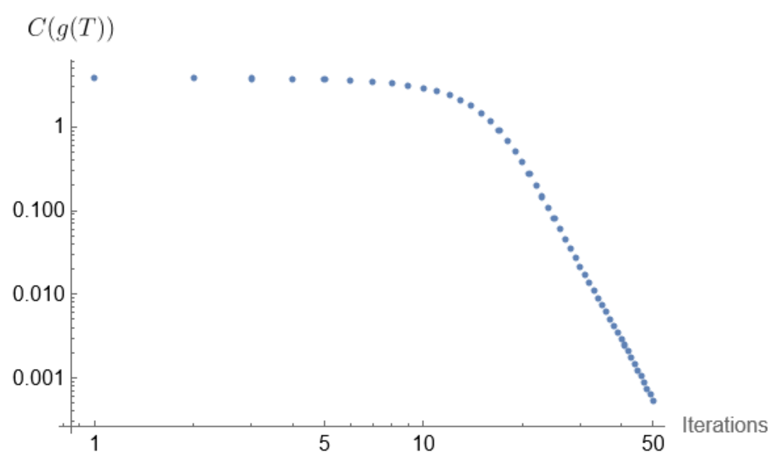


Figure 4.1. Cost function minimization via line-search algorithm for shooting problem on $SO(3)$

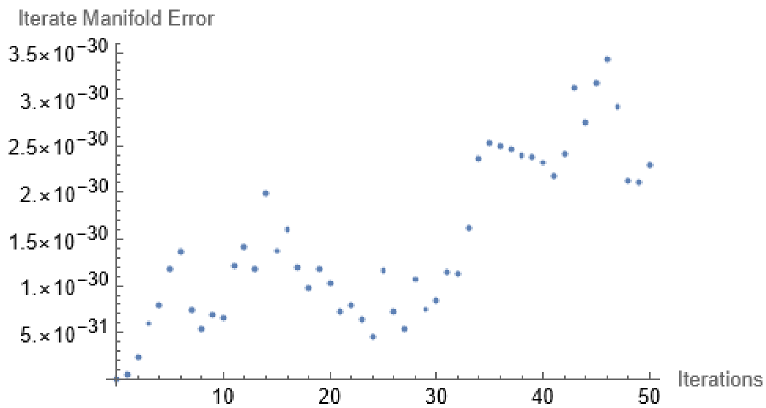


Figure 4.2. Iterate $SO(3)$ manifold error

This example can be visualized as follows. The objective is to find an element g_0 of $SO(3)$ such that under the time $T = 1$ flow of F, $g(1) = g_{\text{target}}$ where $g(0) = g_0$. For this example, g_{target} is chosen to be a $\pi/2$ counterclockwise rotation about the z-axis, i.e., in the xy plane. Thus, we can imagine some test mass located at $\vec{v} \in \mathbb{R}^3$ which is rotated by $g(t)$, which generates a curve $g(t)\vec{v}$. In particular, choosing $\vec{v} = \hat{x}$, the unit vector in the x direction, then the curve produced from rotating the test mass should end at $g_{\text{target}}\hat{x} = \hat{y}$. Each iteration in the algorithm generates such a curve. In Figure 4.3, several such curves are shown, with the initial point in the curve $g_0\hat{x}$ marked. Additionally, the desired terminal point $g_{\text{target}}\hat{x}$ is marked.

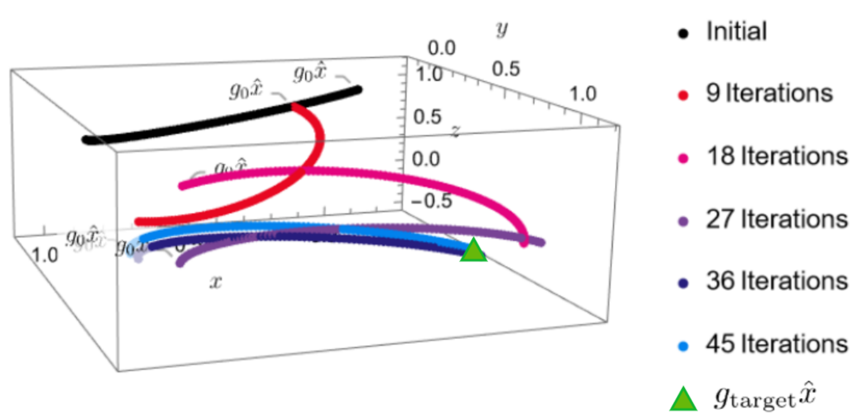


Figure 4.3. Visualization of the shooting problem on $SO(3)$ using a test mass over several iterations

Parameter Sensitivity Example. For our second example, we consider the following problem of the form (4.3.10),

$$\min_{u \in U} C(g(T)) \equiv \frac{1}{2}\|g(T) - g_{\text{target}}\|_F^2,$$
$$\text{such that } \dot{g}(t) = F(g(t), u),\ t \in (0, T),$$
$$g(0) = g_0.$$

Thus, this optimal control problem is to find $u \in U$ such that the vector field $F(\cdot, u)$ steers the initial condition $g_0 \in G$ to some desired terminal-value $g_{\text{target}} \in G$.

