Structure Preserving Discretizations of Classical Field Theories

Brian Tran

Advisors:
Professor Michael Holst
Professor Melvin Leok

University of California, San Diego
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Introduction

The purpose of this thesis is to discuss the construction of discretizations of classical field theories, i.e. a finite dimensional reduction of the infinite dimensional field dynamics. Finite element exterior calculus will serve as the main tool to reduce the problem to a finite dimensional computation. To accurately reflect the physical system, a discretization should preserve the structures inherent in the infinite dimensional system. We will develop two discretization frameworks, a discrete Lagrangian approach and a discrete Hamiltonian approach, which preserve different structures of the full theory and serve different applications.

After providing a background on geometry and field theory in the first chapter, the second chapter discusses how to discretize these theories and the third chapter considers applications and examples.

1 Differential Geometry and Lagrangian Field Theory

The purpose of this chapter is to review concepts in differential geometry and Lagrangian field theory which provide an introduction to the later contents of the paper. In particular, in this chapter we formulate Lagrangian field theories in the language of exterior calculus, and in the subsequent chapters we will see how to discretize such theories.

1.1 Differentiable Manifolds

Manifolds will be the physical space where our theories occur. An n-dimensional manifold M is a topological space with an atlas, $\{U_\eta, \pi_\eta\}_\eta$, consisting of open subsets $U_\eta \subset M$ and homeomorphisms π_η mapping U_η to open subsets of $\mathbb{R}^n$ such that the atlas covers M,

$$M = \cup_\eta U_\eta.$$

Furthermore, the charts in the atlas are connected via transition maps, which are the maps

$$\pi_\eta \circ \pi_\xi^{-1} : \pi_\xi(U_\xi \cap U_\eta) \to \pi_\eta(U_\xi \cap U_\eta).$$

This allows us to describe points on open subsets of M using coordinates on $\mathbb{R}^n$ and the transition functions provide the coordinate transformations between two different charts. If the transitions maps are all differentiable, we say M is a **differentiable manifold.** Throughout the paper, when we refer to "manifold", we assume that it has a differentiable structure, unless otherwise stated.

The tangent space at $x \in M$, denoted T_xM, is the union of all possible tangent vectors at x, which can be constructed as differential operators along the flows of smooth curves on M at x. In some coordinate chart on M, we can parametrize a curve $\gamma(t) = (x^1(t), ..., x^n(t))$ with $\gamma(0) = x$. Considering a smooth function f on M in a neighborhood of x, we can compute the rate of change of f along γ at x,

$$\frac{d}{dt}(f \circ \gamma(t))\Big|_{t=0} = \frac{dx^\alpha}{dt}\Big|_{t=0} \frac{\partial f}{\partial x^\alpha}\Big|_x = \dot{x}^\alpha(0) \frac{\partial}{\partial x^\alpha}[f]\Big|_x.$$

We associate the differential operator $\dot{x}^\alpha \frac{\partial}{\partial x^\alpha}$ with the tangent vector to the curve γ at x. Of course, since $\dot{x}^\alpha$ can be chosen arbitrarily by appropriately choosing the curve γ, the tangent space

$$T_xM = \text{span}\{\frac{\partial}{\partial x^\alpha}\Big|_x\}_\alpha.$$

1.2 Vector Bundles

The dynamics of field theories evolve over vector bundles, defined over some configuration manifold. Informally, a vector bundle is a manifold which decomposes (locally) as the product of a manifold with a vector space. More precisely,

Definition 1.2.1 *A **differentiable vector bundle** consists of differentiable manifolds E (the total space) and M (the base space) with a differentiable projection $\pi : E \to M$ such that for each $x \in M$, the fiber $\pi^{-1}(x)$ is a real k-dimensional vector space and there exists a neighborhood U of x and a diffeomorphism*

$$\varphi : \pi^{-1}(U) \to U \times \mathbb{R}^k,$$

such that for each $x' \in U$, $\varphi|_{\pi^{-1}(x')}$ is a vector space isomorphism between $\pi^{-1}(x')$ and $\mathbb{R}^k$. The bundle is denoted (E, π, M) and has rank k.

Thus, for a neighboorhood U at each point, a bundle admits the local trivialization $\pi^{-1}(U) \simeq U \times \mathbb{R}^k$. Note, we often denote the bundle simply by E.

In a field theory occurring on a vector bundle, a field is a differentiable assignment of a vector $v \in \pi^{-1}(x)$ to each $x \in M$. This is formalized by the notion of a section. A ***section*** of a vector bundle (E, π, M) is a differentiable map $\gamma : M \to E$ such that $\pi \circ \gamma = \mathbb{1}_M$. We denote the space of sections $\Gamma(E)$.

Definition 1.2.2 *A **bundle metric** on a bundle (E, π, M) is a smooth assignment of a scalar product to each fiber $\pi^{-1}(x)$ for all $x \in M$.*

Example 1.2.1 The tangent bundle of a differentiable manifold M, (TM, π, M), is a vector bundle where for $x \in M$, $\pi^{-1}(x) = T_xM$, the tangent space of M at x. In a neighborhood U of M, we have the trivialization $\pi^{-1}(U) \simeq U \times \mathbb{R}^{dim(M)}$. For this bundle, $\Gamma(TM)$ is the space of smooth vector fields on M. If TM has a bundle metric, we say that M is a Riemannian manifold.

Furthermore, given two vector bundles (E_1, π_1, M), (E_2, π_2, M), we construct the product bundle denoted $(E_1 \times E_2, \pi, M)$ where for $x \in M$, the fiber at x is defined $\pi^{-1}(x) := \pi_1^{-1}(x) \times \pi_2^{-1}(x)$. In a similar manner, we can construct the tensor product of two bundles, denoted $(E_1 \otimes E_2, \pi, M)$.

Of particular importance for our purposes is the bundle of differential forms, which we discuss next.

1.3 Exterior Calculus

Let V be a vector space; we denote $Alt^k(V)$ as the space of alternating k-linear maps from V^k to $\mathbb{R}$. The wedge product is a bilinear associative map

$$\wedge : Alt^k(V) \times Alt^l(V) \to Alt^{k+l}(V),$$

where for $\beta \in Alt^k(V),\ \alpha \in Alt^l(V)$, $v_i \in V$, the wedge product is defined by

$$\beta \wedge \alpha\ (v_1, ..., v_{k+l}) := \frac{1}{(k+l)!} \sum_{\sigma \in S_{k+l}} sign(\sigma) \beta(v_{\sigma(1)}, ..., v_{\sigma(k)}) \alpha(v_{\sigma(k+1)}, ..., v_{\sigma(k+l)}).$$

In order to determine a basis for $Alt^k(V)$, consider a basis $\{e_j\}_{j=1,..n}$ for V. A natural basis on $V^* = Alt^1(V)$ is defined by $\alpha^l(e_j) = \delta^l_j$. Then, $Alt^k(V)$ is spanned by a basis $\{\alpha^{l_1} \wedge ... \wedge \alpha^{l_k}\}_{l_1 < ... < l_k}$ where $l_1, ..., l_k \in \{1, ..., n\}$.

Proposition 1.3.1 *The wedge product is* ***graded commutative****, i.e.,*

$$\alpha \wedge \beta = (-1)^{kj}\beta \wedge \alpha, \ \forall \alpha \in Alt^k(V), \beta \in Alt^j(V).$$

Proof. It suffices to prove this on a basis for $Alt^k(V), Alt^j(V)$ since the wedge product is bilinear. Let $\alpha^{l_1} \wedge ... \wedge \alpha^{l_k} \in Alt^k(V)$, $\alpha^{m_1} \wedge ... \wedge \alpha^{m_j} \in Alt^j(V)$ where each $\alpha^i \in Alt^1(V)$. Clearly, by the definition of the wedge product, for $\alpha^i, \alpha^h \in Alt^1(V)$, $\alpha^i \wedge \alpha^h = -\alpha^h \wedge \alpha^i$. Thus,

$$\begin{aligned}\alpha^{l_1} \wedge ... \wedge \alpha^{l_k} \wedge (\alpha^{m_1} \wedge ... \wedge \alpha^{m_j}) &= (-1)^j \alpha^{l_1} \wedge ... \wedge (\alpha^{m_1} \wedge ... \wedge \alpha^{m_j}) \wedge \alpha^{l_k} \\ &= ... \\ &= (-1)^{kj}(\alpha^{m_1} \wedge ... \wedge \alpha^{m_j}) \wedge \alpha^{l_1} \wedge ... \wedge \alpha^{l_k}.\end{aligned}$$

That is, moving j 1-forms through k 1-forms produces kj sign changes. □

Furthermore, assume that V has an inner product, which naturally induces an inner product on the dual space V^*. We define the inner product in $Alt^k(V)$ by its action on the basis: For $\alpha = \alpha^{l_1} \wedge ... \wedge \alpha^{l_k}$ and $\beta = \beta^{m_1} \wedge ... \wedge \beta^{m_k}$,

$$\langle \alpha, \beta \rangle := det\Big(\langle \alpha^{l_i}, \beta^{m_j} \rangle\Big)_{ij}.$$

On a manifold, we take $V = T_xM$ for each $x \in M$. This gives the bundle of differential k-forms $(\Lambda^k M, \pi, M)$ where $\pi^{-1}(x) = Alt^k(T_xM)$. Analogous to a tensor product bundle, this space can be constructed as the k-fold wedge product of the cotangent bundle, $\Lambda^k M = T^*M \wedge ... \wedge T^*M$. A k-form is defined as a section of this bundle, i.e. an element of $\Gamma(\Lambda^k M) =: \Omega^k M$.

A coordinate basis on TM, $\{\partial_i\}_i$, provides a canonical choice of dual basis on T^*M, $\{dx^j\}_j$, satisfying $dx^j(\partial_i) = \delta_i^j$. This accordingly determines a basis for $\Lambda^k M$, $\{dx^{j_1} \wedge ... \wedge dx^{j_k}\}_{j_1 < ... < j_k}$.

Definition 1.3.1 *The* ***exterior derivative*** *is a map*

$$d^k : \Omega^k M \to \Omega^{k+1} M,$$

where for a function $f \in \Omega^0 M$, $df = (\partial_i f)dx^i$, and for $\omega \in \Omega^k M$ with components $\{\omega_{i_1,...,i_k}\}$ with respect to the coordinate basis,

$$d\omega = \sum_{i_1 < ... < i_k} d(\omega_{i_1,...,i_k}) \wedge dx^{i_1} \wedge ... \wedge dx^{i_k},$$

where we omit the superscript k when clear. The exterior derivative satisfies

$$\begin{aligned}&(i)\ d(a\alpha + b\beta) = ad\alpha + bd\beta \ \forall\ \alpha, \beta \in \Omega^k M, \ a, b \in \mathbb{R}; \\ &(ii)\ d(\alpha \wedge \beta) = d\alpha \wedge \beta + (-1)^k \alpha \wedge d\beta, \forall\ \alpha \in \Omega^k M; \\ &(iii)\ d^{k+1} \circ d^k = 0.\end{aligned}$$

In particular, the following sequence forms a cochain complex,

$$0 \to \Omega^0 M \xrightarrow{d} \Omega^1 M \xrightarrow{d} ... \xrightarrow{d} \Omega^n M \to 0. \tag{1.3.1}$$

We now state a fundamental theorem regarding the integration of forms.

Theorem 1.3.1 (Stokes' Theorem) *Let M be a compact, oriented differentiable manifold of dimension n, then for all $\omega \in \Omega^{n-1}M$,*

$$\int_M d\omega = \int_{\partial M} \omega. \tag{1.3.2}$$

Metric Structure

Now, assume M is a compact oriented Riemannian manifold of dimension n. Naturally, the metric on the tangent bundle induces a bundle metric on $\Lambda^k M$, denoted $\langle\ ,\ \rangle$.

Definition 1.3.2 *Define the **Hodge star operator** $\star : \Omega^k M \to \Omega^{n-k} M$ such that, on a k-form $\beta \in \Omega^k M$,*

$$\alpha \wedge \star\beta = \langle \alpha, \beta \rangle vol,\ \forall\ \alpha \in \Omega^k M,$$

where vol is the volume n-form corresponding to the orientation of M.

This defines an L^2 inner product on k-forms: For $\alpha, \beta \in \Omega^k M$,

$$(\alpha, \beta)_{L^2\Omega^k} := \int_M \alpha \wedge \star\beta = \int_M \langle \alpha, \beta \rangle vol.$$

Proposition 1.3.2 *The Hodge star satisfies $\star\star = (-1)^{k(n-k)}$ and is an isometry from the $L^2\Omega^k$ to $L^2\Omega^{n-k}$.*

Proof. Consider $dx^{i_1} \wedge ... \wedge dx^{i_k} \in \Omega^k M$. Then, $\star(dx^{i_1} \wedge ... \wedge dx^{i_k}) = dx^{j_1} \wedge ... \wedge dx^{j_{n-k}}$ where $dx^{i_1} \wedge ... \wedge dx^{i_k} \wedge dx^{j_1} \wedge ... \wedge dx^{j_{n-k}} = vol$. Applying the Hodge star again, we have

$$\star\star\,(dx^{i_1} \wedge ... \wedge dx^{i_k}) = \star(dx^{j_1} \wedge ... \wedge dx^{j_{n-k}}) = \pm dx^{i_1} \wedge ... \wedge dx^{i_k},$$

where the $\pm$ is determined by whether $dx^{j_1} \wedge ... \wedge dx^{j_{n-k}} \wedge dx^{i_1} \wedge ... \wedge dx^{i_k} = \pm vol$. However, by graded commutativity, $vol = dx^{i_1} \wedge ... \wedge dx^{i_k} \wedge dx^{j_1} \wedge ... \wedge dx^{j_{n-k}} = (-1)^{k(n-k)} dx^{j_1} \wedge ... \wedge dx^{j_{n-k}} \wedge dx^{i_1} \wedge ... \wedge dx^{i_k}$ and thus $\star\star = (-1)^{k(n-k)}$.

To show that the Hodge star is an isometry, for $\alpha, \beta \in L^2\Omega^k$,

$$\begin{aligned}
(\alpha, \beta)_{L^2\Omega^k} &= \int_M \alpha \wedge \star\beta = (-1)^{k(n-k)} \int_M (\star\star\alpha) \wedge \star\beta \\
&= (-1)^{k(n-k)}(-1)^{k(n-k)} \int_M (\star\beta) \wedge \star\star\alpha = \int_M (\star\beta) \wedge \star\star\alpha \\
&= (\star\beta, \star\alpha)_{L^2\Omega^{n-k}} = (\star\alpha, \star\beta)_{L^2\Omega^{n-k}},
\end{aligned}$$

where we used graded commutativity $(\star\star\alpha) \wedge \star\beta = (-1)^{k(n-k)}(\star\beta) \wedge \star\star\alpha$. □

Definition 1.3.3 *$d^{k*} : \Omega^k M \to \Omega^{k-1} M$ is the formal adjoint of d^k with respect to the $L^2\Omega^k$ product such that for $\beta \in \Omega^k M$,*

$$(d\alpha, \beta)_{L^2\Omega^k} = (\alpha, d^*\beta)_{L^2\Omega^{k-1}},$$

for all compactly supported $\alpha \in \Omega^{k-1} M$.

Proposition 1.3.3

$$d^{k*} = (-1)^k \star^{-1} d^{n-k} \star,$$
$$d^{k-1*} \circ d^{k*} = 0.$$

Proof. By Stokes' theorem 1.3.2 and property (ii) in Definition 1.3.1, for $\beta \in \Omega^k M$ and $\alpha \in \Omega_c^{k-1} M$,

$$0 = \int_{\partial M} \alpha \wedge \star\beta = \int_M d(\alpha \wedge \star\beta) = \int_M d\alpha \wedge \star\beta + (-1)^{k-1} \int_M \alpha \wedge d \star \beta$$
$$= \int_M d\alpha \wedge \star\beta - (-1)^k \int_M \alpha \wedge \star\star^{-1} d \star \beta = (d\alpha, \beta)_{L^2\Omega^k} - (\alpha, (-1)^k \star^{-1} d \star \beta)_{L^2\Omega^{k-1}}.$$

This gives the first identity. Furthermore,

$$d^{k-1*} \circ d^{k*} = (-1)^{k+1} \star^{-1} d^{n-k+1} \star (-1)^k \star^{-1} d^{n-k} \star = - \star^{-1} d^{n-k+1} d^{n-k} \star = 0.$$

□

Definition 1.3.4 *The **Hodge Laplacian** $\Delta^k : \Omega^k M \to \Omega^k M$ is an operator defined by*

$$\Delta^k := d^{k+1*} d^k + d^{k-1} d^{k*}. \tag{1.3.3}$$

*Furthermore, we say that $\alpha \in \Omega^k M$ is **harmonic** if $\Delta\alpha = 0$.*

Proposition 1.3.4 *For $\alpha \in \Omega_c^k M$,*

$$\Delta\alpha = 0 \iff d^*\alpha = 0 \text{ and } d\alpha = 0.$$

Proof.

($\Longleftarrow$) Clearly, $d^*\alpha = 0$ and $d\alpha = 0$ implies $(d^*d + dd^*)\alpha = 0$.
($\Longrightarrow$) Using the L^2 inner product and the adjoint property,

$$0 = (\Delta\alpha, \alpha) = ((d^*d + dd^*)\alpha, \alpha) = (d^*d\alpha, \alpha) + (dd^*\alpha, \alpha)$$
$$= (d^*\alpha, d^*\alpha) + (d\alpha, d\alpha) = \|d^*\alpha\|^2 + \|d\alpha\|^2,$$

which implies $d^*\alpha = 0, d\alpha = 0$. □

We define the Hilbert space $H\Omega^k$ and its dual:

$$H\Omega^k M = \{\omega \in L^2\Omega^k M \mid d^k\omega \in L^2\Omega^{k+1} M\},$$
$$H^*\Omega^k M = \{\omega \in L^2\Omega^k M \mid d^{k*}\omega \in L^2\Omega^{k-1} M\},$$

with inner products ($\alpha, \beta \in H\Omega^k M;\ \sigma, \tau \in H^*\Omega^k M$),

$$(\alpha, \beta)_{H\Omega^k} = (\alpha, \beta)_{L^2\Omega^k} + (d\alpha, d\beta)_{L^2\Omega^{k+1}},$$
$$(\sigma, \tau)_{H^*\Omega^k} = (\sigma, \tau)_{L^2\Omega^k} + (d^*\sigma, d^*\tau)_{L^2\Omega^{k-1}}.$$

The spaces $H\Omega^k$ form the Hilbert de Rham cochain complex under the map d (and similarly a dual complex for d^*):

$$0 \longrightarrow H\Omega^0 \xrightarrow{d} H\Omega^1 \xrightarrow{d} ... \xrightarrow{d} H\Lambda^n \longrightarrow 0,$$
$$0 \longleftarrow H^*\Omega^0 \xleftarrow{d^*} H^*\Omega^1 \xleftarrow{d^*} ... \xleftarrow{d^*} H^*\Omega^n \longleftarrow 0.$$

As more notation, we define the space of L^2 harmonic k-forms, L^2 k-cocyles (closed forms), and L^2 k-coboundaries (exact forms) in $H\Omega^k$, respectively:

$$\mathfrak{H}^k := \{\omega \in H\Omega^k \cap \mathring{H}^*\Omega^k \mid d\omega = 0, \delta\omega = 0\},$$
$$\mathfrak{Z}^k := \{\omega \in H\Omega^k \mid d\omega = 0\},$$
$$\mathfrak{B}^k := d[H\Omega^{k-1}].$$

To end this section, we make some final remarks regarding the structure of the de Rham complex 1.3.1. The Hodge decomposition theorem states that the space of k-forms admits the decomposition

$$\Omega^k M \cong d[\Omega^{k-1}M] \oplus d^*[\Omega^{k+1}M] \oplus H^k(M), \tag{1.3.4}$$

where $H^k(M)$ is the space of harmonic k-forms over M. Analogously, the Hilbert de Rham complex can be decomposed

$$H\Omega^k M \cong \mathfrak{B}^k \oplus \mathfrak{B}^{*k} \oplus \mathfrak{H}^k, \tag{1.3.5}$$

where $B^{*k} = d^*[H\Omega^{k+1}]$. Furthermore, the Hodge decomposition 1.3.4 implies that the de Rham cohomology $H^k_{dR} := ker(d^k)/d[\Omega^{k-1}]$ is isomorphic to the space of harmonic forms $H^k(M)$, i.e. each cohomology class $[\alpha] \in H^k_{dR}$ corresponds to a harmonic form. When discretizing the de Rham complex, it will then be important to preserve the cochain complex structure to ensure that the Hodge decomposition still applies in the discretized space.

Vector-Valued Differential Forms

Recall in the definition of differential forms, forms take values in $M \times \mathbb{R}$, i.e. they take values in $\mathbb{R}$ at each point in M. However, more generally, forms can take values in an arbitrary vector bundle.

Definition 1.3.5 *Let (E, π, M) be a vector bundle. Then an **E-valued differential k-form** is a section of the bundle $E \otimes \Lambda^k M$. We denote the space of E-valued k-forms*

$$\Omega^k(M, E) := \Gamma(E \otimes \Lambda^k M).$$

In the case of a trivial vector bundle $E = M \times V$, we use the notation

$$\Omega^k(M|V) := \Omega^k(M, M \times V).$$

Definition 1.3.6 *Let $[\cdot,\cdot]$ be a smooth pointwise binary operation on the fibers of (E,π,M), i.e. $[\cdot,\cdot]_x : \pi^{-1}(x)\times\pi^{-1}(x)\to\pi^{-1}(x)$. Then, we extend the wedge product to vector-valued forms $[\cdot\wedge\cdot]:\Omega^k(M,E)\times\Omega^l(M,E)\to\Omega^{k+l}(M,E)$ such that for $\beta\in\Omega^k(M,E)$, $\alpha\in\Omega^l(M,E)$, $v_1,...,v_{k+l}\in\Gamma(TM)$,*

$$[\beta\wedge\alpha](v_1,...,v_{k+l}) := \frac{1}{(k+l)!}\sum_{\sigma\in S_{k+l}} sign(\sigma)[\beta(v_{\sigma(1)},...,v_{\sigma(k)}),\alpha(v_{\sigma(k+1)},...,v_{\sigma(k+l)})].$$

Definition 1.3.7 *Let $\langle\ ,\ \rangle_E$ be a bundle metric on E and let $\langle\ ,\ \rangle_{\Lambda^k M}$ be a bundle metric on $\Lambda^k M$. For $\eta\otimes\omega,\eta'\otimes\omega'\in\Gamma(E\otimes\Lambda^k M)$, define*

$$\langle\eta\otimes\omega,\eta'\otimes\omega'\rangle := \langle\eta,\eta'\rangle_E\langle\omega,\omega'\rangle_{\Lambda^k M}.$$

In particular, this determines a metric on the basis of $E\otimes\Lambda^k M$ and by linear extension provides a bundle metric on $E\otimes\Lambda^k M$.

The above definitions will allow us to work with theories which involve forms with values in vector spaces other than $\mathbb{R}$ (e.g. Yang-Mills theory, see section 1.5).

1.4 Lagrangian Field Theory

A Lagrangian field theory characterizes the configuration of a field $u\in\Gamma(E)$ as the stationary point of an associated action $S[u]$, where $S:\Gamma(E)\to\mathbb{R}$ is defined as the integral of a Lagrangian density. The condition for stationarity is that the variation of S vanishes for all proper variations. To make this precise, we define the following derivative:

Definition 1.4.1 (Gâteaux Derivative) *Let X and Y be locally convex topological vector spaces and suppose $F:X\to Y$. Then, F is said to be Gâteaux differentiable at $u\in X$ if there exists a linear operator $\delta F(u):X\to Y$ satisfying*

$$\lim_{\epsilon\to 0}\frac{1}{\epsilon}\|F(u+\epsilon v)-F(u)-\epsilon\delta F(u)\cdot v\|_Y = 0,\ \forall\ v\in X.$$

*If it exists, we call $\delta F(u)$ the **Gâteaux derivative (or variation)** of F at u and it can be computed directly via the formula*

$$\delta F(u)\cdot v = \frac{d}{d\epsilon}\Big|_{\epsilon=0} F(u+\epsilon v).$$

For a field theory defined over some vector bundle (E,π,M), the action $S=\int\mathcal{L}$ where $\mathcal{L}:J^1(E)\to\Omega^n M$ is the Lagrangian density (Lagrangian for short), where $n:=dim(M)$. $J^1(E)$ is the first jet-bundle of E which in coordinates involves the coordinates on M, the coordinates on E (the field), and the first derivatives of the field.

For our purposes, we consider a specific class of Lagrangians. We take as our configuration bundle $\Lambda^k M$ and the analog of the jet-bundle to be $\Lambda^k M\times\Lambda^{k+1}M\times\Lambda^{k-1}M$ over the base space M. Thus,

$$\mathcal{L}:\Gamma(\Lambda^k M\times\Lambda^{k+1}M\times\Lambda^{k-1}M)\to\Omega^n M.$$

We construct the action

$$S[u] := \int_M \mathcal{L}(u, du, d^*u), \tag{1.4.1}$$

where the solution u satisfies the stationary condition $\delta S(u) \cdot v = 0$ for all proper variations, i.e. v vanishing on the boundary.

Lemma 1.4.1 *Let M be an oriented Riemannian manifold and $Z : \Omega^s M \to \Omega^n M$ be Gâteaux differentiable at u, then there exists $\partial Z : \Omega^s M \to \Omega^s M$ such that $\delta Z(u) \cdot v = \partial Z(u) \wedge \star v$ for all $v \in \Omega^s M$.*

Proof. By the definition of the Gâteaux derivative, $\delta Z(u)$ is a linear operator from $\Omega^s M$ to $\Omega^n M$. Writing $v \in \Omega^s M$ in components, $v = \sum v_{i_1,\dots,i_s} dx^{i_1} \wedge \dots \wedge dx^{i_s}$, summing over $i_1 < \dots < i_s$. Since $\delta Z(u)$ maps v linearly into an n-form,

$$\delta Z(u) \cdot v = \Big(\sum a_{i_1,\dots,i_s} v_{i_1,\dots,i_s} \Big) vol,$$

where the a-coefficients depend on u. Then, taking

$$\partial Z(u) = \sum \frac{a_{i_1,\dots,i_s}}{\|dx^{i_1} \wedge \dots \wedge dx^{i_s}\|^2} dx^{i_1} \wedge \dots \wedge dx^{i_s},$$

we verify $\partial Z(u) \wedge \star v = \delta Z(u) \cdot v$,

$$\begin{aligned}
\partial Z(u) \wedge \star v &= \Big(\sum \frac{a_{i_1,\dots,i_s}}{\|dx^{i_1} \wedge \dots \wedge dx^{i_s}\|^2} dx^{i_1} \wedge \dots \wedge dx^{i_s} \Big) \wedge \star \Big(\sum v_{i_1,\dots,i_s} dx^{i_1} \wedge \dots \wedge dx^{i_s} \Big) \\
&= \sum \Big(\frac{a_{i_1,\dots,i_s} v_{i_1,\dots,i_s}}{\|dx^{i_1} \wedge \dots \wedge dx^{i_s}\|^2} (dx^{i_1} \wedge \dots \wedge dx^{i_s}) \wedge \star (dx^{i_1} \wedge \dots \wedge dx^{i_s}) \Big) \\
&= \sum \frac{a_{i_1,\dots,i_s} v_{i_1,\dots,i_s}}{\|dx^{i_1} \wedge \dots \wedge dx^{i_s}\|^2} \|dx^{i_1} \wedge \dots \wedge dx^{i_s}\|^2 vol \\
&= \sum \Big(a_{i_1,\dots,i_s} v_{i_1,\dots,i_s} \Big) vol = \delta Z(u) \cdot v,
\end{aligned}$$

where we used the definition of the Hodge star and the fact that $(dx^{i_1} \wedge \dots \wedge dx^{i_s}) \wedge \star (dx^{j_1} \wedge \dots \wedge dx^{j_s}) \neq 0$ only if $(i_1, \dots, i_s) = (j_1, \dots, j_s)$ and thus, only the terms in both sums with the same indices interact. □

Remark A similar result can be proven for differential forms with values in a vector bundle. In this case, the metric $\wedge\star$ gets replaced with the metric on the tensor product bundle $\langle\ ,\ \rangle_{E \otimes \Lambda^k M}$. In particular, there exists ∂Z such that $\delta Z(u) \cdot v = \langle \partial Z(u), v \rangle_{E \otimes \Lambda^k M}$. The next theorem holds in this more general case as well.

Theorem 1.4.1 (Euler-Lagrange Equation) *The condition for the stationarity of the action 1.4.1 for all proper variations is given by*

$$\frac{\partial}{\partial u} \mathcal{L}(u, du, d^*u) + d^* \frac{\partial}{\partial (du)} \mathcal{L}(u, du, d^*u) + d \frac{\partial}{\partial (d^*u)} \mathcal{L}(u, du, d^*u) = 0, \tag{1.4.2}$$

where the ∂ notation is as in the previous lemma.

Proof. From the action $S[u] = \int_M \mathcal{L}(u, du, d^*u)$,

$$\begin{aligned}\delta S[u] \cdot v &= \frac{d}{d\epsilon}\Big|_{\epsilon=0} S[u + \epsilon v] \\ &= \int_M \delta_1\mathcal{L}(u, du, d^*u) \cdot v + \delta_2\mathcal{L}(u, du, d^*u) \cdot dv + \delta_3\mathcal{L}(u, du, d^*u) \cdot d^*v,\end{aligned}$$

where δ_i denotes the variation in the i^{th} argument. By Lemma 1.4.1 and the adjoint property of d and d^* (holds since v vanishes on the boundary),

$$\begin{aligned}\delta S[u] \cdot v &= \int_M \partial_1\mathcal{L}(u, du, d^*u) \wedge \star v + \partial_2\mathcal{L}(u, du, d^*u) \wedge \star dv + \partial_3\mathcal{L}(u, du, d^*u) \wedge \star d^*v \\ &= \int_M \partial_1\mathcal{L}(u, du, d^*u) \wedge \star v + d^*\partial_2\mathcal{L}(u, du, d^*u) \wedge \star v + d\partial_3\mathcal{L}(u, du, d^*u) \wedge \star v \\ &= \int_M \Big(\partial_1\mathcal{L}(u, du, d^*u) + d^*\partial_2\mathcal{L}(u, du, d^*u) + d\partial_3\mathcal{L}(u, du, d^*u)\Big) \wedge \star v.\end{aligned}$$

In order for this variation to vanish for arbitrary v,

$$\partial_1\mathcal{L}(u, du, d^*u) + d^*\partial_2\mathcal{L}(u, du, d^*u) + d\partial_3\mathcal{L}(u, du, d^*u) = 0.$$

□

Remark We can also include explicit coordinate dependence to the Lagrangian $\mathcal{L}(x, u, du, d^*u),\ x \in M$, which would have the same associated Euler-Lagrange equation. Furthermore, we could consider a theory governing multiple fields, $\{u^A\}_{A=1,...,s}$. In this case, we would get an equation from each condition $\delta_A S[u^1, ..., u^s] \cdot v = 0$. Explicitly,

$$\frac{\partial}{\partial u^A}\mathcal{L} + d^*\frac{\partial}{\partial(du^A)}\mathcal{L} + d\frac{\partial}{\partial(d^*u^A)}\mathcal{L} = 0,\ \ A = 1, ..., s.$$

Example 1.4.1 Consider the Lagrangian

$$\mathcal{L}(u, du, d^*u) = \frac{1}{2}du \wedge \star du + \frac{1}{2}d^*u \wedge \star d^*u + f \wedge \star u,$$

where $u, f \in \Omega^k M$. Compute the variations

$$\delta_1\mathcal{L}(u, du, d^*u) \cdot v = \frac{d}{d\epsilon}\Big|_{\epsilon=0}\mathcal{L}(u + \epsilon v, du, d^*u) = f \wedge \star v,$$

$$\delta_2\mathcal{L}(u, du, d^*u) \cdot dv = \frac{d}{d\epsilon}\Big|_{\epsilon=0}\mathcal{L}(u, du + \epsilon dv, d^*u) = du \wedge \star dv,$$

$$\delta_3\mathcal{L}(u, du, d^*u) \cdot d^*v = \frac{d}{d\epsilon}\Big|_{\epsilon=0}\mathcal{L}(u, du, d^*u + \epsilon d^*v) = d^*u \wedge \star d^*v.$$

By lemma 1.4.1, $\partial_1\mathcal{L}(u, du, d^*u) = f$, $\partial_2\mathcal{L}(u, du, d^*u) = du$, $\partial_3\mathcal{L}(u, du, d^*u) = d^*u$. Thus, the corresponding Euler-Lagrange equation 1.4.2 is the Poisson equation (for a k-form):

$$\Delta u = (d^*d + dd^*)u = -f.$$

Note, for a Lorentzian (spacetime) manifold, this equation instead has the interpretation of a wave equation $\Box u = -f$.

Noether's Theorem

When discretizing a physical theory, it is important to consider its conservation laws, as they shape the behavior of the system. If our discretization in some way respects the conserved structures of a system, the numerical simulation will be more robust. In a Lagrangian theory, Noether's theorem states that the symmetries of an action correspond to a conservation law.

Let M be an n-dimensional differentiable manifold and X be a generator for a transformation on M. Denote $\tilde{X}$ as the lifted action of X on ΛM.

Definition 1.4.2 *We say X is a **continuous symmetry** of the action $S : \Omega^k \to \mathbb{R}$ if for all $\phi \in \Omega^k M$, the variation of $S[\phi]$ in the symmetry direction over any submanifold U, $\dim(U) = \dim(M)$, vanishes up to an exterior derivative,*

$$S'[\phi] \cdot \tilde{X}(\phi) = \int_U dK(\phi), \tag{1.4.3}$$

for some $K : \Omega^k M \to \Omega^{n-1} M$, where 1.4.3 varies smoothly w.r.t. U.

Theorem 1.4.2 (Noether's Theorem) *Let X be a continuous symmetry of $S : \Omega^k M \to \mathbb{R}$. Then, for $u \in \Omega^k M$ satisfying the Euler-Lagrange equation 1.4.2, there exists $\mathfrak{J} : \Omega^k M \to \Omega^{n-1} M$ such that $d\mathfrak{J}(u) = 0$, given by*

$$\mathfrak{J}(u) = \Big(\tilde{X}(u) \wedge \star \partial_2 \mathcal{L}(u, du, d^* u) - \partial_3 \mathcal{L}(u, du, d^* u) \wedge \star \tilde{X}(u)\Big) - K(u). \tag{1.4.4}$$

Proof. The basic idea is to obtain an expression for the variation in the symmetry direction in two different ways and subtract to obtain the conservation law. Let U be a submanifold of M, $\dim(U) = \dim(M)$. Since X is a symmetry of the action, there exists $K : \Omega^k M \to \Omega^{n-1} M$ such that

$$S'[\phi] \cdot \tilde{X}(\phi) = \int_U dK(\phi), \ \forall \ \phi \in \Omega^k M.$$

We compute the variation $S'[\phi] \cdot v$ for any perturbation v. Note that it is not necessarily a proper variation and thus, d^* and d are not necessarily adjoint.

$$\begin{aligned} S'[u] \cdot v &= \int_U \partial_1 \mathcal{L}(z) \wedge \star v + \partial_2 \mathcal{L}(z) \wedge \star dv + \partial_3 \mathcal{L}(z) \wedge \star d^* v \\ &= \int_U \Big(\partial_1 \mathcal{L}(z) + d^* \partial_2 \mathcal{L}(z) + d\partial_3 \mathcal{L}(z)\Big) \wedge \star v + \int_{\partial U} v \wedge \star \partial_2 \mathcal{L}(z) - \partial_3 \mathcal{L}(z) \wedge \star v \\ &= \int_{\partial U} v \wedge \star \partial_2 \mathcal{L}(z) - \partial_3 \mathcal{L}(z) \wedge \star v = \int_U d\Big(v \wedge \star \partial_2 \mathcal{L}(z) - \partial_3 \mathcal{L}(z) \wedge \star v\Big), \end{aligned}$$

where we used that u satisfies 1.4.2 and denote $z := (u, du, d^* u)$. Thus,

$$0 = S'[u] \cdot v\Big|_{v = \tilde{X}(u)} - S'[\phi] \cdot \tilde{X}(\phi)\Big|_{\phi = u} = \int_U d\Big(\tilde{X}(u) \wedge \star \partial_2 \mathcal{L}(z) - \partial_3 \mathcal{L}(z) \wedge \star \tilde{X}(u) - K(u)\Big),$$

since U is arbitrary and the integrand varies smoothly with U, the expression 1.4.4 satisfies $d\mathfrak{J}(u) = 0$. One can also easily check by the definition of the wedge product and Hodge star that $\mathfrak{J}(u) \in \Omega^{n-1} M$. □

Remark 1.4.1 We refer to $\mathfrak{J}$ as a conserved current, since $d\mathfrak{J}(u) = 0$ is a conservation law. To see this in coordinates, since $\mathfrak{J}(u) \in \Omega^{n-1}M$, it can be written as a linear combination of n basis forms,

$$\mathfrak{J}(u) = \mathfrak{J}^1 \partial_1 \lrcorner vol^n + ... + \mathfrak{J}^n \partial_n \lrcorner vol^n,$$

where $vol^n := dx^1 \wedge ... \wedge dx^n$. Thus, $0 = d\mathfrak{J}(u) = \partial_\alpha \mathfrak{J}^\alpha vol^n$. With x^1 as time t,

$$\frac{\partial}{\partial t}\mathfrak{J}^1 + \sum_{k=2}^{n} \partial_k \mathfrak{J}^k = 0,$$

which is the classical form of a conservation law.

Remark 1.4.2 Note that since $\mathfrak{J}(u)$ is a closed form, we could also add an exact form $d\alpha$ to the Noether current. Thus, Noether's theorem actually specifies an equivalence class of closed forms,

$$[\mathfrak{J}(u)] := \{\omega \in \ker(d^{n-1}) \mid \mathfrak{J}(u) - \omega \in d[\Omega^{n-2}M]\},$$

i.e. an element of the $(n-1)$ de Rham cohomology $H^{n-1}_{dR}(M) := Z^{n-1}/B^{n-1}$.

Example 1.4.2 (Energy Momentum Current of Scalar Field)
To illustrate Noether's theorem, we consider a scalar field theory. Let M be an $n+1$ dimensional Lorentzian manifold with Minkowski metric $\eta = diag(-1\ 1\ 1\ 1)$. For a scalar field $\phi \in \Omega^0 M$, $d^*\phi = 0$. Thus, the action has the form $S[\phi] = \int_M \mathcal{L}(\phi, d\phi)$. Since $\mathcal{L}(\phi, d\phi) \in \Omega^{n+1}M$,

$$\mathcal{L}(\phi, d\phi) = L(\phi, d\phi) d^{n+1}x,$$

for some $L : \Gamma(\Omega^k M \times \Omega^{k+1}M) \to M \times \mathbb{R}$, where $d^{n+1}x := dx^0 \wedge ... \wedge dx^n$. For a translation in spacetime (generated by $X_\nu = \partial_\nu$), the fields transform as $\tilde{X}_\nu(\phi) = \partial_\nu \phi$ and likewise the Lagrangian transforms as $(\partial_\nu L) d^{n+1}x$. Thus,

$$S'[\phi] \cdot \tilde{X}_\nu(\phi) = \int_U (\partial_\nu L(\phi, d\phi)) d^{n+1}x = \int_U d(L(\phi, d\phi)\partial_\nu \lrcorner d^{n+1}x),$$

i.e., translations are symmetries of the action, which arises from the fact that the Lagrangian does not explicitly depend on the coordinates. By Noether's theorem, for a solution $u \in \Omega^0 M$ of 1.4.2, for each symmetry X_ν, $\nu \in \{0, 1, ..., n\}$,

$$T_\nu(u) = \partial_\nu u \wedge \star \partial_2 \mathcal{L}(u, du) - L(u, du)\partial_\nu \lrcorner d^{n+1}x$$

is a conserved current. Thinking of each current $T_\nu(u)$ as the components of a single object, we have the energy momentum current $T(u)$. Clearly, $T(u)$ is a $\Omega^n M$ valued 1-form, i.e. an element of $\Gamma(\Lambda^n M \times \Lambda^1 M)$: for any vector $Z = Z^\nu \partial_\nu \in TM$, $T(u) \cdot Z = T_\nu(u) Z^\nu \in \Omega^n M$. Intuitively, the energy-momentum current takes in a direction, specified by the vector Z, and returns the conserved n-form current corresponding to the translational symmetry in that direction.