We again take $G = SO(3)$. We will assume that F is a parameter-dependent left-invariant vector field $F(g,u) = gX(u)$, where $u \in \mathbb{R}^3$ parametrizes $\mathfrak{so}(3)$ as

$$X(u) = \begin{pmatrix} 0 & -u_z & u_y \\ u_z & 0 & -u_x \\ -u_y & u_x & 0 \end{pmatrix}.$$

For simplicity, we take $g_0 = \text{Id}_{3\times 3} = g_{\text{target}}$ since the analytic answer is known: F should be the zero vector field, since $g_0 = g_{\text{target}}$ and hence, the optimal value of u is $u = (0,0,0)^T$. We take an initial guess of $u = (1,2,-1)^T$. We again take $T = 1$ with $\Delta t = 0.01$, using the same retraction as the previous example. We combine the parameter sensitivity, obtained from Algorithm 2, with a simple vector space line-search algorithm,

$$u \leftarrow u - \gamma \frac{d}{du} C,$$

with a fixed line-search step size $\gamma = 0.1$. The cost function $C(g(T))$ over 50 iterations is shown in Figure 4.4.

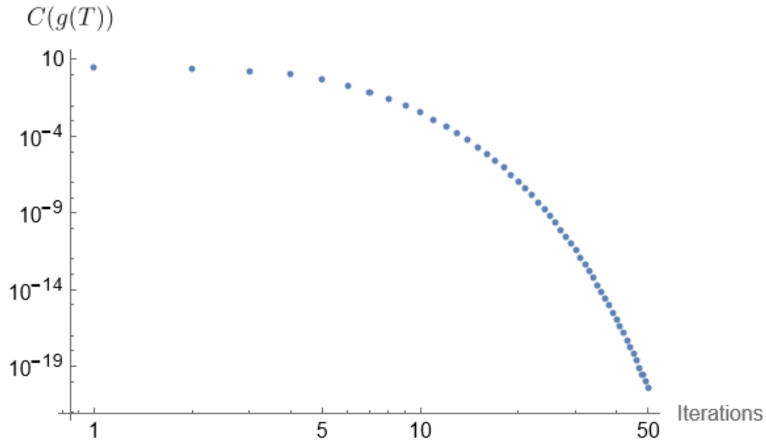


Figure 4.4. Cost function minimization via line-search algorithm for optimal control problem on $SO(3)$

4.4 Conclusion and Future Research Directions

In this paper, we developed continuous and discrete global Type II variational principles on the cotangent bundle of a Lie group G. In the discrete setting, the Type II variational principle leads to a structure-preserving variational integrator on T^*G which we showed to be symplectic and momentum-preserving. Subsequently, we applied these Type II variational principles to the class of adjoint Hamiltonian systems on T^*G. This results in a structure-preserving method to perform adjoint sensitivity analysis on Lie groups, allowing one to exactly compute sensitivities in optimization problems subject to the dynamics of an ODE on G.

One research direction which we are currently pursuing is to explore the geometry of adjoint sensitivity analysis in the infinite-dimensional setting, with the application of PDE-constrained optimization in mind. It would be interesting to synthesize this line of research with the ideas presented in this paper, to develop Hamiltonian integrators for PDEs where the solutions are valued in Lie groups, algebras, or more generally, solutions which are stationary sections over principal and fibre bundles associated to a structure group G, such as gauge field theories (see, for example, [53; 92]). It would be particularly interesting to extend the Type II multisymplectic Hamiltonian variational integrators developed in [112] to apply to the setting of Lie groups-valued fields, in order to investigate the role of multisymplectic integrators for adjoint sensitivity analysis in both space and time.

Another natural research direction would be to explore the applications of geometric structure-preserving adjoint sensitivity analysis on Lie groups. One such application is the training of neural networks via backpropagation. In particular, if a neural network is viewed as a discretization of a *neural ODE* [31], then backpropagation can be viewed as a discretization of the corresponding adjoint equation [88]. As is discussed in [88], utilizing symplectic methods to perform backpropagation leads to efficient methods for training neural networks. It would be interesting to utilize the methods presented in this paper to perform symplectic backpropagation of neural networks where the neural ODE evolves over a Lie group, which would arise in group-equivariant neural networks [33; 64] where a Lie group symmetry is a fundamental feature of the neural network. In particular, the reduction theory for adjoint systems on Lie groups that was developed in this paper would be relevant.

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Chapter 4, in full, is currently being prepared for submission for publication of the material. Tran, Brian; Leok, Melvin. The dissertation author was the primary investigator and first author of this material.

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