With this energy-momentum current, we can for example calculate the energy for a scalar wave with Lagrangian $\mathcal{L}(u, du) = -\frac{1}{2} du \wedge \star du - U(u) d^{n+1}x$. Computing the current corresponding to the time symmetry,

$$\begin{aligned} T_0(u) &= \partial_0 u \wedge \star \partial_2 \mathcal{L}(u, du) - L(u, du)\partial_0 \lrcorner d^{n+1}x = -\partial_0 u \wedge \star du - L(u, du)\partial_0 \lrcorner d^{n+1}x \\ &= -\partial_0 u \wedge \star(\partial_0 u \; dx^0 + \partial_1 u \; dx^1 + ... + \partial_n u \; dx^n) - L(u, du)\partial_0 \lrcorner d^{n+1}x \\ &= -\partial_0 u \wedge (-\partial_0 u \; dx^1 \wedge ... \wedge dx^n + ...) - L(u, du) dx^1 \wedge ... \wedge dx^n \\ &= ((\partial_0 u)^2 - L(u, du)) dx^1 \wedge ... \wedge dx^n + ... \end{aligned}$$

(omitting some terms since we are only calculating the energy T_0^0). As in remark 1.4.1, since $T_0(u) \in \Omega^n M$, it can be written as $T_0(u) = T_0^\mu(u)\partial_\mu \lrcorner d^{n+1}x$. From the Minkowski metric, $L(u, du) = \frac{1}{2}(\partial_0 u)^2 - \frac{1}{2}\sum_{k=1}^n (\partial_k u)^2 - U(u)$. Consequently, the energy is (as expected)

$$T_0^0(u) = (\partial_0 u)^2 - L(u, du) = \frac{1}{2}(\partial_0 u)^2 + \frac{1}{2}\sum_{k=1}^n (\partial_k u)^2 + U(u),$$

and satisfies the conservation law $\partial_0 T_0^0(u) + \sum_{k=1}^n \partial_k T_0^k(u) = 0$.

1.5 Connection and Curvature

In a vector bundle, there is no natural way to compare vectors with different base points. Consequently, differentiation of a section of the bundle in a direction is not necessarily well-defined. This leads to the idea of a connection.

For a vector bundle (E, π, M), a connection provides the notion of differentiation of a section of E in some direction $Z \in TM$.

Definition 1.5.1 *A **connection** on (E, π, M) is a linear map*

$$D : \Gamma(E) \to \Gamma(E \otimes T^*M),$$

such that for all $f \in C^\infty M$, $Z, Z' \in TM$, $\alpha \in \Gamma(E)$,

$$\begin{aligned} &(i)\; D\alpha \cdot (fZ) = fD\alpha \cdot Z; \\ &(ii)\; D\alpha \cdot (Z + Z') = D\alpha \cdot Z + D\alpha \cdot Z'; \\ &(iii)\; D(f\alpha) \cdot Z = Z(f)\alpha + fD\alpha \cdot Z. \end{aligned}$$

*We say $D\alpha \cdot Z =: D_Z\alpha$ is the **covariant derivative** of α in the direction Z.*

In the notation of vector-valued differential forms, $D : \Omega^0(M, E) \to \Omega^1(M, E)$. To see this more explicitly, we determine an expression for the connection.

Proposition 1.5.1 *The connection can be expressed $D = d + A$, where A is a matrix-valued 1-form*

Proof. Using a basis $\{\partial_\alpha\}$ on TM and a basis $\{e_j\}$ on E, define the Christoffel symbols by $\Gamma^i_{\alpha j} e_i := D_{\partial_\alpha} e_j$, where i, j run from 1 to the rank of E and α runs

from 1 to $\dim(M)$. Then, for $Z = Z^\alpha \partial_\alpha \in TM$, $\beta = \beta^j e_j \in \Gamma(E)$,

$$\begin{aligned} D\beta \cdot Z = D_Z \beta = D_Z(\beta^j e_j) &\overset{(iii)}{=} Z(\beta^i)e_i + \beta^j D_Z(e_j) = Z(\beta^i)e_i + \beta^j D_{Z^\alpha \partial_\alpha} e_j \\ &\overset{(i)}{=} Z(\beta^i)e_i + Z^\alpha \beta^j D_{\partial_\alpha} e_j = Z(\beta^i)e_i + Z^\alpha \beta^j \Gamma^i_{\alpha j} e_i. \end{aligned}$$

To remove the Z dependence and obtain an expression for D, recall that for a scalar function f, $df \cdot Z = Z(f)$. Furthermore, defining $A^i_j = \Gamma^i_{\alpha j} dx^\alpha$, we have that $A^i_j \cdot Z = \Gamma^i_{\beta j} dx^\beta \cdot (Z^\alpha \partial_\alpha) = Z^\alpha \Gamma^i_{\beta j} \delta^\beta_\alpha = Z^\alpha \Gamma^i_{\alpha j}$. Thus,

$$\begin{aligned} D\beta \cdot Z &= Z(\beta^i)e_i + Z^\alpha \beta^j \Gamma^i_{\alpha j} e_i \\ &= d(\beta^i) \cdot Z \; e_i + A^i_j \cdot Z \beta^j e_i \\ &= (d(\beta^i)e_i + A^i_j \beta^j e_i) \cdot Z, \\ \therefore D\beta &= (d\beta^i + A^i_j \beta^j) \; e_i. \end{aligned}$$

With $A = (A^i_j)$ acting on β by matrix multiplication, we have $D = d + A$. □

Note that in this definition the exterior derivative moves through the vector structure and acts on the components. We refer to A as the **connection one-form** or **potential**; it is a 1-form valued in the endomorphisms of the bundle. Since A is a matrix-valued one-form, $D : \Omega^0(M, E) \to \Omega^1(M, E)$ as expected. The derivative can be uniquely extended to E-valued k-forms by

$$\begin{aligned} D : \Omega^k(M, E) &\to \Omega^{k+1}(M, E), \\ \beta &\mapsto d\beta + A \wedge \beta, \end{aligned}$$

or in components, $D\beta = (d\beta^i + A^i_j \wedge \beta^j) \; e_i$. The $\wedge$ can be omitted for $k = 0$.

Definition 1.5.2 *The* ***curvature*** *of the connection is given by*

$$F = D^2 : \Omega^0(M, E) \to \Omega^2(M, E).$$

Furthermore, if $F = 0$, we say the connection is flat.

Proposition 1.5.2 *The curvature is given by*

$$F = dA + A \wedge A = dA + \frac{1}{2}[A \wedge A], \tag{1.5.1}$$

where $[\cdot, \cdot]$ is the commutator (in general, the Lie-bracket).

Proof. For $\beta \in \Gamma(E)$,

$$\begin{aligned} F\beta = D^2\beta &= (d + A \wedge)(d + A)\beta = (d + A \wedge)(d\beta + A\beta) \\ &= d^2\beta + d(A\beta) + A \wedge d\beta + A \wedge A\beta \\ &= 0 + (dA)\beta + (-1)A \wedge d\beta + A \wedge d\beta + A \wedge A\beta \\ &= (dA + A \wedge A)\beta. \end{aligned}$$

Thus, $F = dA + A \wedge A$, and the second equality holds since

$$A \wedge A = A_\alpha A_\beta dx^\alpha \wedge dx^\beta = \frac{1}{2}(A_\alpha A_\beta - A_\beta A_\alpha)dx^\alpha \wedge dx^\beta = \frac{1}{2}[A \wedge A].$$

Note that in general $A \wedge A \neq 0$ since matrix multiplication is non-commutative. □

Remark 1.5.1 The curvature satisfies the Bianchi identity $DF = 0$, which can be shown by treating F as an element of $\Omega^0(M, E)^* \otimes \Omega^2(M, E)$ and using the induced connection on this space (I omit the details of the proof here; for the proof, see [10]). Note that on the space $\Omega^0(M, E)^* \otimes \Omega^k(M, E)$, D acts via the adjoint action, $D\eta = d\eta + [A \wedge \eta]$.

Yang-Mills Theory

Yang-Mills theory governs the dynamics of the connection of a bundle and is used in the Standard Model to describe the electromagnetic, weak, and strong interactions.

(This section assumes some background with Lie groups, algebras, and their representation; see the appendix for details) To provide a rough sketch of the Yang-Mills theory, consider matter fields, defined as sections of a bundle (E, π, M) which carries a fiber-wise representation of a Lie group G. Gauge transformations are maps from M to G which form a group under pointwise multiplication in G and induces a transformation in the matter fields. The Yang-Mills theory describes the dynamics of a connection (gauge potential) in a manner consistent with the gauge transformations and allows for the dynamics of the matter fields to be coupled with the gauge potential.

Let G be a compact semi-simple Lie Group (these assumptions allow for the Killing form to be a negative definite bilinear form on the Lie algebra). Then, in Yang-Mills theory, we take the connection one-form to be a $\mathfrak{g}$-valued 1-form, i.e. $A \in \Gamma(\mathfrak{g} \otimes T^*M) = \Omega^1(M|\mathfrak{g})$. The pure Yang-Mills action is

$$S_{YM}[A] := -\int_M tr'(F_A \wedge \star F_A), \tag{1.5.2}$$

where tr' is the Killing-form on $\mathfrak{g}$ and the Hodge star operates on the differential form part of the curvature 2-form $F_A := dA + \frac{1}{2}[A \wedge A]$ (here, $[\cdot, \cdot]$ is the Lie-bracket on $\mathfrak{g}$).

We further suppose that the connection respects a metric structure on E, in the sense that $d\langle\alpha, \beta\rangle_E = \langle D\alpha, \beta\rangle_E + \langle\alpha, D\beta\rangle_E$. With this assumption, a simple calculation shows that for any $Z \in TM$, $A \cdot Z$ is skew symmetric. Using this skew symmetry and a similar calculation of the adjoint d^* to d, the adjoint to D with respect to $-\int_M tr'(\ \wedge\star\ )$ is

$$D^* := d^* + A\lrcorner.$$

To determine the equation governing the dynamics of the connection, we compute a proper variation of the action.

Theorem 1.5.1 (Yang-Mills Equation) *The Euler-Lagrange equation corresponding to the action 1.5.2 is given by*

$$D^*F_A = 0. \tag{1.5.3}$$

Proof. The stationary condition for the action is given by

$$0 = \delta S_{YM}[A] \cdot B = \int_M \delta_1 \mathcal{L}(A, dA) \cdot B + \delta_2 \mathcal{L}(A, dA) \cdot dB$$

for all proper variations, where

$$\begin{aligned}\mathcal{L}(A, dA) &= -tr'(F_A \wedge \star F_A) = -tr'((dA + \frac{1}{2}[A \wedge A]) \wedge \star(dA + \frac{1}{2}[A \wedge A])) \\ &= -tr'(dA \wedge \star dA + dA \wedge \star[A \wedge A] + \frac{1}{4}[A \wedge A] \wedge \star[A \wedge A]).\end{aligned}$$

Thus,

$$\begin{aligned}\delta_1 \mathcal{L}(A, dA) \cdot B &= \frac{d}{d\epsilon}\Big|_{\epsilon=0} \mathcal{L}(A + \epsilon B, dA) \\ &= -\frac{d}{d\epsilon}\Big|_{\epsilon=0} tr'\Big(dA \wedge \star dA + dA \wedge \star[(A + \epsilon B) \wedge (A + \epsilon B)] \\ &\quad + \frac{1}{4}[(A + \epsilon B) \wedge (A + \epsilon B)] \wedge \star[(A + \epsilon B) \wedge (A + \epsilon B)]\Big) \\ &= -tr'\Big(dA \wedge \star([B \wedge A] + [A \wedge B]) + \frac{1}{4}[A \wedge A] \wedge \star(2[B \wedge A] + 2[A \wedge B])\Big) \\ &= -tr'\Big((dA + \frac{1}{2}[A \wedge A]) \wedge \star([B \wedge A] + [A \wedge B])\Big) \\ &= -2\ tr'\Big(F_A \wedge \star[A \wedge B]\Big),\end{aligned}$$

where we used the symmetry of the inner product and the fact that $[A \wedge B] = [B \wedge A]$ (we get commutativity from the anticommutativity of the Lie bracket with the anticommutativity of the wedge product on one-forms). Similarly,

$$\begin{aligned}\delta_2 \mathcal{L}(A, dA) \cdot dB &= \frac{d}{d\epsilon}\Big|_{\epsilon=0} \mathcal{L}(A, dA + \epsilon dB) \\ &= -\frac{d}{d\epsilon}\Big|_{\epsilon=0} tr'\Big((dA + \epsilon dB) \wedge \star(dA + \epsilon dB) + (dA + \epsilon dB) \wedge \star[A \wedge A] + \frac{1}{4}[A \wedge A] \wedge \star[A \wedge A]\Big) \\ &= -tr'\Big(2\ dA \wedge \star dB + [A \wedge A] \wedge \star dB\Big) = -2\ tr'\Big((dA + \frac{1}{2}[A \wedge A]) \wedge \star dB\Big) = -2\ tr'(F_A \wedge \star dB).\end{aligned}$$

Thus, recalling that D acts on B in the adjoint action,

$$\begin{aligned}0 &= \int_M \delta_1 \mathcal{L}(A, dA) \cdot B + \delta_2 \mathcal{L}(A, dA) \cdot dB = -2 \int_M tr'\Big(F_A \wedge \star(dB + [A \wedge B])\Big) \\ &= -2 \int_M tr'(F_A \wedge \star DB) = -2 \int_M tr'(D^*F_A \wedge \star B).\end{aligned}$$

In order for this to vanish for arbitrary proper variations B, $D^*F_A = 0$. □

We could make several possible modifications. One such modification is the incorporation of a source term $J \in \Omega^1(M|\mathfrak{g})$,

$$S_{YM}[A] = \int_M -tr'\Big(\frac{1}{2}F_A \wedge \star F_A - A \wedge \star J\Big),$$

which gives the equation $D^*F_A = J$. Another possible modification is the inclusion of a matter field, for example

$$S[A, \Psi] = \int_M -k\ tr'(F_A \wedge \star F_A) + (D\Psi)^\dagger \wedge \star(D\Psi) - m^2\Psi^\dagger \wedge \star\Psi,$$

where k is a coupling constant. Variation in A gives a modified form of the Yang-Mills equation and variation in Ψ governs the dynamics of the matter field $D^*D\Psi - m^2\Psi = 0$.

One important aspect of the Yang-Mills theory is that it is a gauge theory. Given a solution A of the equation 1.5.1 and a gauge transformation Φ, $A' = \Phi \cdot A$ is also a solution (where the action of Φ is in the appropriate representation). Furthermore, if the action for a matter field ψ is invariant under global G actions, coupling to the gauge fields makes the action for the matter field invariant under local G actions (and hence $(\Phi \cdot A, \Phi \cdot \psi)$ is a solution if (A, ψ) is).

In the next chapter, we will review the finite element method and introduce a method for modeling Lagrangian field theories using the finite element exterior calculus framework. In chapter 3, we will return to Yang-Mills theory as an application of this method.

2 | Structure Preserving Discretizations of Field Theories

In this chapter, we briefly review the finite element method and then discuss the Finite Element Exterior Calculus (FEEC) framework introduced in [1] as a finite element method which preserves the structure of the de Rham complex. We then apply this framework to Lagrangian field theories by introducing a discrete Euler-Lagrange equation, which admits a weak form of a local conservation law. For time dynamic fields, we will instead use a semi-discrete Euler-Lagrange equation and then show that this semi-discrete equation has a Hamiltonian structure. Consequently, we can fully discretize the problem by symplectic integration of the time dynamics. Furthermore, we will see that the discrete time evolution admits globally conserved charges. Lastly, we will consider additional extensions to both frameworks which allow for handling more general field theories (e.g. coupled theories or theories over vector bundles).

The main motivation for this chapter is to discretize a field theory to make it computationally solvable, while preserving the structures inherent in the full infinite dimensional problem.

2.1 Review: Finite Element Method

Consider a variational problem: find $u \in V$ such that $\delta J(u) \cdot v = 0 \ \forall v \in V$, where V is some function space and J is a functional on V. Generally, the function space is infinite dimensional and hence the solution cannot always be determined analytically. We approximate this problem by the Galerkin method: restrict the domain to a finite dimensional subspace $V_h \subset V$ and find $u_h \in V_h$ such that $\delta J(u_h) \cdot v = 0 \ \forall v \in V_h$. The finite dimensional subspace should satisfy the completeness condition $\lim_{h \to 0} V_h = V$. Of course, in computation, we cannot let $h \to 0$ since this recovers the original infinite-dimensional problem. However, we can choose h sufficiently small to resolve the scale of the system that we are interested in. Since the new problem is defined on a finite dimensional space, it is computationally tractable.

The finite element method is an example of the above method where the variational problem is defined on a domain M: find $u \in V(M)$ such that $A(u, v) = L(v) \ \forall v \in V(M)$, where $V(M)$ is a function space defined over M. To produce a finite dimensional subspace, we triangulate the domain $f : M \to M_h$ and define a finite set of basis functions over M_h, resulting in a finite subspace $V_h(M_h) \subset V(M)$. To illustrate this method, we consider a classical example.

Example 2.1.1 (Poisson's Equation)
Consider Poisson's equation, find $u \in H_0^2(M)$ such that $\nabla^2 u = -f$ for some $f \in L^2(M)$. To obtain a variational formulation of the problem, multiply the equation by a test function $v \in H_0^1(M)$ and integrate over M. Applying integration by parts (Green's identity), the solution of the variational problem requires one lower degree of differentiability. Thus, the variational problem is

to find $u \in H_0^1(M)$ such that

$$A(u,v) := \int_M \nabla u \cdot \nabla v \ vol = \int_M fv \ vol =: L(v) \ \forall v \in H_0^1(M).$$

To approximate this problem, triangulate the domain and define a finite set of basic functions $\{\phi_j\}$. Writing our approximate solution in terms of the basis $u_h = \sum_j c_j \phi_j$ and taking $v = \phi_k$, our new problem becomes

$$\sum_j c_j \int_{M_h} \nabla \phi_j \cdot \nabla \phi_k \ vol = \int_{M_h} f\phi_k \ vol.$$

Defining $K = (\int \nabla \phi_j \cdot \nabla \phi_k \ vol)_{jk}$, $\vec{c} = (c_j)_j$, $\vec{f} = (\int f\phi_k \ vol)_k$, we have in matrix form

$$K\vec{c} = \vec{f}.$$

Thus, assuming K is invertible, we can solve for the vector of coefficients $\vec{c} = K^{-1}\vec{f}$ which determines our solution $u_h = \sum_j c_j \phi_j$.

The preceding discussion provides a rough sketch of the finite element method and how it is used to solve variational problems. For brevity, we omit many key issues such as well-posedness and error estimates; for a more detailed discussion, see for example [18].

2.2 Finite Element Exterior Calculus

In the framework of FEEC, we take the function space to be the de Rham complex $V(M) = H\Omega(M)$. Thus, in some sense, FEEC is just a specific finite element method. However, it is worth noting that FEEC unifies many different finite element families (e.g. Lagrange, curl, and divergence elements) and hence can be applied to many problems. When determining a finite subspace $\Omega_h(M_h) \subset H\Omega(M)$, it is important to preserve the algebraic and topological structure of the de Rham complex.

A proper discrete de Rham complex must satisfy compatibility conditions which preserve the structure of the original de Rham complex. The discrete complex must be a subcomplex of the de Rham complex, i.e. that $\Omega_h^k \subset H\Omega^k$ and $d\Omega_h^k \subseteq \Omega_h^{k+1}$. Furthermore, there must exist a bounded cochain projection $\Pi_h : H\Omega \to \Omega_h$, i.e. a bounded projection map which commutes with the exterior derivative $d^k \circ \Pi_h^k = \Pi_h^{k+1} \circ d^k$. This is summarized by the following commuting diagram:

$$\begin{array}{ccccccccccc} 0 & \longrightarrow & H\Omega^0 & \xrightarrow{d} & H\Omega^1 & \xrightarrow{d} & \dots & \xrightarrow{d} & H\Omega^n & \longrightarrow & 0 \\ & & \downarrow{\scriptstyle \Pi_h} & & \downarrow{\scriptstyle \Pi_h} & & & & \downarrow{\scriptstyle \Pi_h} & & \\ 0 & \longrightarrow & \Omega_h^0 & \xrightarrow{d} & \Omega_h^1 & \xrightarrow{d} & \dots & \xrightarrow{d} & \Omega_h^n & \longrightarrow & 0 \end{array} \tag{2.2.1}$$

The subcomplex condition ensures that the discrete sequence is a cochain complex and hence, admits a Hodge decomposition, in analogy to 1.3.5,

$$\Omega_h^k \cong \mathfrak{B}_h^k \oplus \mathfrak{B}_h^{*k} \oplus \mathfrak{H}_h^k.$$

Furthermore, the existence of a cochain projection ensures that the cohomologies of the discrete complex are isomorphic to the cohomologies of the original complex. To accurately discretize a physical system on domains with nontrivial cohomology, it is important to preserve the cohomology of the original space, since each cohomology class in the k^{th} cohomology corresponds to a harmonic k-form. This has importance in physical applications as harmonic forms affect how a system behaves (for example, many electromagnetic devices have nontrivial cohomologies and the resulting harmonic forms govern their operation). If the cohomology of the discrete complex is not isomorphic to the cohomology of the original complex, then our discretization has a differing number of harmonic forms than the original problem, which may drastically alter how the system evolves.

One example of a discrete de Rham complex is based on the space of polynomial k-forms of degree at most r, $\mathcal{P}_r\Lambda^k$. Furthermore, define the reduced space $P_r^-\Lambda^k = \{\omega \in \mathcal{P}_r\Lambda^k \mid \kappa\omega \in \mathcal{P}_r\Lambda^{k-1}\}$ (κ is the Koszul differential). The space of polynomial forms over the triangulation of a manifold $f : M \to K_h$ gives rise to finite element spaces $\Omega_h^k(M) = \mathcal{P}_r\Lambda^k(K_h)$ or $\mathcal{P}_r^-\Lambda^k(K_h)$ by taking shape functions to be the polynomial forms over simplices $\sigma \in K_h$. Explicitly,

$$\mathcal{P}_r\Lambda^k(K_h) = \{\omega \in H\Omega^k \mid \omega|_T \in P_r\Lambda^k \ \forall \sigma \in K_h\},$$
$$\mathcal{P}_r^-\Lambda^k(K_h) = \{\omega \in H\Omega^k \mid \omega|_T \in P_r^-\Lambda^k \ \forall \sigma \in K_h\}.$$

Many of these discrete de Rham complexes can be shown to be equivalent to classical finite element spaces, such as the Lagrange and curl elements. Since the discrete complex of polynomial forms is finite dimensional, the infinite dimensional problem gets reduced to a computationally tractable problem. For a detailed discussion of these finite element spaces, see [2].

2.3 Lagrangian Framework: Discrete Euler-Lagrange

With the FEEC framework established, we apply it to modeling Lagrangian field theories discussed in the first chapter.

To discretize a theoery governed by an action $S : V \to \mathbb{R}$, there are two broad approaches within the Lagrangian framework. One approach would be to discretize the Euler-Lagrange equation arising from the action, e.g. by applying the finite difference method to the Euler-Lagrange equation. However, this approach is not compatible with the variational structure of the problem. The other approach is to discretize the variational structure directly, by working with the variational problem $\delta S[u] \cdot v = 0 \ \forall \ v \in V$. This approach is compatible with the variational structure in the sense that variation and discretization commute. Generally, having a discretization which preserves the variational structure produces a more robust numerical method. For example, to discretize Lagrangian mechanics, there are a class of integrators which respect the variational structure of the problem, producing numerical methods which are symplectic maps that also have near-exact energy conservation (for further discussion of variational integrators, see [3]). Keeping this in mind, we will discretize our field theories by working with their variational structure.

The first step in applying FEEC to Lagrangian field theories is putting the Euler-Lagrange equations in weak (variational) form. Recall that the action governing a field theory has the form $S[u] = \int_M \mathcal{L}(u, du, d^*u)$. To obtain the weak form of the Euler-Lagrange equation, operate equation 1.4.2 with $\wedge \star v$, integrate over M, and apply the adjoint property of d and d^*. Thus, the weak formulation of the Euler-Lagrange equation is to find $u \in H\Omega^k \cap \mathring{H}^*\Omega^k$ such that for all $v \in H\Omega^k \cap \mathring{H}^*\Omega^k$,

$$\begin{aligned} 0 &= \int_M \partial_1\mathcal{L}(\hat{u}) \wedge \star v + \partial_2\mathcal{L}(\hat{u}) \wedge \star dv + \partial_3\mathcal{L}(\hat{u}) \wedge \star d^*v \\ &= (\partial_1\mathcal{L}(\hat{u}), v)_{L^2\Omega^k} + (\partial_2\mathcal{L}(\hat{u}), dv)_{L^2\Omega^{k+1}} + (\partial_3\mathcal{L}(\hat{u}), d^*v)_{L^2\Omega^{k-1}}, \end{aligned} \tag{2.3.1}$$

where for brevity $\hat{u} := (u, du, d^*u)$. Note that the above equation was already obtained in chapter 1 by computing the variation $\delta S[u] \cdot v = 0$.

However, in general, this formulation of the problem is not well-posed (e.g. in Yang-Mills theory, gauge freedom creates uniqueness issues, or for Poisson's equation, the corresponding functional is unbounded due to the space of harmonic forms $\mathfrak{H}^k$). To avoid these issues, as noted in [1], we instead use a mixed formulation of the problem. We introduce a Lagrange multiplier $q \in \mathfrak{D}^k \subset H^k\Omega$ to enforce orthogonality of the solution to $\mathfrak{D}^k$ (which we will call the gauge space, since this process is analogous to gauge fixing used in gauge field theories). Also, we introduce a multiplier $p \in H\Omega^{k-1}$ to enforce σ to be weakly equivalent to d^*u. This gives the modified action

$$\bar{S}[u, \sigma, \bar{p}, \bar{q}] = \int_M \mathcal{L}(u, du, \sigma) - \sigma \wedge \star\bar{p} + u \wedge \star d\bar{p} + u \wedge \star\bar{q}. \tag{2.3.2}$$

Varying $\bar{S}$ with respect to each argument and requiring them to vanish independently provides a mixed formulation of the weak Euler-Lagrange equation:

Definition 2.3.1 (Mixed Formulation of the Euler-Lagrange Equation)
Find $(u, \sigma, \bar{p}, \bar{q}) \in H\Omega^k \times H\Omega^{k-1} \times H\Omega^{k-1} \times \mathfrak{D}^k$ *such that*

$$\begin{aligned} (\partial_1\mathcal{L}(\hat{u}^\sigma), v) + (\partial_2\mathcal{L}(\hat{u}^\sigma), dv) + (d\bar{p}, v) + (\bar{q}, v) &= 0, \ \forall\ v \in H\Omega^k, \\ (\partial_3\mathcal{L}(\hat{u}^\sigma), \tau) - (\bar{p}, \tau) &= 0, \ \forall\ \tau \in H\Omega^{k-1}, \\ (\sigma, p) - (u, dp) &= 0, \ \forall\ p \in H\Omega^{k-1}, \\ (u, q) &= 0, \ \forall\ q \in \mathfrak{D}^k, \end{aligned} \tag{2.3.3}$$

where $\hat{u}^\sigma := (u, du, \sigma)$.

Comparing the mixed formulation 2.3.3 to the weak form 2.3.1, the mixed formulation has the benefit of working with $H\Omega$ and $\mathfrak{D}$, rather than an intersection space $H\Omega^k \cap \mathring{H}^*\Omega^k$. Consequently, along with resolving existence and uniqueness issues arising in the weak formulation, the mixed formulation can be discretized much more simply.

Remark 2.3.1 Another possible modification is to introduce a multiplier to enforce weak equivalence to du. Thus, all of the derivatives of the field are

replaced by weak equivalents, resulting in a generalized Hamilton-Pontryagin principle. Explicitly, this is produced by the modified action

$$\bar{S}[u, \sigma_d, \sigma_{d^*}, p_d, p_{d^*}, q] = \int_M \mathcal{L}(u, \sigma_d, \sigma_{d^*}) + (du - \sigma_d) \wedge \star p_d - \sigma_{d^*} \wedge \star p_{d^*} + u \wedge \star dp_{d^*} + u \wedge \star q.$$

With the mixed formulation 2.3.3, we can now apply the finite element method: restrict $H\Omega$ to Ω_h (e.g. take Ω_h to be the space of polynomial differential forms defined over a triangulation of M) and $\mathfrak{D}^k$ to $\mathfrak{D}_h^k := \Pi_h^k \mathfrak{D}^k$. This then gives a Discrete-Euler Lagrange equation within the FEEC framework:

Definition 2.3.2 (Discrete Euler-Lagrange Equation)
Find $(u_h, \sigma_h, \bar{p}_h, \bar{q}_h) \in \Omega_h^k \times \Omega_h^{k-1} \times \Omega_h^{k-1} \times \mathfrak{D}_h^k$ *such that*

$$\begin{aligned} (\partial_1 \mathcal{L}(\hat{u}_h^\sigma), v) + (\partial_2 \mathcal{L}(\hat{u}_h^\sigma), dv) + (d\bar{p}_h, v) + (\bar{q}_h, v) &= 0, \ \forall\ v \in \Omega_h^k, \\ (\partial_3 \mathcal{L}(\hat{u}_h^\sigma), \tau) - (\bar{p}_h, \tau) &= 0, \ \forall\ \tau \in \Omega_h^{k-1}, \\ (\sigma_h, p) - (u_h, dp) &= 0, \ \forall\ p \in \Omega_h^{k-1}, \\ (u_h, q) &= 0, \ \forall\ q \in \mathfrak{D}_h^k, \end{aligned} \tag{2.3.4}$$

where $\hat{u}_h^\sigma := (u_h, du_h, \sigma_h)$.

Thus, given an action $S[u] = \int_M \mathcal{L}(u, du, d^*u)$, equation 2.3.4 provides a set of equations which can be solved for an approximate solution u_h of the variational problem $\delta S[u] \cdot v = 0$. Note that since this mixed formulation arises from the action 2.3.2, it respects the variational structure of Lagrangian field theories.

The discrete equations introduced in this section allow for discretization of Lagrangian field theories within the framework of FEEC, where the fields are sections of the bundle of differential forms ΛM. Since exterior calculus generalizes vector calculus, these equations can be applied to many problems of physical interest. One can also use the above equations in theories which involve coupled fields $S[u_1, ..., u_n]$, producing a set of discrete equations for each variation. In section 2.7 below, we will consider coupled theories explicitly and also theories which involve vector bundle valued differential forms. Before returning to these ideas, we next consider how conservation properties are affected by discretization.

2.4 Lagrangian Framework: Conservation Laws under Discretization

Having developed a discrete equation for the Euler-Lagrange, we would like to understand how this discretization affects the conservation laws arising from Noether's theorem. The two main points we consider in this section are:

- Determining a bound for the error in the conservation law from the approximate solution
- An exact discrete conservation law admitted by the approximate solution

It is clear why one would one the first point to hold; it would ensure that the actual conserved current is approximately conserved by the discrete solution. The second point, however, requires slightly more elaboration. If the approximate solution satisfies an exact discrete conservation law, it would ensure that the system behaves similarly to the original system, in that symmetries of the theory generate conserved currents both in the smooth and discretized cases. Furthermore, if the exact discrete conservation law is quantifiably close to the smooth conservation law, this would reinforce the first point (as an example of this, although variational integrators do not exactly conserve the true energy, they do admit an exact discrete conserved energy which ensures that the energy of the approximate solution remains exceptionally close to the actual energy for sufficiently long times).

Bound for Conservation of Noether Current

From Noether's theorem 1.4.2, for a continuous symmetry of the action, there exists a conserved current $\mathfrak{J}(u)$, where u is the solution of the associated Euler-Lagrange equation. Conservation of $\mathfrak{J}(u)$ is the statement $d\mathfrak{J}(u) = 0$. Consequently, for an approximation u_h of the solution, we would like to determine to what extent $d\mathfrak{J}(u_h) \approx 0$.

To determine a bound on $d\mathfrak{J}(u_h)$, define the negative Sobolev norm $\|\cdot\|_{H^{-*}\Omega^k}$, for a k-form ω,

$$\|\omega\|_{H^{-*}\Omega^k} := \sup_{v \in H^*\Omega^k \setminus \{0\}} \frac{(\omega, v)_{L^2\Omega^k}}{\|v\|_{H^*\Omega^k}}.$$

Theorem 2.4.1 (Bound for Conservation of Noether Current)
Let $u \in \Omega^k$ be a solution of the Euler-Lagrange equation over a compact oriented manifold M and let X be a continuous symmetry of the associated action. Furthermore, suppose $\|\partial_2 \mathcal{L}(u, du, d^*u)\|_{L^2\Omega^{k+1}}$, $\|\partial_3 \mathcal{L}(u, du, d^*u)\|_{L^2\Omega^{k-1}}$, and $\|\tilde{X}(u)\|_{L^2\Omega^k}$ are bounded. Then, for an approximation u_h of u,

$$\begin{aligned}\|d\mathfrak{J}(u_h)\|_{H^{-*}\Omega^{|M|}} \leq C\Big[&\|K(u_h) - K(u)\|_{L^2\Omega^{|M|-1}} + \|\tilde{X}(u_h) - \tilde{X}(u)\|_{L^2\Omega^k} \\ &+ \Big(1 + \|\tilde{X}(u_h) - \tilde{X}(u)\|_{L^2\Omega^k}\Big)\Big(\|\partial_3\mathcal{L}([u_h]) - \partial_3\mathcal{L}([u])\|_{L^2\Omega^{k-1}} + \|\partial_2\mathcal{L}([u_h]) - \partial_2\mathcal{L}([z])\|_{L^2\Omega^{k+1}}\Big)\Big],\end{aligned} \tag{2.4.1}$$

for some constant C independent of u_h, where K and $\mathfrak{J}$ are as defined in theorem 1.4.2, $|M| := dim(M)$, $[u] := (u, du, d^*u)$, and $[u_h] := (u_h, du_h, d^*u_h)$.

Proof. Since u is a solution of 1.4.2, by Noether's theorem, for the symmetry X, there exists a current $\mathfrak{J}(u)$ such that $d\mathfrak{J}(u) = 0$. Thus,

$$\|d\mathfrak{J}(u_h)\|_{H^{-*}\Omega^{|M|}} = \|d\mathfrak{J}(u_h) - d\mathfrak{J}(u)\|_{H^{-*}\Omega^{|M|}} = \|d\big(\mathfrak{J}(u_h) - \mathfrak{J}(u)\big)\|_{H^{-*}\Omega^{|M|}}.$$

For $v \in H^*\Omega^{|M|}$,

$$\begin{aligned}(d\big(\mathfrak{J}(u_h) - \mathfrak{J}(u)\big), v)_{L^2\Omega^{|M|}} &= \int_{\partial M}\Big[(\mathfrak{J}(u_h) - \mathfrak{J}(u)) \wedge \star v\Big] + (\mathfrak{J}(u_h) - \mathfrak{J}(u), d^*v)_{L^2\Omega^{|M|-1}} \\ &\leq \|\mathfrak{J}(u_h) - \mathfrak{J}(u)\|_{L^2\Omega^{|M|-1}}(\|v\|_{L^2\Omega^{|M|}} + \|d^*v\|_{L^2\Omega^{|M|-1}}) \leq 2\|\mathfrak{J}(u_h) - \mathfrak{J}(u)\|_{L^2\Omega^{|M|-1}}\|v\|_{H^*\Omega^{|M|}}.\end{aligned}$$

Thus, by definition of the H^{-*} norm,

$$\|d\mathfrak{J}(u_h)\|_{H^{-*}\Omega^{|M|}} = \|d\mathfrak{J}(u_h) - d\mathfrak{J}(u)\|_{H^{-*}\Omega^{|M|}} \leq 2\|\mathfrak{J}(u_h) - \mathfrak{J}(u)\|_{L^2\Omega^{|M|-1}}.$$

Using the formula for $\mathfrak{J}$ and the triangle inequality,

$$\begin{aligned}\frac{1}{2}\|d\mathfrak{J}(u_h)\|_{H^{-*}\Omega^{|M|}} &\leq \|K(u_h) - K(u)\| + \|\tilde{X}(u_h) \wedge \star\partial_2\mathcal{L}([u_h]) - \tilde{X}(u) \wedge \star\partial_2\mathcal{L}([u])\| \\ &\quad + \|\partial_3\mathcal{L}([u_h]) \wedge \star\tilde{X}(u_h) - \partial_3\mathcal{L}([u]) \wedge \star\tilde{X}(u)\| \\ &\leq \|K(u_h) - K(u)\| + \|(\tilde{X}(u_h) - \tilde{X}(u)) \wedge \star\partial_2\mathcal{L}([u])\| + \|\tilde{X}(u_h) \wedge \star(\partial_2\mathcal{L}([u_h]) - \partial_2\mathcal{L}([u]))\| \\ &\quad + \|\partial_3\mathcal{L}([u]) \wedge \star(\tilde{X}(u_h) - \tilde{X}(u))\| + \|(\partial_3\mathcal{L}([u_h]) - \partial_3\mathcal{L}([u])) \wedge \star\tilde{X}(u_h)\|,\end{aligned}$$

where the norms are taken in the appropriate L^2 spaces. By the definition of the wedge product, we have a Cauchy-Schwarz-like estimate on the wedge product, $\|u \wedge \star v\| \leq C'\|u\|\|\star v\|$ for some constant C'. Furthermore, using the fact that the Hodge star is an isometry and the assumptions on boundedness,

$$\begin{aligned}\frac{1}{2}\|d\mathfrak{J}(u_h)\|_{H^{-*}\Lambda^{|M|}} &\leq \|K(u_h) - K(u)\| + C_1\Big(\|\tilde{X}(u_h) - \tilde{X}(u)\| \\ &\quad + \|\tilde{X}(u_h)\|\big(\|\partial_3\mathcal{L}([u_h]) - \partial_3\mathcal{L}([u])\| + \|\partial_2\mathcal{L}([u_h]) - \partial_2\mathcal{L}([u])\|\big)\Big) \\ &\leq \|K(u_h) - K(u)\| + C_1\Big(\|\tilde{X}(u_h) - \tilde{X}(u)\| \\ &\quad + (\|\tilde{X}(u)\| + \|\tilde{X}(u_h) - \tilde{X}(u)\|)\big(\|\partial_3\mathcal{L}([u_h]) - \partial_3\mathcal{L}([u])\| + \|\partial_2\mathcal{L}([u_h]) - \partial_2\mathcal{L}([u])\|\big)\Big) \\ &\leq \|K(u_h) - K(u)\| + C_2\Big(\|\tilde{X}(u_h) - \tilde{X}(u)\| \\ &\quad + \big(1 + \|\tilde{X}(u_h) - \tilde{X}(u)\|\big)\big(\|\partial_3\mathcal{L}([u_h]) - \partial_3\mathcal{L}([u])\| + \|\partial_2\mathcal{L}([u_h]) - \partial_2\mathcal{L}([u])\|\big)\Big).\end{aligned}$$

Taking $C = 2\max\{1, C_2\}$ gives the desired result.

□

This result states that the conservation law approximately holds for the approximate solution: the extent to which the conservation law is not exact is bounded by the difference of quantities involving the approximate solution from the actual solution. In other words, as $u_h \to u$, $d\mathfrak{J}(u_h) \to 0$. Also, as can be seen from the above derivation, a similar bound holds for $\|\mathfrak{J}(u_h) - \mathfrak{J}(u)\|_{H\Omega^{|M|-1}}$, considering the solution u fixed.

Corollary 2.4.1 *Assuming the conditions of the theorem, suppose furthermore that $\partial_2\mathcal{L}$ and $\partial_3\mathcal{L}$ have a Lipschitz bound in their second and third arguments (independent of the first argument), then*

$$\begin{aligned}\|d\mathfrak{J}(u_h)\|_{H^{-*}\Omega^{|M|}} \leq C\Big[&\|K(u_h) - K(u)\| + \|\tilde{X}(u_h) - \tilde{X}(u)\| \\ &+ (1 + \|\tilde{X}(u_h) - \tilde{X}(u)\|)(\|du_h - du\| + \|d^*u_h - d^*u\|)\Big].\end{aligned}$$

In particular, this applies for Lagrangians purely quadratic in du and d^*u (which is the case for many Lagrangians).

Exact Discrete Noether's Theorem

Recall that in discretizing the Euler-Lagrange equation, we first considered the weak formulation of the problem: rather than looking for strong solutions of equation 1.4.2, we look for solutions which satisfy 2.3.1 for all test functions v. Consequently, in order to determine an exact discrete conservation law, we first consider a weak analog of Noether's theorem.

Definition 2.4.1 *Let X be a generator of a transformation on M. We say X is a weak symmetry of the an action $S : \Omega^k M \to \mathbb{R}$ if there exists $K : \Omega^k M \to \Omega^{|M|-1} M$ such that*

$$S'[\phi] \cdot \tilde{X}(\phi) = \int_M dK(\phi).$$

The difference between this definition and a continuous symmetry is that that the weak symmetry is only required to hold when integrated over all of M.

Theorem 2.4.2 (Weak Noether's Theorem) *Given a weak symmetry X of an action $S : \Omega^k M \to \mathbb{R}$, for a weak solution $u \in V := H\Omega^k \cap \mathring{H}^* \Omega^k$ of 2.3.1,*

$$0 = \int_M \partial_1 \mathcal{L}(\hat{u}) \wedge \star \tilde{X}(u) + \partial_2 \mathcal{L}(\hat{u}) \wedge \star d\tilde{X}(u) + \partial_3 \mathcal{L}(\hat{u}) \wedge \star d^* \tilde{X}(u) - dK(u),$$

and

$$0 = \int_M \partial_1 \mathcal{L}(\hat{u}) \wedge \star (I - P_V)\tilde{X}(u) + \partial_2 \mathcal{L}(\hat{u}) \wedge \star d(I - P_V)\tilde{X}(u) + \partial_3 \mathcal{L}(\hat{u}) \wedge \star d^*(I - P_V)\tilde{X}(u) - dK(u),$$

where P_V denotes orthogonal projection into V and $\hat{u} := (u, du, d^* u)$. Furthermore, if u is a strong solution to the Euler-Lagrange equation 1.4.2,

$$0 = \int_M d\Big[\tilde{X}(u) \wedge \star \partial_2 \mathcal{L}(\hat{u}) - \partial_3 \mathcal{L}(\hat{u}) \wedge \star \tilde{X}(u) - K(u)\Big].$$

Proof. The proof is similar to the proof for Noether's theorem 1.4.2. For the first equation, obtain two expressions for $S'[u] \cdot \tilde{X}(u)$ (one by directly computing the variation and one by the definition of the weak symmetry) and subtract

$$S'[u] \cdot v\Big|_{v = \tilde{X}(u)} - S'[\phi] \cdot \tilde{X}(\phi)\Big|_{\phi = u} = 0.$$

For the second equation, since u is a weak solution, equation 2.3.1 holds for all $v \in V$ so in particular it holds for $v = P_V \tilde{X}(u)$. Subtracting this to the first equation gives the second.

Lastly, for the third equation, since we assume u is a strong solution, we can proceed as in the case of the original Noether's theorem. However, since the weak symmetry only holds over all M, we do not have the local current $\mathfrak{J}$ satisfying $d\mathfrak{J}(u) = 0$ everywhere. □

We now extend this weak theorem to the discrete mixed formulation 2.3.4. Of course, since defining the mixed formulation .

Theorem 2.4.3 (Discrete Noether Theorem for 2.3.4) *Suppose that X is a weak symmetry for the modified action 2.3.2 up to terms involving the gauge space $q \in \mathfrak{D}^k$, i.e.*

$$\bar{S}'[\phi,\tau,p,q]\cdot\tilde{X}(\phi,\tau,p,q) = \int_M dK(\phi,\tau,p) + \tilde{X}(\phi)\wedge\star q + \phi\wedge\star\tilde{X}(q),\ \forall\ (\phi,\tau,p,q).$$

Then, for a solution $(u_h,\sigma_h,\bar{p}_h,\bar{q}_h)$ of 2.3.4, the following exact discrete conservation law holds

$$\begin{aligned}0 = \int_M \Big[&- dK(u_h,\sigma_h,\bar{p}_h) + \partial_1\mathcal{L}(\hat{u}_h^\sigma)\wedge\star(I-P_h^k)\tilde{X}(u_h) + \partial_2\mathcal{L}(\hat{u}_h^\sigma)\wedge\star d(I-P_h^k)\tilde{X}(u_h)\\ &- \bar{q}_h\wedge\star P_h^k\tilde{X}(u_h) + \partial_3\mathcal{L}(\hat{u}_h^\sigma)\wedge\star(I-P_h^{k-1})\tilde{X}(\sigma_h) - \bar{p}_h\wedge\star(I-P_h^{k-1})\tilde{X}(\sigma_h)\\ &+ u_h\wedge\star d(I-P_h^{k-1})\tilde{X}(\bar{p}_h) - \sigma_h\wedge\star(I-P_h^{k-1})\tilde{X}(\bar{p}_h)\Big],\end{aligned}$$

where $\hat{u}_h^\sigma := (u_h, du_h, \sigma_h)$ and $P_h^k := P_{\Omega_h^k}$.

Proof. As in the other cases, compute $\bar{S}'(u_h,\sigma_h,\bar{p}_h,\bar{q}_h)\cdot\tilde{X}(u_h,\sigma_h,\bar{p}_h,\bar{q}_h)$ in two ways and subtract. Furthermore, we can additionally subtract the first three equations of 2.3.4 with $v = P_h^k\tilde{X}(u_h)$, $\tau = P_h^{k-1}\tilde{X}(\sigma_h)$, $p = P_h^{k-1}\tilde{X}(\bar{p})$. □

Remark 2.4.1 Suppose instead that X is a total weak symmetry for the modified action, including the gauge terms,

$$\bar{S}'[\phi,\tau,p,q]\cdot\tilde{X}(\phi,\tau,p,q) = \int_M dK(\phi,\tau,p,q),\ \forall\ (\phi,\tau,p,q),$$

then the term $-\bar{q}_h\wedge\star P_h^k\tilde{X}(u_h)$ in the above conservation law would be replaced by $\bar{q}_h\wedge\star(I-P_h^k)\tilde{X}(u_h) + u_h\wedge\star(I-P_{\mathfrak{D}_h^k})\tilde{X}(\bar{q}_h)$.

The discrete Noether theorem is similar to the original theorem 1.4.2. For the original theorem, we "project" out the part of the variation $S'[u]\cdot v$ which vanishes (the part which satisfies the Euler-Lagrange equation). The entire variation in general does not vanish since $v = \tilde{X}(u)$ is not necessarily zero on the boundary. Likewise, in the discrete theorem, we project out the part of the variation which vanishes but the entire variation does not since in general $\tilde{X}(u_h,\sigma_h,\bar{p}_h,\bar{q}_h) \notin \Omega_h^k\times\Omega_h^{k-1}\times\Omega_h^{k-1}\times\mathfrak{D}_h^k$.

2.5 Hamiltonian Framework: Discrete Field Dynamics

In the previous sections, we have considered how FEEC could be used to construct discretizations of the Euler-Lagrange variational problem and its related conservation properties. These considerations involved no dynamics, i.e. the evolution of a system over time. Although the FEEC framework is capable of solving problems on spacetime meshes, often we want to evolve the system in time separately (e.g. for a non-relativistic theory or for interpretation of the dynamics). To simulate the time dynamics of field theories, we will utilize the Hamiltonian structure of the dynamics to evolve the system by symplectic

integration. Along with preserving the symplectc structure of the field theory, utilizing the Hamiltonian formulation has the practical advantage of being first order as opposed to second order in time differentiation (so we only need to specify initial conditions at a single time). Furthermore, as discussed in [13], whereas the Lagrangian formulation is ill-posed due to gauge freedom (we can solve this by manually fixing the gauge), the Hamiltonian formulation introduces an additional constraint which automatically produces a well-posed formulation of the dynamics.

For a dynamical field theory, we describe the evolution of a time-dependent field $u(t) \in \Omega^k R$ by the action

$$S[u] = \int dt \int_R \mathcal{L}(u, \dot{u}, du, d^*u), \tag{2.5.1}$$

where the geometric operators act in the spatial domain R. The corresponding Euler-Lagrange equation is given by varying the action, $\delta S = 0$,

$$\frac{\partial \mathcal{L}}{\partial u} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{u}} + d^*\frac{\partial \mathcal{L}}{\partial (du)} + d\frac{\partial \mathcal{L}}{\partial (d^*u)} = 0. \tag{2.5.2}$$

To see the Hamiltonian structure in the dynamics of this system, introduce the conjugate momentum field,

$$\pi := \frac{\partial \mathcal{L}}{\partial \dot{u}}.$$

Furthermore, assume the above expression is invertible for $\dot{u}$ so we can determine $\dot{u}(u, \pi, du, d^*u)$. Then, the Hamiltonian density $\mathcal{H}(u, \pi) \in \Omega^{dim(R)} R$ is given by the Legendre transform of the Lagrangian:

$$\mathcal{H}(u, \pi) = \pi \wedge \star \dot{u}(u, \pi, du, d^*u) - \mathcal{L}(u, \dot{u}(u, \pi, du, d^*u), du, d^*u), \tag{2.5.3}$$

with u and π considered as independent.

Proposition 2.5.1 *The dynamics of the action 2.5.1 carry a Hamiltonian structure, given by*

$$\dot{\pi} = -\frac{\delta \mathcal{H}}{\delta u}, \ \dot{u} = \frac{\delta \mathcal{H}}{\delta \pi}, \tag{2.5.4}$$

where, using the ∂ notation of lemma 1.4.1,

$$\frac{\delta}{\delta z} := \frac{\partial}{\partial z} + d^*\frac{\partial}{\partial (dz)} + d\frac{\partial}{\partial (d^*z)}. \tag{2.5.5}$$

Proof. Since the Hamiltonian 2.5.3 does not depend on the derivatives of π,

$$\frac{\delta \mathcal{H}}{\delta \pi} = \frac{\partial \mathcal{H}}{\partial \pi} = \dot{u} + \pi\frac{\partial \dot{u}}{\partial \pi} - \frac{\partial \mathcal{L}}{\partial \dot{u}}\frac{\partial \dot{u}}{\partial \pi} = \dot{u} + \pi\frac{\partial \dot{u}}{\partial \pi} - \pi\frac{\partial \dot{u}}{\partial \pi} = \dot{u}.$$

Furthermore,

$$\frac{\delta \mathcal{H}}{\delta u} = \pi\frac{\delta \dot{u}}{\delta u} - \frac{\partial \mathcal{L}}{\partial \dot{u}}\frac{\delta \dot{u}}{\delta u} - \frac{\delta \mathcal{L}}{\delta u} = -\frac{\delta \mathcal{L}}{\delta u} = -\Big(\frac{\partial \mathcal{L}}{\partial u} + d^*\frac{\partial \mathcal{L}}{\partial (du)} + d\frac{\partial \mathcal{L}}{\partial (d^*u)}\Big) \overset{(i)}{=} -\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{u}} = -\dot{\pi},$$

where, at (i), we used the Euler-Lagrange equation 2.5.2.

Clearly, upon substitution, the dynamical equations are equivalent to the Euler-Lagrange equation 2.5.2,

$$0 = \frac{\delta \mathcal{H}}{\delta u} + \dot{\pi} = -\frac{\delta \mathcal{L}}{\delta u} + \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{u}} = -\Big(\frac{\partial \mathcal{L}}{\partial u} + d^* \frac{\partial \mathcal{L}}{\partial (du)} + d\frac{\partial \mathcal{L}}{\partial (d^* u)} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{u}}\Big).$$

□

Thus, the time dynamics of the system carry a Hamiltonian structure which evolve over the phase space $T^*(\Omega^k R)$, the cotangent bundle of the manifold of k-forms. Unlike particle dynamics, this is an infinite dimensional phase space.

To obtain a semi-discrete equation for the action 2.5.1, perform a similar discretization procedure as the previous discrete Euler-Lagrange equation in the spatial domain,

Definition 2.5.1 (Semi-Discrete Euler-Lagrange Equation)
Find $(u_h(t), \sigma_h(t), \bar{p}_h(t)) \in \Omega_h^k \times \Omega_h^{k-1} \times \Omega_h^{k-1}$ *such that for each* t,

$$\begin{aligned}(\partial_1 \mathcal{L}(\hat{u}_h^\sigma(t)), v) - (\frac{d}{dt}\partial_2 \mathcal{L}(\hat{u}_h^\sigma(t)), v) + (\partial_3 \mathcal{L}(\hat{u}_h^\sigma(t)), dv) + (d\bar{p}_h(t), v) = 0, \ \forall\ v \in \Omega_h^k, \\ (\partial_4 \mathcal{L}(\hat{u}_h^\sigma(t)), \tau) - (\bar{p}_h(t), \tau) = 0, \ \forall\ \tau \in \Omega_h^{k-1}, \\ (\sigma_h(t), p) - (u_h(t), dp) = 0, \ \forall\ p \in \Omega_h^{k-1},\end{aligned} \tag{2.5.6}$$

where $\hat{u}_h^\sigma(t) := (u_h(t), \dot{u}_h(t), du_h(t), \sigma_h(t))$.

This provides a spatial discretization of the evolution problem. Subsequently, one can discretize in time to obtain a complete discretization of the evolution problem. Of course, one could use a simple finite difference in time, such as a forward difference, to completely discretize the problem. However, this ignores the Hamiltonian structure of the field theory. As we will see explicitly in the examples, the time evolution of the semi-discrete equation 2.5.6 has a Hamiltonian structure. This is a reflection of the fact that the time dynamics of the field carry a Hamiltonian structure in the smooth case. As a result, we can symplectically integrate the time dynamics of the system.

To make the Hamiltonian form of the semi-discrete equation manifest, we can eliminate the coefficients of σ_h and $\bar{p}_h$ in the mixed formulation to obtain a system of ODE's for the coefficients of u_h (this is done, for example, in [9] to rewrite the mixed semi-discrete form of the heat equation into a system of ODE's for the coefficients of the solution). We can then define a natural derivative operator which is similar to the derivative for the smooth Hamiltonian theory and generates a Hamiltonian structure for the discrete counterpart.

Theorem 2.5.1 *The semi-discrete Euler-Lagrange equation 2.5.6 carries a Hamiltonian structure,*

$$\dot{\pi}_i = -\frac{\hat{\delta}\mathcal{H}_h}{\hat{\delta} u^i}, \ \dot{u}^i = \frac{\hat{\delta}\mathcal{H}_h}{\hat{\delta}\pi_i}, \tag{2.5.7}$$

where the field coefficients π_i, u^i, the derivative $\hat{\delta}/\hat{\delta}z^i$, and the Hamiltonian $\mathcal{H}_h$ will be defined in the proof.

Furthermore, the Hamiltonian structure of the mixed semi-discrete equation is isomorphic (in the sense of weak equivalence) to the Hamiltonian structure of the smooth dynamics after projection into the discrete space Ω_h; i.e., the semi-discrete Euler-Lagrange equation preserves the Hamiltonian structure of the field theory.

Proof. Consider a basis $\{\varphi^\mu_{k-1}\}^\mu$ for Ω^{k-1}_h and $\{\varphi^\mu_k\}^\mu$ for Ω^k_h. Expand $u_h(t) = u^\mu(t)\varphi^\mu_k$, $\sigma_h(t) = \sigma^\mu(t)\varphi^\mu_{k-1}$, $\bar{p}_h(t) = \bar{p}^\mu(t)\varphi^\mu_{k-1}$. Substituting into the semi-discrete equation 2.5.6 with $v = \varphi^\alpha_k, \tau = \varphi^\beta_{k-1}, p = \varphi^\gamma_{k-1}$ yields the system,

$$\begin{aligned}(\partial_1\mathcal{L}, \varphi^\alpha_k) - (\frac{d}{dt}\partial_2\mathcal{L}, \varphi^\alpha_k) + (\partial_3\mathcal{L}, d\varphi^\alpha_k) + \bar{p}^\mu(d\varphi^\mu_{k-1}, \varphi^\alpha_k) = 0,\\ (\partial_4\mathcal{L}, \varphi^\beta_{k-1}) - \bar{p}^\mu(\varphi^\mu_{k-1}, \varphi^\beta_{k-1}) = 0,\\ \sigma^\mu(\varphi^\mu_{k-1}, \varphi^\gamma_{k-1}) - u^\mu(\varphi^\mu_k, d\varphi^\gamma_{k-1}) = 0,\end{aligned}$$

where $\mathcal{L}$ is evaluated at $(u_h, \dot{u}_h, du_h, \sigma_h)$. Introducing the matrices $M := (\varphi^i_{k-1}, \varphi^j_{k-1})^j_i$, $Z := (d\varphi^i_{k-1}, \varphi^j_k)^j_i$ and the vectors $\vec{F}_1 := (\partial_1\mathcal{L}, \varphi^\alpha_k)^\alpha$, $\vec{F}_3 := (\partial_3\mathcal{L}, d\varphi^\alpha_k)^\alpha$, $\vec{F}_4 := (\partial_4\mathcal{L}, \varphi^\beta_{k-1})^\beta$, this system can be written

$$\begin{aligned}\vec{F}_1 - (\frac{d}{dt}\partial_2\mathcal{L}, \varphi^\alpha_k)^\alpha + \vec{F}_3 + Z\vec{p} = 0,\\ \vec{F}_4 - M\vec{p} = 0,\\ M\vec{\sigma} - Z^T\vec{u} = 0.\end{aligned}$$

Since M is clearly positive definite (hence, invertible), the second equation allows us to eliminate $\vec{p}$ from the first equation and the third equation determines the coefficients of σ_h in terms of the coefficients of u_h, $\vec{\sigma} = M^{-1}Z^T\vec{u}$. Thus, we can completely eliminate σ_h and $\bar{p}_h$ from the system to give

$$\vec{F}_1 - (\frac{d}{dt}\partial_2\mathcal{L}, \varphi^\alpha_k)^\alpha + \vec{F}_3 + ZM^{-1}\vec{F}_4 = 0, \tag{2.5.8}$$

which is evaluated at $(u_h, \dot{u}_h, du_h, \sigma_h(u_h))$ with $\sigma_h(u_h) = (M^{-1}Z^T\vec{u})_i\varphi^i_{k-1}$.

As before, define the conjugate momentum field $\pi_h := \partial_2\mathcal{L}$ which we can expand $\pi_h = \pi_i\varphi^i_k$. To see the Hamiltonian structure, introduce the field parameters $\Pi_i := (\pi_h, \varphi^i_k) = (\partial_2\mathcal{L}, \varphi^i_k)$, $U^i := (u_h, \varphi^i_k)$, and the Hamiltonian

$$\mathcal{H}_h := \Big(\dot{u}(u,\pi) \wedge \star\pi - \mathcal{L}(u, \dot{u}(u,\pi), du, \sigma_h(u))\Big)_{u\mapsto u_h, \pi\mapsto\pi_h}. \tag{2.5.9}$$

Note that functions of u_h and π_h are characterized as functions of the field parameters U^i and Π_i. Also, define a weak analog of the derivative 2.5.5, for $W^i := (w, \varphi^i_k)$ and $F = F(w, \dot{w}, dw, d^*w)$,

$$\frac{\hat{\delta}F}{\hat{\delta}W^i} := (\frac{\partial F}{\partial w}, \varphi^i_k) + (\frac{\partial F}{\partial(dw)}, d\varphi^i_k) + \Big(ZM^{-1}(\frac{\partial F}{\partial(d^*w)}, \varphi^\beta_{k-1})^\beta\Big)^i\Big|_{d^*w\mapsto\sigma_h(w)}.$$

Then, since $\mathcal{H}_h$ does not depend on the derivatives of π,

$$\begin{aligned}
\frac{\hat{\delta}\mathcal{H}_h}{\hat{\delta}\Pi_i} &= (\frac{\partial \mathcal{H}_h}{\partial \pi}, \varphi_k^i) = (\dot{u}_h, \varphi_k^i) + (\pi_h \frac{\partial \dot{u}_h}{\partial \pi}, \varphi_k^i) - (\frac{\partial \mathcal{L}}{\partial \dot{u}} \frac{\partial \dot{u}}{\partial \pi}, \varphi_k^i) \\
&= (\dot{u}_h, \varphi_k^i) + (\frac{\partial \dot{u}_h}{\partial \pi} \pi_h, \varphi_k^i) - (\pi_h \frac{\partial \dot{u}_h}{\partial \pi}, \varphi_k^i) = (\dot{u}_h, \varphi_k^i) = \frac{d}{dt}(u_h, \varphi_k^i) = \dot{U}^i, \\
\frac{\hat{\delta}\mathcal{H}_h}{\hat{\delta}U^i} &= (\frac{\partial \mathcal{H}_h}{\partial u}, \varphi_k^i) + (\frac{\partial \mathcal{H}_h}{\partial (du)}, d\varphi_k^i) + ZM^{-1}\Big((\frac{\partial \mathcal{H}}{\partial (d^*u)}, \varphi_{k-1}^\beta)^\beta\Big)^i \Big|_{d^*u \mapsto \sigma_h(u_h)} \\
&= (\pi_h \frac{\partial \dot{u}_h}{\partial u}, \varphi_k^i)) - (\frac{\partial \mathcal{L}}{\partial \dot{u}} \frac{\partial \dot{u}_h}{\partial u}, \varphi_k^i) - (\frac{\partial \mathcal{L}}{\partial u}, \varphi_k^i) - (\frac{\partial \mathcal{L}}{\partial (du)}, d\varphi_k^i) - ZM^{-1}\Big((\frac{\partial \mathcal{L}}{\partial (d^*u)}, \varphi_{k-1}^\beta)^\beta\Big)^i \Big|_{d^*u \mapsto \sigma_h(u_h)} \\
&= -(\frac{\partial \mathcal{L}}{\partial u}, \varphi_k^i) - (\frac{\partial \mathcal{L}}{\partial (du)}, d\varphi_k^i) - ZM^{-1}\Big((\frac{\partial \mathcal{L}}{\partial (d^*u)}, \varphi_{k-1}^\beta)^\beta\Big)^i \Big|_{d^*u \mapsto \sigma_h(u_h)} \\
&= -(\partial_1 \mathcal{L}, \varphi_k^i) - (\partial_3 \mathcal{L}, d\varphi_k^i) - ZM^{-1}\Big((\partial_4 \mathcal{L}, \varphi_{k-1}^\beta)^\beta\Big)^i \\
&= -(\vec{F}_1 + \vec{F}_3 + ZM^{-1}\vec{F}_4)^i = -(\frac{d}{dt}\partial_2 \mathcal{L}, \varphi_k^i) = -\frac{d}{dt}(\pi_h, \varphi_k^i) = -\dot{\Pi}_i,
\end{aligned}$$

where we used the fact that the bases are time-independent, the chain rule, $\pi = \partial \mathcal{L}/\partial \dot{u}$, and equation 2.5.8. Note since $\Pi_i = (\pi_h, \varphi_k^i) = \pi^j(\varphi_k^j, \varphi_k^i)$ (and similar for U^i), we have $\vec{\Pi} = M'\vec{\pi}$ and $\vec{U} = M'\vec{u}$ where $M' = (\varphi_k^j, \varphi_k^i)_j^i$. Thus, the Hamiltonian structure can be expressed in terms of the coefficients of the fields,

$$\begin{aligned}
\dot{u}^i = (M'^{-1})_j^i \dot{U}^j = (M'^{-1})_j^i \frac{\hat{\delta}\mathcal{H}}{\hat{\delta}\Pi_j} =: \frac{\hat{\delta}\mathcal{H}}{\hat{\delta}\pi_i}, \\
\dot{\pi}^i = (M'^{-1})_j^i \dot{\Pi}_j = -(M'^{-1})_j^i \frac{\hat{\delta}\mathcal{H}}{\hat{\delta}U^j} = -\frac{\hat{\delta}\mathcal{H}}{\hat{\delta}u_i}.
\end{aligned}$$

Lastly, to see that the Hamiltonian structure is equivalent to the Hamiltonian structure of the smooth theory after projection, project the smooth Hamilton's equations 2.5.4 into Ω_h:

$$\begin{aligned}
(\dot{u}, \varphi_k^i)\Big|_{\Omega_h} &= (\frac{\delta \mathcal{H}}{\delta \pi}, \varphi_k^i)\Big|_{\Omega_h} = (\frac{\partial \mathcal{H}}{\partial \pi}, \varphi_k^i)\Big|_{\Omega_h} = \frac{\hat{\delta}\mathcal{H}_h}{\hat{\delta}\Pi_i}, \\
(\dot{\pi}, \varphi_k^i)\Big|_{\Omega_h} &= (\frac{\delta \mathcal{H}}{\delta u}, \varphi_k^i)\Big|_{\Omega_h} = -\Big((\partial_u \mathcal{L}, \varphi_k^i) + (d^* \partial_{du} \mathcal{L}, \varphi_k^i) + (d\partial_{d^*u} \mathcal{L}, \varphi_k^i)\Big)\Big|_{\Omega_h} \\
&= -\Big((\partial_1 \mathcal{L}, \varphi_k^i) + (\partial_3 \mathcal{L}, d\varphi_k^i) + (\partial_4 \mathcal{L}, d^*\varphi_k^i)\Big)\Big|_{\Omega_h} \\
&= -\Big((\vec{F}_1)^i + (\vec{F}_2)^i + (\partial_4 \mathcal{L}, d^*\varphi_k^i)\Big) \\
&\cong -\Big(\vec{F}_1 + \vec{F}_2 + ZM^{-1}\vec{F}_4\Big)^i = \frac{\hat{\delta}\mathcal{H}_h}{\hat{\delta}U^i},
\end{aligned}$$

where, by construction of the mixed formulation, we have the weak equivalence $(\partial_4 \mathcal{L}, d^*\varphi_k^i)^i \cong ZM^{-1}\vec{F}_4$. □

Thus, in order to evolve the semi-discrete Euler Lagrange equation in time, we introduce the conjugate field (and its associated components / parameters) to rewrite the time evolution in Hamiltonian form. Subsequently, we use a symplectic integrator to evolve the system in time, which preserves the symplectic structure of the dynamics over $T^*(\Omega_h^k R)$. This time-symplectic discrete Euler-Lagrange method completely discretizes the evolution problem 2.5.1 while simultaneously preserving the de Rham structure of the spatial manifold and the Hamiltonian structure of the time dynamics. We will use this method for the applications in Chapter 3. Note that although in general the Hamiltonian structure is non-canonical, it is shown in [14] that a symplectic integrator applied to a non-canonical Hamiltonian system results in a conjugate symplectic method, which shares similar structure preserving properties.

Furthermore, there is an interesting physical connection between Hamiltonian field theory and the discrete Hamiltonian structure. When developing Hamiltonian field theory, one considers a collection of particles governed by a Hamiltonian and takes the continuum limit as the number of particles go to infinity to recover the infinite dimensional field theory formulation. Conversely, our discretization begins with the Hamiltonian for the field theory over $T^*(\Omega^k R)$ and restricts to a finite dimensional subspace, which results in a finite dimensional Hamiltonian system of "particles" evolving in real phase space $\mathbb{R}^{2N}$ (here, the "particles" represent the coefficients of the solution in the basis expansion). In particular, the theory of Hamiltonian mechanics for particles applies to the evolution of our coefficient "particles".

2.6 Hamiltonian Framework: Discrete Charge Conservation

Recall that in the Lagrangian framework we derived a discrete Noether's theorem which said there exists a conserved current $\mathfrak{J}$ which weakly satisfied $d\mathfrak{J} = 0$. In spacetime, this has the interpretation of a local conservation law $\partial_t \rho + \nabla \cdot J = 0$. In the time dynamic Hamiltonian framework, we can derive a different type of conservation law. Instead of a local conservation law for a conserved current, we get a discrete analog of global charge conservation $\dot{Q}(t) = 0$, for each time t_n,

$$Q^{n+1} = Q^n.$$

For example, in electromagnetism Q could be the total energy of the system (obtained by integrating the energy density over the spatial domain) or for Schrödinger's equation Q could be the total probability. The difference between these types of conservation laws provides a distinction between the Lagrangian and Hamiltonian framework, depending on which structures one wishes to preserve under discretization (see the summary at the end of the chapter for a more thorough discussion of how the two approaches compare).

In order to understand Noether's theorem for Hamiltonian mechanics, we must further develop the theory of symplectic structures and its symmetries to express the theorem concisely. After developing this theory, we discuss how Noether's theorem holds for our semi-discrete formulation of the field dynamics. For the full discrete problem where we apply an integrator for the time evolution, one can utilize integrators discussed in the literature which admit exact discrete

Noether's theorems, e.g. see [12].

Symplectic Geometry, Symmetries, and Conservation

Recall that the phase space dynamics of the fields occur on $T^*(\Omega^k R)$. This space (and more generally the cotangent bundle of a manifold) is an example of a symplectic manifold.

Definition 2.6.1 *A symplectic manifold (S, ω) is a manifold S with a closed, non-degenerate two form $\omega \in \Omega^2 S$.*

We refer to ω as the symplectic form. Since ω is a two form, it can be viewed as an antisymmetric bilinear functional on TS,

$$\omega : TS \times TS \to \Omega^0 S.$$

Definition 2.6.2 *A Hamiltonian system (S, ω, H) is a symplectic manifold (S, ω) with a smooth function H, the Hamiltonian, which specifies the Hamiltonian vector field X_H, satisfying*

$$X_H \lrcorner \omega = -dH,$$

or, equivalently $\omega(X_H, \cdot) = -dH(\cdot)$.

In local coordinates, $\omega_{IJ}(X_H)^I = -dH_J$ which can be inverted to give $(X_H)^I = \omega^{IJ} dH_J = \omega^I_J \nabla^J H =: (\omega^\sharp \cdot \nabla H)^I$ The dynamics of the system in phase space are trajectories along the flow of X_H; in coordinates $\xi \in S$,

$$\dot{\xi} = X_H = \omega^\sharp \cdot \nabla_\xi H.$$

Define the Poisson bracket acting on the space of smooth functions in phase space,

$$\begin{aligned} \{\cdot, \cdot\} : \Omega^0 S \times \Omega^0 S &\to \Omega^0 S, \\ \{F, G\} &:= \omega(X_F, X_G). \end{aligned}$$

The time evolution of a function over phase space along the trajectories ξ of the system is given by

$$\frac{d}{dt} F = X_H[F] = \langle \nabla_\xi F, \dot{\xi} \rangle = \langle \nabla_\xi F, \omega^\sharp \cdot \nabla_\xi H \rangle = \omega(X_F, X_H) = \{F, H\},$$

where $X_H[F]$ denotes differentiation of F along the flow of X_H.

Definition 2.6.3 *A symmetry of a Hamiltonian system (S, ω, H) is vector field X_F satisfying: there exists $F \in \Omega^0 S$ such that $X_F \lrcorner \omega = -dF$ and $X_F[H] = 0$.*

By the definition of a symmetry,

$$0 = X_F[H] = \{H, F\} = -\{F, H\} = -X_H[F] = -\frac{d}{dt} F,$$

which is a simple statement of Noether's theorem in the Hamiltonian formulation (i.e. that a symmetry of the Hamiltonian generates a conserved charge). Furthermore, the converse holds: for a conserved quantity Q, by the non-degeneracy of the symplectic form, there exists a corresponding Hamiltonian vector field X_Q which is a symmetry.

In our semi-discrete formulation of field theories, the time continuous dynamics evolve over the finite dimensional phase space $T^*(\Omega_h^k R)$ which carries a Hamiltonian structure, parametrized by the field parameters (U^i, Π_i). Clearly, by the definition of the discrete Hamiltonian $\mathcal{H}_h$ in 2.5.9, a symmetry of the smooth Hamiltonian by transforming the fields (u_h, π_h) induces a symmetry of the discrete Hamiltonian as a transformation on the parameters (U^i, Π_i). Thus, by Noether's theorem, this symmetry gives rise to a conserved charge over the evolution of the system. Another way to see this explicitly is to show that the semi-discrete system has a canonical Hamiltonian structure given by a symplectic form ω. To do this, introduce the particle Lagrangian

$$L_h(U^i, \Pi_i) := \int_R \mathcal{L}(u_h(U^i), \dot{u}_h(U^i, \Pi_i), du_h(U^i), d\sigma_h(U^i)),$$

and the corresponding particle Hamiltonian, by the Legendre transform,

$$H_h(U^i, \Pi_i) = U^i \Pi_i - L_h(U^i, \Pi_i).$$

Here, the equations of motion are simply

$$\dot{U}^i = \frac{\partial H_h}{\partial \Pi_i}, \ \dot{\Pi}_i = -\frac{\partial H_h}{\partial U_i},$$

which possesses a canonical Hamiltonian structure with $\omega = d\Pi_i \wedge dU^i$ over the manifold $T^*(\mathbb{R}^{2N})$, where N is the dimension of Ω_h^k. Using the chain rule, the equations of motion generated by this canonical structure are weakly equivalent to the equations of motion generated by the non-canonical structure 2.5.7.

For a discrete Noether's theorem in the fully discretized problem, apply a Hamiltonian integrator which admits a discrete Noether's theorem, which can be found in the literature (or, at least, integrators which admit excellent error bounds on the conservation and long time stability). For a specific reference, see [12], where the authors show that for a symmetry, the discrete flow of a Hamiltonian variational integrator preserves the momentum map $J^{n+1} = J^n$.

2.7 Extensions

So far, we have considered field theories which govern the dynamics of a field, described as the section of the bundle $\Lambda^k M$, and the corresponding discretization of such theories. To provide more flexibility and handle more general problems, we can consider several extensions:

- How to form a basis for differential forms over manifolds which can be decomposed as a cross product $M = M_1 \times M_2$;
- Discretizing an action which governs multiple coupled fields $S[u^1, ..., u^N]$;

- More generally, consider fields which are vector-valued differential forms, i.e. sections of $\Lambda^k M \otimes (E, \pi, M)$.

Tensor Product Elements

In some problems, the domain of interest can be decomposed as a Cartesian product, $M = M_1 \times M_2$. For example, a foliation of spacetime is the product of spatial hypersurfaces with a time axis, $M = \Omega \times \mathbb{R}$ (the cost of such a foliation is losing Lorentz invariance). The ability to construct finite elements on such product spaces is permitted by the following lemma.

Lemma 2.7.1 *Let M_1 be a k_1-dimensional manifold and M_2 be a k_2-dimensional manifold. Then, the complex*

$$0 \to (\Omega M_1 \otimes \Omega M_2)^0 \xrightarrow{d} (\Omega M_1 \otimes \Omega M_2)^1 \xrightarrow{d} \dots \xrightarrow{d} (\Omega M_1 \otimes \Omega M_2)^{k_1+k_2} \to 0 \quad (2.7.1)$$

is a subcomplex of the de Rham Complex on $M_1 \times M_2$,

$$0 \to \Omega^0(M_1 \times M_2) \xrightarrow{d} \Omega^1(M_1 \times M_2) \xrightarrow{d} \dots \xrightarrow{d} \Omega^{k_1+k_2}(M_1 \times M_2) \to 0,$$

where $(\Omega M_1 \otimes \Omega M_2)^k := \bigoplus_{i+j=k} \pi_1^* \Omega^i M_1 \wedge \pi_2^* \Omega^j M_2$ (π_1 and π_2 are the canonical projections on $M_1 \times M_2$).

Proof. To show that the complex 2.7.1 is a subcomplex of the de Rham complex on $M_1 \times M_2$, we must show that $(\Omega M_1 \otimes \Omega M_2)^k$ is a subset of $\Omega^k(M_1 \times M_2)$, $d \circ d|_{(\Omega M_1 \otimes \Omega M_2)^k} = 0$, and $d(\Omega M_1 \otimes \Omega M_2)^k \subseteq (\Omega M_1 \otimes \Omega M_2)^{k+1}$.

The projection maps π_1 and π_2 are the canonical projections $\pi_1 : M_1 \times M_2 \to M_1$ and $\pi_2 : M_1 \times M_2 \to M_2$. π_1^* denotes the pullback of forms on M_1 to $M_1 \times M_2$ (likewise, π_2^*). Thus, $\pi_1^* \Omega^i M_1 \subseteq \Omega^i(M_1 \times M_2)$ and $\pi_2^* \Omega^j M_2 \subseteq \Omega^j(M_1 \times M_2)$. This of course implies that $(\Omega M_1 \otimes \Omega M_2)^k \subseteq \Omega^k(M_1 \times M_2)$. In particular then, d^k restricted to $(\Omega M_1 \otimes \Omega M_2)^k$ satisfies $d^{k+1} \circ d^k = 0$.

To see that $d(\Omega M_1 \otimes \Omega M_2)^k \subseteq (\Omega M_1 \otimes \Omega M_2)^{k+1}$, consider an element $\pi_1^* \alpha \wedge \pi_2^* \beta \in (\Omega M_1 \otimes \Omega M_2)^k$, where $\alpha \in \Omega^i M_1$, $\beta \in \Omega^j M_2$, $i + j = k$,

$$\begin{aligned} d_{M_1 \times M_2}(\pi_1^* \alpha \wedge \pi_2^* \beta) &= d_{M_1 \times M_2} \pi_1^* \alpha \wedge \pi_2^* \beta + (-1)^i \pi_1^* \alpha \wedge d_{M_1 \times M_2} \pi_2^* \beta \\ &= \pi_1^* d_{M_1} \alpha \wedge \pi_2^* \beta + (-1)^i \pi_1^* \alpha \wedge \pi_2^* d_{M_2} \beta, \end{aligned}$$

where we used the fact that the exterior derivative commutes with pullback. Thus, since $\pi_1^* d\alpha \wedge \pi_2^* \beta \in \pi_1^* \Omega^{i+1} M_1 \wedge \pi_2^* \Omega^j M_2$ and $\pi_1^* \alpha \wedge \pi_2^* d\beta \in \pi_1^* \Omega^i M_1 \wedge \pi_2^* \Omega^{j+1} M_2$, their (graded) sum lies in $(\Omega M_1 \otimes \Omega M_2)^{k+1}$. □

By the lemma, given finite element subcomplexes $\Omega_h M_1 \subset \Omega M_1$ and $\Omega_h M_2 \subset \Omega M_2$, the tensor product complex $\Omega_h M_1 \otimes \Omega_h M_2$ gives a finite element approximation of $\Omega(M_1 \times M_2)$. This discretization is summarized by the following commuting diagram

$$\begin{array}{ccccccccc}
0 & \longrightarrow & \Omega^0(M_1 \times M_2) & \xrightarrow{d} & \Omega^1(M_1 \times M_2) & \xrightarrow{d} & \dots & \xrightarrow{d} & \Omega^{k_1+k_2}(M_1 \times M_2) \longrightarrow 0 \\
 & & \downarrow{\scriptstyle \pi_*} & & \downarrow{\scriptstyle \pi_*} & & & & \downarrow{\scriptstyle \pi_*} \\
0 & \longrightarrow & (\Omega M_1 \otimes \Omega M_2)^0 & \xrightarrow{d} & (\Omega M_1 \otimes \Omega M_2)^1 & \xrightarrow{d} & \dots & \xrightarrow{d} & (\Omega M_1 \otimes \Omega M_2)^{k_1+k_2} \longrightarrow 0 \\
 & & \downarrow{\scriptstyle \Pi_h} & & \downarrow{\scriptstyle \Pi_h} & & & & \downarrow{\scriptstyle \Pi_h} \\
0 & \to & (\Omega_h M_1 \otimes \Omega_h M_2)^0 & \xrightarrow{d} & (\Omega_h M_1 \otimes \Omega_h M_2)^1 & \xrightarrow{d} & \dots & \xrightarrow{d} & (\Omega_h M_1 \otimes \Omega_h M_2)^{k_1+k_n} \to 0
\end{array}$$

Thus, with a basis $\{\phi_j\}_j$ for $\Omega_h M_1$ and a basis $\{\psi_k\}_k$ for $\Omega_h M_2$, we can construct a basis for $\Omega_h(M_1 \times M_2)$, $\{\pi_1^*\phi_j \wedge \pi_2^*\psi_k\}_{j,k}$. Note, also, since the mapping $\alpha \otimes \beta \to \pi_1^*\alpha \wedge \pi_2^*\beta$ is injective, we can equivalently work with the basis $\{\phi_j \otimes \psi_k\}_{j,k}$ where we define $d(\alpha \otimes \beta) = d\alpha \otimes \beta + (-1)^{deg(\alpha)}\alpha \otimes d\beta$.

This process allows us to create basis functions over complicated decomposable domains as the tensor product of basis functions over simpler domains. As an example, one can create basis functions for the n-cube $[0,1]^n$ by combining the simpler basis functions on the unit interval $[0,1]$.

Coupling

Many interesting systems involve multiple fields which interact, i.e., the dynamics of the fields are coupled. For examples, see chapter 3 below.

In the simplest case of coupling, consider two fields ϕ and ψ, respectively governed by actions $S_1[\phi] = \int \mathcal{L}_1(\phi, d\phi, d^*\phi)$ and $S_2[\psi] = \int \mathcal{L}_2(\psi, d\psi, d^*\psi)$. To couple these theories, we construct a new Lagrangian as a sum of the original Lagrangians plus a Lagrangian which describes the interaction between the two

$$S[\phi, \psi] = \int \mathcal{L}_1(\phi, d\phi, d^*\phi) + \mathcal{L}_2(\psi, d\psi, d^*\psi) + \mathcal{L}_{int}(\phi, d\phi, d^*\phi, \psi, d\psi, d^*\psi).$$

Of course, in the case that $\mathcal{L}_{int} \equiv 0$, the variations in ϕ and ψ are independent and the two systems decouple. To see this explicitly, by the Euler-Lagrange equation 1.4.2, we get the following equations for ϕ and ψ respectively

$$\Big(\frac{\partial}{\partial\phi} + d^*\frac{\partial}{\partial(d\phi)} + d\frac{\partial}{\partial(d^*\phi)}\Big)\mathcal{L}_1(\hat{\phi}) = -\Big(\frac{\partial}{\partial\phi} + d^*\frac{\partial}{\partial(d\phi)} + d\frac{\partial}{\partial(d^*\phi)}\Big)\mathcal{L}_{int}(\hat{\phi}, \hat{\psi}),$$
$$\Big(\frac{\partial}{\partial\psi} + d^*\frac{\partial}{\partial(d\psi)} + d\frac{\partial}{\partial(d^*\psi)}\Big)\mathcal{L}_2(\hat{\psi}) = -\Big(\frac{\partial}{\partial\psi} + d^*\frac{\partial}{\partial(d\psi)} + d\frac{\partial}{\partial(d^*\psi)}\Big)\mathcal{L}_{int}(\hat{\phi}, \hat{\psi}),$$

where $\hat{\phi} := (\phi, d\phi, d^*\phi)$. In the uncoupled case, the right hand side of both equations would be zero. Thus, the dynamics of the coupled fields is governed by their usual Euler-Lagrange equations but sourced by an interaction term.

For multiple fields $u^1, ..., u^N$, respectively governed by the Lagrangians $\mathcal{L}_1, ..., \mathcal{L}_N$, we get the following coupled action

$$S[u^1, ..., u^N] = \int \sum_{k=1}^{N} \mathcal{L}_k(\hat{u}^k) + \mathcal{L}_{int}(\hat{u}^1, ..., \hat{u}^N).$$

Defining the total Lagrangian $\mathcal{L}(\hat{u}^1, ..., \hat{u}^N) := \sum_{k=1}^N \mathcal{L}_k(\hat{u}^k) + \mathcal{L}_{int}(\hat{u}^1, ..., \hat{u}^N)$, the fields $u^1, ..., u^N$ are governed by the N-coupled equations

$$\Big(\frac{\partial}{\partial u^k} + d^* \frac{\partial}{\partial (du^k)} + d \frac{\partial}{\partial (d^* u^k)}\Big)\mathcal{L}(\hat{u}^1, ..., \hat{u}^N) = 0, \quad k = 1, ..., N.$$

The results from the previous sections of this chapter generalize to this case naturally (discretizations and their conservation laws). To do this, we use the following notation. For the coupled action $S[u^1, ..., u^N]$, we say each $u^k \in \Omega^{\alpha_k}$, i.e. u^1 is an α_1 form, etc (since the coupled fields do not have to be the same degree). Furthermore, denote $\partial_{k,1} := \frac{\partial}{\partial u^k}$, $\partial_{k,2} := \frac{\partial}{\partial (du^k)}$, $\partial_{k,3} := \frac{\partial}{\partial (d^* u^k)}$. Then, the discrete Euler-Lagrange equation is

Definition 2.7.1 (Coupled Discrete Euler-Lagrange Equation)
Find $(u_h^k, \sigma_h^k, \bar{p}_h^k, \bar{q}_h^k) \in \Omega_h^{\alpha_k} \times \Omega_h^{\alpha_k - 1} \times \Omega_h^{\alpha_k - 1} \times \mathfrak{D}_h^{\alpha_k}$, $k = 1, ..., N$, *such that*

$$\begin{aligned}
(\partial_{k,1}\mathcal{L}(\hat{u}^\sigma), v) + (\partial_{k,2}\mathcal{L}(\hat{u}^\sigma), dv) + (d\bar{p}_h^k, v) + (\bar{q}_h^k, v) = 0, \ \forall\ v \in \Omega_h^{\alpha_k}, \quad (2.7.2)\\
(\partial_{k,3}\mathcal{L}(\hat{u}^\sigma), \tau) - (\bar{p}_h^k, \tau) = 0, \ \forall\ \tau \in \Omega_h^{\alpha_k - 1},\\
(\sigma_h^k, p) - (u_h^k, dp) = 0, \ \forall\ p \in \Omega_h^{\alpha_k - 1},\\
(u_h^k, q) = 0, \ \forall\ q \in \mathfrak{D}_h^{\alpha_k},
\end{aligned}$$

where $\hat{u}^\sigma := (u_h^1, du_h^1, \sigma_h^1, ..., u_h^N, du_h^N, \sigma_h^N)$ *and* $\mathcal{L}$ *is the total Lagrangian.*

Thus, the above system consists of $4N$ coupled equations which can be used to discretize the coupled theory. The coupled semi-discrete case follows similarly.

In chapter 3 below, we will use these equations 2.7.2 to discretize the dynamics of matter fields coupled to gauge fields.

Vector Bundles

Another possible extension which provides more flexibility is to consider more general function spaces. For the systems we consider (e.g. Yang-Mills), we will need to extend our current theory to vector bundle valued forms, i.e. elements of $\Omega^k(M, E) := \Gamma(\Lambda^k M \otimes E)$.

Let M be a n-dimensional manifold and E a vector bundle over M with metric $\langle\ ,\ \rangle_E$. The L^2 inner product on $\Omega^k(M, E)$ is given by

$$(\alpha, \beta)_{L^2\Omega^k(M,E)} := \int_M \star\langle \alpha, \beta \rangle_{\Lambda^k M \otimes E}.$$

The Hilbert spaces $H\Omega^k(M, E)$ and $H^*\Omega^k(M, E)$ are defined analogously, where instead of the exterior derivative we use a general connection D.

Our goal is to discretize a generalized version of the de Rham sequence,

$$0 \longrightarrow \Omega^0(M, E^0) \xrightarrow{D} \Omega^1(M, E^1) \xrightarrow{D} ... \xrightarrow{D} \Omega^n(M, E^n) \longrightarrow 0, \quad (2.7.3)$$

where each E^k is a vector bundle over M with a bundle metric. To be completely general, we allow the connection to map between different vector-bundle valued

forms. Recall that in the case where the connection mapped forms to forms valued in the same vector bundle, the connection could be expressed $D = d + A\wedge$ where the exterior derivative acts through the vector structure and A is a 1-form valued in the endomorphisms of the vector bundle. For the connection in this more general setting, the connection is instead expressed $D^k = (d^k, f^k) + A^k\wedge$, where f^k is a vector bundle homomorphism from E^k to E^{k+1} and A^k is a 1-form valued in the homomorphisms from E^k to E^{k+1}.

The main issue in discretizing the sequence 2.7.3 is that in general, it is not a complex, $D^{k+1} \circ D^k \neq 0$. This is problematic within our FEEC framework since one of the compatibility conditions for a discretization is that there exists a bounded cochain projection between the original sequence and the discrete sequence, which is not well-defined if the sequence is not a complex. Consequently, we will assume that the sequence is a cochain complex, i.e. that the connection is flat $D^{k+1} \circ D^k = 0$.

Thus, a discretization of 2.7.3 is given by finding bounded projections Π_h^k to finite dimensional spaces $\Omega_h^k(M, E^k)$ such that $D^k\Omega_h^k(M, E^k) \subset \Omega_h^k(M, E^{k+1})$ and the following diagram commutes

$$\begin{array}{ccccccccc} 0 & \longrightarrow & H\Omega^0(M,E^0) & \xrightarrow{D} & H\Omega^1(M,E^1) & \xrightarrow{D} & \ldots & \xrightarrow{D} & H\Omega^n(M,E^n) \longrightarrow 0 \\ & & \downarrow{\scriptstyle \Pi_h} & & \downarrow{\scriptstyle \Pi_h} & & & & \downarrow{\scriptstyle \Pi_h} \\ 0 & \longrightarrow & \Omega_h^0(M,E^0) & \xrightarrow{D} & \Omega_h^1(M,E^1) & \xrightarrow{D} & \ldots & \xrightarrow{D} & \Omega_h^n(M,E^n) \longrightarrow 0 \end{array}$$

In general, the choice of discretization will depend on the connections and vector bundles in consideration for the problem at hand. Assuming we can find a projection for real-valued forms Π_h and a projection ξ_h from sections of the vector bundle $\Gamma(E^k)$ to a finite subspace $\Gamma_h(E^k)$ which commute with the connection, the following provides a discretization of 2.7.3

$$\begin{array}{ccccccccc} 0 & \longrightarrow & H\Omega^0(M,E^0) & \xrightarrow{D} & H\Omega^1(M,E^1) & \xrightarrow{D} & \ldots & \xrightarrow{D} & H\Omega^n(M,E^n) \longrightarrow 0 \\ & & \downarrow{\scriptstyle (\Pi_h,\xi_h)} & & \downarrow{\scriptstyle (\Pi_h,\xi_h)} & & & & \downarrow{\scriptstyle (\Pi_h,\xi_h)} \\ 0 & \longrightarrow & \Omega_h^0 M \otimes \Gamma_h(E^0) & \xrightarrow{D} & \Omega_h^1 M \otimes \Gamma_h(E^1) & \xrightarrow{D} & \ldots & \xrightarrow{D} & \Omega_h^n M \otimes \Gamma_h(E^n) \longrightarrow 0 \end{array}$$

In particular, for trivial vector bundles $E^k = M \times \mathbb{V}^k$ where each $\mathbb{V}^k$ is finite dimensional, a simple choice would be

$$\begin{array}{ccccccccc} 0 & \longrightarrow & H\Omega^0(M|\mathbb{V}^0) & \xrightarrow{D} & H\Omega^1(M|\mathbb{V}^1) & \xrightarrow{D} & \ldots & \xrightarrow{D} & H\Omega^n(M|\mathbb{V}^n) \longrightarrow 0 \\ & & \downarrow{\scriptstyle (\Pi_h,\mathbb{1})} & & \downarrow{\scriptstyle (\Pi_h,\mathbb{1})} & & & & \downarrow{\scriptstyle (\Pi_h,\mathbb{1})} \\ 0 & \longrightarrow & \Omega_h^0(M) \otimes \mathbb{V}^0 & \xrightarrow{D} & \Omega_h^1(M) \otimes \mathbb{V}^1 & \xrightarrow{D} & \ldots & \xrightarrow{D} & \Omega_h^n(M) \otimes \mathbb{V}^n \longrightarrow 0 \end{array}$$

(we use this choice in the next chapter to discretize the Yang-Mills equation, since locally the gauge potential is a one form valued in a trivial bundle $M \times \mathfrak{g}$).

2.8 Summary

In this chapter, we presented two broad approaches for simulating classical field theories, which both involve using FEEC (and extensions) to make the problem finite dimensional.

In the Lagrangian framework, we discretized the variational problem $\delta S = 0$ using the discrete Euler-Lagrange equation 2.3.4 which is naturally compatible with the variational structure. One advantage of this framework is that, since all of the operators were formulated via exterior calculus, it applies directly to problems defined over domains in spacetime (Lorentzian manifolds) and hence, respects the structure of relativistic field theories. Furthermore, the discrete Noether's theorem in this framework was a weak equivalent of the local current conservation law $d\mathfrak{J} = 0$. However, in order to make the problem well-posed, we had to manually introduce a gauge space $\mathfrak{D}$ to fix the gauge for the solution (the specific choice of $\mathfrak{D}$ depends on the problem at hand).

On the other hand, in the Hamiltonian framework, we discretized the variational problem by singling out the time coordinate t and considering the evolution of the field configuration as t varies. By singling out the time coordinate, this approach is not compatible with a relativistic structure. However, often we want to simulate the dynamics of a system and in particular, this approach respects the symplectic structure of the dynamics. In this framework, instead of local current conservation, Noether's theorem gives global charge conservation. Furthermore, the initial value problem of the Hamiltonian formulation is well-posed without manually imposing any constraints.

While the two different approaches have some similarities (e.g. both utilize FEEC), they preserve different structures inherent in classical field theories and thus the choice of discretization should depend on which structures one wishes to preserve. In the next chapter, we use the Lagrangian framework to spell out a discretization of the Yang-Mills theory (due to its compatibility with the spacetime structure). However, in the actual examples, we are interested in the time dynamics of the systems and hence, use the Hamiltonian framework.

Some interesting directions to consider in the future would be to see how these discretizations are related to quantization of field theories, and to see if there is a generalization of the discrete Hamiltonian framework to a discrete covariant Hamiltonian framework which preserves the multisymplectic structure of a field theory.

3 Applications

3.1 Yang-Mills Theory

In this section, we will apply the theory in chapter 2 to develop a FEEC discretization for Yang-Mills theories. For physical applications, the choice of the Lie group $U(1)$ corresponds to the electromagnetic interaction, $SU(2)$ corresponds to the weak interaction, and $SU(3)$ corresponds to the strong interaction. We set all of the relevant physical constants to unity, e.g. $\hbar = c = \epsilon_0 = 1$.

Recall the Yang-Mills action for a gauge field $A \in \Omega^1(M|\mathfrak{g})$, with source $J \in \Omega^1(M|\mathfrak{g})$,

$$S_{YM}[A] := \int_M \frac{1}{2}\langle F_A, F_A\rangle - \langle A, J\rangle,$$

where $\langle\ ,\ \rangle := -tr'(\ \wedge\star\ )$. The corresponding Euler-Lagrange equation is $D^*F_A = J$. In order to apply our discretization, write the variation in weak form, for $\beta \in \Omega^1(M|\mathfrak{g})$ proper,

$$\begin{aligned}
0 = \delta S_{YM}[A]\cdot\beta &= \int_M \langle D^*F_A, \beta\rangle - \langle J, \beta\rangle \\
&= \int_M \langle d^*(dA + \frac{1}{2}[A\wedge A]), \beta\rangle - \langle [A\lrcorner(dA + \frac{1}{2}[A\wedge A])], \beta\rangle - \langle J, \beta\rangle \\
&= \int_M \langle dA, d\beta\rangle + \frac{1}{2}\langle [A\wedge A], d\beta\rangle - \langle [A\lrcorner dA], \beta\rangle - \frac{1}{2}\langle [A\lrcorner[A\wedge A]], \beta\rangle - \langle J, \beta\rangle \\
&= \Big(dA, d\beta\Big)_2 + \frac{1}{2}\Big([A\wedge A], d\beta\Big)_2 - \Big([A\lrcorner\star\, dA], \beta\Big)_2 - \frac{1}{2}\Big([A\lrcorner[A\wedge A]], \beta\Big)_2 - \Big(J, \beta\Big)_1,
\end{aligned}$$

where $(\ ,\ )_k := (\ ,\ )_{\Omega^k(M|\mathfrak{g})}$. Thus, the weak formulation of the Yang-Mills equation is to find $A \in H\Omega^1(M|\mathfrak{g})$ such that for all $\beta \in \mathring{H}\Omega^1(M|\mathfrak{g})$,

$$(dA, d\beta) + \frac{1}{2}([A\wedge A], d\beta) - ([A\lrcorner dA], \beta) - \frac{1}{2}([A\lrcorner[A\wedge A]], \beta) = (J, \beta),$$

Note that this equation is in general nonlinear in A (except when G is abelian). Physically, these nonlinearities in nonabelian Yang-Mills theories correspond to self-interactions of the gauge particles. As a result of the nonlinearity, the discretization of this equation will result in a nonlinear system. Applying the discrete Euler-Lagrange equation: Find $(A_h, \bar{q}_h) \in \Omega^1_h(M|\mathfrak{g}) \times \mathfrak{D}^1_h(M|\mathfrak{g})$ such that for all $(\beta, q) \in \Omega^1_h(M|\mathfrak{g}) \times \mathfrak{D}^1_h(M|\mathfrak{g})$,

$$\begin{aligned}
(dA_h, d\beta) + \frac{1}{2}([A_h\wedge A_h], d\beta) - ([A_h\lrcorner dA_h], \beta) - \frac{1}{2}([A_h\lrcorner[A_h\wedge A_h]], \beta) + (\bar{q_h}, \beta) = (J, \beta), \\
(A_h, q) = 0. \qquad (3.1.1)
\end{aligned}$$

In order to compute with this discrete equation, consider a finite element basis for the Lie-algebra valued 1-forms, $\{\varphi^\mu \otimes t^a\}_{\mu,a}$ for $\Omega^1_h(M|\mathfrak{g})$ and a basis $\{e^\sigma \otimes$

$t^a\}_{\sigma,a}$ for $\mathfrak{D}^1_h(M|\mathfrak{g})$. Expand $A_h = A^a_\mu \varphi^\mu \otimes t^a$, $\bar{q}_h = \bar{q}^a_\sigma e^\sigma \otimes t^a$, and taking $\beta = \varphi^\mu \otimes t^a$, $q = e^\sigma \otimes t^a$, we can write 3.1.1 in component form.

$$\begin{aligned}
\Big(J, \varphi^\xi \otimes t^c\Big) &= A^a_\mu \Big(d\varphi^\mu \otimes t^a, d\varphi^\xi \otimes t^c\Big) + \frac{1}{2} A^a_\mu A^b_\nu \Big([(\varphi^\mu \otimes t^a) \wedge (\varphi^\nu \otimes t^b)], d\varphi^\xi \otimes t^c\Big) \\
&\quad - A^a_\mu A^b_\nu \Big([(\varphi^\mu \otimes t^a) \lrcorner (d\varphi^\nu \otimes t^b)], \varphi^\xi \otimes t^c\Big) \\
&\quad - \frac{1}{2} A^a_\mu A^b_\nu A^d_\rho \Big([\varphi^\mu \otimes t^a \lrcorner [(\varphi^\nu \otimes t^b) \wedge (\varphi^\rho \otimes t^d)]], \varphi^\xi \otimes t^c\Big) \\
&\quad + \bar{q}^a_\sigma \Big(e^\sigma \otimes t^a, \varphi^\xi \otimes t^c\Big) \\
&= A^a_\mu \Big(d\varphi^\mu \otimes t^a, d\varphi^\xi \otimes t^c\Big) + \frac{1}{2} A^a_\mu A^b_\nu \Big((\varphi^\mu \wedge \varphi^\nu) \otimes [t^a, t^b], d\varphi^\xi \otimes t^c\Big) \\
&\quad - A^a_\mu A^b_\nu \Big((\varphi^\mu \lrcorner d\varphi^\nu) \otimes [t^a, t^b], \varphi^\xi \otimes t^c\Big) \\
&\quad - \frac{1}{2} A^a_\mu A^b_\nu A^d_\rho \Big(\varphi^\mu \lrcorner (\varphi^\nu \wedge \varphi^\rho) \otimes [t^a, [t^b, t^d]]], \varphi^\xi \otimes t^c\Big) \\
&\quad + \bar{q}^a_\sigma \Big(e^\sigma \otimes t^a, \varphi^\xi \otimes t^c\Big), \\
0 &= A^\alpha_\mu \Big(\varphi^\mu \otimes t^a, e^\sigma \otimes t^b\Big).
\end{aligned}$$

Or, written as matrix-vector equations,

$$\begin{aligned}
K\vec{A} + B(\vec{A}) + G\vec{q} &= \vec{J}, \\
G^T \vec{A} &= 0,
\end{aligned} \tag{3.1.2}$$

where

$$\begin{aligned}
\vec{A} &:= (A^a_\mu)^{(\mu,a)}, \\
\vec{q} &:= (\bar{q}^a_\sigma)^{(\sigma,a)}, \\
\vec{J} &:= (J, \varphi^\xi \otimes t^c)^{(\xi,c)}, \\
K &:= (d\varphi^\mu \otimes t^a, d\varphi^\xi \otimes t^c)^{(\xi,c)}_{(\mu,a)}, \\
G &:= (e^\sigma \otimes t^a, \varphi^\xi \otimes t^c)^{(\xi,c)}_{(\sigma,a)}, \\
B(\vec{r}) &:= (\frac{1}{2} r^a_\mu r^b_\nu \Big((\varphi^\mu \wedge \varphi^\nu) \otimes [t^a, t^b], d\varphi^\xi \otimes t^c\Big) \\
&\quad - r^a_\mu r^b_\nu \Big((\varphi^\mu \lrcorner d\varphi^\nu) \otimes [t^a, t^b], \varphi^\xi \otimes t^c\Big) \\
&\quad - \frac{1}{2} r^a_\mu r^b_\nu r^d_\rho \Big(\varphi^\mu \lrcorner (\varphi^\nu \wedge \varphi^\rho) \otimes [t^a, [t^b, t^d]]], \varphi^\xi \otimes t^c\Big))^{(\xi,c)}.
\end{aligned}$$

Note that due to the nonlinear operator B, the system 3.1.2 is nonlinear and thus in general, we must apply a nonlinear method to compute the solution. However, in the case that the gauge group is abelian (e.g. in electromagnetism), the Lie bracket is trivial, so $B \equiv 0$, making 3.1.2 a linear system.

With the above formulation, we have a procedure for computing a FEEC solution to the Yang-Mills equation:

- Define the domain M for the problem of interest;
- Triangulate M;
- Define the basis functions $\{\varphi\}$ and $\{e\}$ over the triangulation of M;
- Assemble $\vec{J}$, K, G, and B;
- Solve the system 3.1.2 for $\vec{A}$ and $\vec{q}$;
- Express the solution $A_h = (\vec{A})^a_\mu(\varphi^\mu \otimes t^a)$.

Coupling to matter

Naturally, the Yang-Mills gauge theory of the Lie group G can be coupled to matter fields which transform under a representation of G. Coupling of the matter fields to the gauge fields physically describes massive particles which interact with force carriers (such as photons in electromagnetism, W and Z bosons in the weak interaction, and gluons in the strong interaction).

Let $\mathcal{L}_m(\psi, d\psi, d^*\psi)$ be the Lagrangian for a matter field $\psi \in \Omega^k(M, E)$, where the fibers of E, $\pi^{-1}(x)$, carry a representation ρ_x of G. Suppose that $\mathcal{L}_m$ is invariant under global G transformations, i.e. the transformation $\psi(x) \mapsto \rho_x(g)\psi(x)$ is a symmetry of the Lagrangian for all $g \in G$. To promote this global symmetry to a local symmetry, i.e. for $\mathcal{L}_m$ to be invariant under gauge transformations $\psi(x) \mapsto \rho_x(g(x))\psi(x)$ for all $g : M \to G$, the matter Lagrangian must be modified by making the formal substitution $\mathcal{L}_m(\psi, d\psi, d^*\psi) \mapsto \mathcal{L}_m(\psi, D_A\psi, D_A^*\psi)$, known as the **principle of minimal coupling**. On the matter fields $\Omega^k(M, E)$, D_A acts via the representation ρ, weighted by the "charge" of the matter field, q,

$$D_A\psi = d\psi + q\rho(-iA)\psi,$$

where we use the modified notation $D = d - iA$. The total action of the coupled theory is then

$$S = \int \frac{1}{g}\mathcal{L}_{YM}(A, dA) + \mathcal{L}_m(\psi, D_A\psi, D_A^*\psi),$$

where g is some coupling parameter. This can also be expanded in the form,

$$S = \int \frac{1}{g}\mathcal{L}_{YM}(A, dA) + \mathcal{L}_m(\psi, d\psi, d^*\psi) + \mathcal{L}_{int}(A, \psi).$$

Variation in A and ψ give the coupled equations

$$D^*F_A = J(A, \psi), \tag{3.1.3}$$
$$\Big(\frac{\partial}{\partial\psi} + d^*\frac{\partial}{\partial(d\psi)} + d\frac{\partial}{\partial(d^*\psi)}\Big)\mathcal{L}_m(\psi, d\psi, d^*\psi) = F(A, \psi),$$

where $J := -g\partial_A \mathcal{L}_{int}(A, \psi)$ and $F := -\partial_\psi \mathcal{L}_{int}(A, \psi)$. Thus, the gauge field A is sourced by a current J which arises from its interaction with matter, and the matter field evolves with a forcing term F due to the gauge field.

Discretizing this system is similar to the pure Yang-Mills case. Analogous to system 3.1.2, we get the equations for $\vec{A}$,

$$K\vec{A} + B(\vec{A}) + G\vec{q} = \vec{J}(\vec{A}, \vec{\psi}),$$
$$G^T\vec{A} = 0,$$

which are coupled to the equations for ψ, obtained by assembling the discrete Euler-Lagrange equations for ψ.

Example: Maxwell-Schrödinger System

In this section, we consider an example of discretizing a system involving Yang-Mills gauge fields coupled to matter. For our example, we will take the Yang-Mills theory to be over $U(1)$, an abelian group.

Consider the Schrödinger system for a particle with charge q and mass m coupled to electromagnetism, the $U(1)$ Yang-Mills theory. Since $\mathfrak{u}(1) \simeq \mathbb{R}$, the gauge potential A will be a real-valued one-form (up to a factor of i, depending on convention). Furthermore, since $U(1)$ is Abelian, the Lie bracket on $\mathfrak{u}(1)$ is trivial and hence, the adjoint action becomes

$$DB = dB - i[A \wedge B] = dB,$$

and the curvature of the connection is simply $F_A = dA$.

Since the theory is nonrelativistic, we split the domain into spatial and temporal components. Consider the respective actions for the Schrödinger and Maxwell systems,

$$\begin{aligned} S_S[\psi, \psi^*] &= \int dt \int_R i\psi^* \star \frac{\partial}{\partial t}\psi - \frac{1}{2m} d\psi \wedge \star d\psi^* - V(x, |\psi|)\psi \star \psi^*, \\ S_M[A] &= -\int_M \frac{1}{2} d'A \wedge' \star' d'A \\ &= \frac{1}{2}\int dt \int_R (\frac{\partial}{\partial t}\mathcal{A} + d\phi) \wedge \star(\frac{\partial}{\partial t}\mathcal{A} + d\phi) - d\mathcal{A} \wedge \star d\mathcal{A}, \end{aligned}$$

where the primed operators act on the spacetime manifold M, the unprimed operators act on the spatial manifold R, the gauge potential is split into components $A := (-\phi, \mathcal{A}) = (-\phi, \mathcal{A}^1, \mathcal{A}^2, \mathcal{A}^3)$, and V is the external potential.

Variation of the first action in ψ^* gives the Schrödinger equation (variation in ψ gives the conjugate equation),

$$\begin{aligned} i\frac{\partial}{\partial t}\psi &= \frac{1}{2m} d^* d\psi + V(x, |\psi|)\psi \\ &= -\frac{1}{2m} \star d \star d\psi + V(x, |\psi|)\psi, \end{aligned}$$

while variation in ϕ and $\mathcal{A}$ give two of Maxwell's equation (without source),

$$d^*(\frac{\partial}{\partial t}\mathcal{A} + d\phi) = 0,$$
$$d^*d\mathcal{A} + \frac{\partial}{\partial t}(\frac{\partial}{\partial t}\mathcal{A} + d\phi) = 0.$$

Or, defining the 1-form $E := -(\frac{\partial}{\partial t}\mathcal{A} + d\phi)$ and the 2-form $B := d\mathcal{A}$, these equations are the familiar $-d^*E = 0, d^*B - \partial_t E = 0$. For electromagnetism, the (trivial) Bianchi identity for the connection $d'd'A = 0$ gives the other Maxwell's equations $d^*B = 0, dE + \partial_t B = 0$. The first pair of equations are the dynamical equations while the second pair are geometric constraints.

Why would we be motivated to couple these systems together? Physically, coupling these two systems would allow us to incorporate the electromagnetic interaction into the Schrodinger equation (e.g. to describe nonrelativistic matter laser interaction). Furthermore, note that the Schrödinger action is invariant under the global $U(1)$ transformation, $\psi \mapsto e^{i\alpha}\psi,\ \forall \alpha \in \mathbb{R}$. If we try to promote this symmetry to local gauge transformations, $\psi \mapsto e^{i\alpha(t,x)}\psi$, one can check that the action $S_S[\psi, \psi^*]$ is no longer invariant. In order for the action to remain invariant under gauge transformations, one has to couple the $U(1)$ gauge field A to the Schrödinger action.

To couple these systems, we use the principle of minimal coupling, making the formal subtitution $\mathcal{L}(\psi, \partial_t\psi, d\psi) \mapsto \mathcal{L}(\psi, D_\phi\psi, D_\mathcal{A}\psi)$. For $(\psi(t), \phi(t), \mathcal{A}(t)) \in \Omega^0(R|\mathbb{C}) \times \Omega^0(R) \times \Omega^1(R)$, the total action is

$$S[\psi, \psi^*, \phi, \mathcal{A}] = \int dt \int_R i\psi^* \star (\partial_t + iq\phi)\psi + \frac{1}{2m}(d - iq\mathcal{A})\psi \wedge \star(d - iq\mathcal{A})\psi^* \\ - V(x, |\psi|)\psi \star \psi^* + \frac{1}{2}(\frac{\partial}{\partial t}\mathcal{A} + d\phi) \wedge \star(\frac{\partial}{\partial t}\mathcal{A} + d\phi) - \frac{1}{2}d\mathcal{A} \wedge \star d\mathcal{A}. \tag{3.1.4}$$

One can check that this action is invariant under $U(1)$ gauge transformations with the following representations for a generator α,

$$\begin{aligned} \psi(t,x) &\overset{\alpha}{\mapsto} e^{iq\alpha(t,x)}\psi(t,x), \\ \phi(t,x) &\overset{\alpha}{\mapsto} \phi(t,x) - \frac{\partial}{\partial t}\alpha(t,x), \\ \mathcal{A}(t,x) &\overset{\alpha}{\mapsto} \mathcal{A}(t,x) + d\alpha(t,x). \end{aligned} \tag{3.1.5}$$

Variation in $\psi^*, \phi, \mathcal{A}$ gives the following equations, respectively,

$$\begin{aligned} i\frac{\partial}{\partial t}\psi &= -\frac{1}{2m} \star (d - iq\mathcal{A}\wedge) \star (d - iq\mathcal{A})\psi + (V(x, |\psi|) + q\phi)\psi, \\ d^*(\frac{\partial}{\partial t}\mathcal{A} + d\phi) &= q|\psi|^2, \\ d^*d\mathcal{A} + \frac{\partial}{\partial t}(\frac{\partial}{\partial t}\mathcal{A} + d\phi) &= -\frac{q^2}{m}\mathcal{A}|\psi|^2 + \frac{q}{m}\ Im(\psi^* d\psi), \end{aligned} \tag{3.1.6}$$

which is an example of equation 3.1.3. Defining the momentum operator $p_{\mathcal{A}} := -i \star (d - iq\mathcal{A})$, the total potential $U := V + q\phi$, the corresponding Hamiltonian $\mathcal{H} := p_{\mathcal{A}}^2/2m + U$, the charge density $\rho(\psi) := q|\psi|^2$, and the current one form $J(\psi, \mathcal{A}) := -q^2\mathcal{A}|\psi|^2/m + q\ Im(\psi^* d\psi)/m$, we can rewrite the above equations in a more familiar form:

$$\begin{aligned} i\frac{\partial}{\partial t}\psi &= \mathcal{H}(x, \psi, \phi, \mathcal{A})\psi, \\ \star d \star E &= \rho(\psi), \\ \star d \star B - \frac{\partial}{\partial t}E &= J(\psi, \mathcal{A}). \end{aligned} \tag{3.1.7}$$

That is, the matter field ψ evolves under a Hamiltonian which is coupled to the electromagnetic field, and the electromagnetic fields are sourced by a charge density and current which are coupled to the matter field. These are the complete dynamical equations for the Maxwell-Schrödinger system (the other two geometric constraints from Maxwell's equations still hold).

To see that the potentials propagate as waves, we can use the Lorenz gauge $\frac{\partial}{\partial t}\phi - d^*\mathcal{A} = 0$ (the $U(1)$ gauge symmetry 3.1.5 allows gauge freedom in the problem). The system then becomes

$$\begin{aligned} i\frac{\partial}{\partial t}\psi &= \mathcal{H}(x, \psi, \phi, \mathcal{A})\psi, \\ \frac{\partial^2}{\partial t^2}\phi &= \rho(\psi) - \Delta^0\phi, \\ \frac{\partial^2}{\partial t^2}\mathcal{A} &= J(\psi, \mathcal{A}) - \Delta^1\mathcal{A}, \end{aligned} \tag{3.1.8}$$

where Δ^k is the Hodge-Laplacian on k-forms, $d^*d + dd^*$ (note that the Hodge-Laplacian differs from the usual vector calculus Laplacian ∇^2 by a minus sign).

Discretization The discretization of this system is straight-forward; apply the coupled form of the semi-discrete Euler-Lagrange equation 2.5.6 to the action 3.1.4. Then, with a basis $\{\varphi_0^k\}_k$ for 0-forms and $\{\varphi_1^k\}_k$ for 1-forms, expand $\psi_h = \psi_k(t)\varphi_0^k$, $\phi_h = \phi_k(t)\varphi_0^k$, $\mathcal{A}_h = A_k(t)\varphi_1^k$. This gives the following system

$$\begin{aligned} i\frac{d\psi_k}{dt}(\varphi_0^k, \varphi_0^j) = &-\frac{1}{2m}\Big(- \psi_k(d\varphi_0^k, d\varphi_0^j) - iqA_m\psi_k(\varphi_1^m \lrcorner d\varphi_0^k, \varphi_0^j) + iqA_m\psi_k(\varphi_1^m\varphi_0^k, d\varphi_0^j) \\ &- q^2\psi_k A_l A_m(\varphi_0^k\varphi_1^l \lrcorner \varphi_1^m, \varphi_0^j)\Big) + (V(\psi)\psi, \varphi_0^j) + q\phi_m\psi_k(\varphi_0^m\varphi_0^k, \varphi_0^j), \\ \frac{dA_k}{dt}(\varphi_1^k, d\varphi_0^j) + &\phi_k(d\varphi_0^k, d\varphi_0^j) = q\psi_k^*\psi_m(\varphi_0^k\varphi_0^m, \varphi_0^j), \\ A_k(d\varphi_1^k, d\varphi_1^j) + &\frac{d^2A_k}{dt^2}(\varphi_1^k, \varphi_1^j) + \frac{d\phi_k}{dt}(d\varphi_0^k, \varphi_1^j) = -\frac{q^2}{m}A_m\psi_k^*\psi_l(\varphi_1^m\varphi_0^k\varphi_0^l, \varphi_1^j) + \frac{q}{m}Im(\psi_k^*\psi_m)(\varphi_0^k d\varphi_0^m, \varphi_1^j). \end{aligned}$$

To discretize this system in time, we use the Hamiltonian framework discussed in chapter 2. We will also assume the external potential $V(\psi) \equiv 0$. From the Lagrangian of the action 3.1.4, we get the following conjugate momenta

$\xi := \partial\mathcal{L}/\partial\dot{\psi} = i\psi^*$, $\pi := \partial\mathcal{L}/\partial\dot{\mathcal{A}} = \partial_t\mathcal{A}+d\phi$, $\theta := \partial\mathcal{L}/\partial\dot{\phi} = 0$. The Hamiltonian is

$$\mathcal{H}_h = \xi \wedge \star\dot{\psi} + \pi \wedge \star\dot{\mathcal{A}} - \mathcal{L},$$

Then, in terms of the components of the basis expansion of the fields and their momenta $\Big((\vec{\psi},\vec{\xi}),(\vec{A},\vec{\pi}),(\vec{\phi},\vec{\theta})\Big)$, we get a matrix system of the form

$$\begin{aligned}
iM_{kj}\frac{d\psi_k}{dt} &= -\frac{1}{2m}(-K_{kj}\psi_k - iqB_{mkj}A_m\psi_k - q^2Z_{klmj}\psi_kA_lA_m + qU_{mkj}\phi_m\psi_k),\\
-iM_{kj}\frac{d\xi_k}{dt} &= -\frac{1}{2m}(-K_{kj}\xi_k + iqB_{mkj}A_m\xi_k - q^2Z_{klmj}\xi_kA_lA_m + qU_{mkj}\phi_m\xi_k),\\
M'_{kj}\frac{dA_k}{dt} &= M'_{kj}\pi_k - S^T_{kj}\phi_k,\\
-M'_{kj}\frac{d\pi_k}{dt} &= K'_{kj}A_k + \frac{q^2}{m}J_{mklj}A_m\frac{\xi_k}{i}\psi_l - \frac{q}{m}J'_{kmj}Im(\frac{\xi_k}{i}\psi_m),\\
M_{kj}\frac{d\phi_k}{dt} &= 0,\\
0 = -M_{kj}\frac{d\theta_k}{dt} &= qU_{kmj}\frac{\xi_k}{i}\psi_m - S_{kj}\pi_k,
\end{aligned}$$

where

$$\begin{aligned}
M_{ab} = (\varphi_0^a,\varphi_0^b),\ M'_{ab} = (\varphi_1^a,\varphi_1^b),\\
K_{ab} = (d\varphi_0^a,d\varphi_0^b),\ K'_{ab} = (d\varphi_1^a,d\varphi_1^b),\\
J_{abcd} = (\varphi_1^a\varphi_0^b\varphi_0^c,\varphi_1^d),\ J'_{abc} = (\varphi_0^a d\varphi_0^b,\varphi_1^c),\\
Z_{abcd} = (\varphi_0^a\varphi_1^b\lrcorner\varphi_1^c,\varphi_0^d),\ S_{ab} = (\varphi_1^a,d\varphi_0^b),\\
B_{abc} = (\varphi_1^a\lrcorner d\varphi_0^b,\varphi_0^c) - (\varphi_1^a\varphi_0^b,d\varphi_0^c),\\
U_{abc} = (\varphi_0^a\varphi_0^b,\varphi_0^c).
\end{aligned}$$

Thus, given an initial configuration $\Big((\vec{\psi},\vec{\xi}),(\vec{A},\vec{\pi}),(\vec{\phi},\vec{\theta})\Big)(0)$, we have a well-posed Hamiltonian system which we can apply a symplectic integration scheme to fully discretize. Note that once we assemble the matrices M, M', K, K', J, J', Z, S, B, and U, the remaining computation of the problem becomes relatively straight forward. Furthermore, the Hamiltonian framework automatically imposes the gauge condition $\dot{\phi} = 0$. If we instead want to impose a different gauge, we would impose the gauge at the level of the Lagrangian and then recompute the corresponding Hamiltonian equations.

The images from figure 3.1 were produced using this discretization of the Maxwell-Schrödinger system on a cylinder. Assuming the cylinder is infinite along its axis, dimensional reduction reduces the problem from a 3-dimensional domain to a 2-dimensional domain.

From Noether's theorem under the $U(1)$ symmetry 3.1.5, we expect the probability $P = \frac{1}{i}\int\star(\xi\psi) = \frac{1}{i}M_{ab}\xi_a\psi_b$ satisfies $\dot{P}(t) = 0$. The corresponding plot for the total probability is shown in figure 3.2.

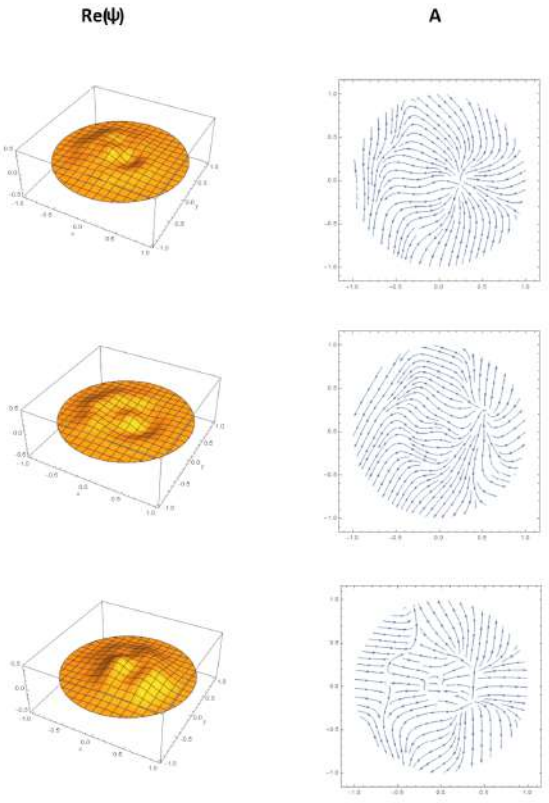

Figure 3.1: Snapshots of evolution of coupled Maxwell-Schrodinger System

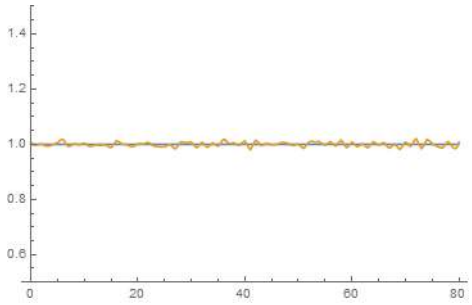

Figure 3.2: Approximate Conservation of Total Probability $P(t)$

3.2 Plasma Physics

In this section, we consider applications of our framework to modeling plasmas (charge particles are completely ionized resulting in free movement). In particular, we will use particle-in-cell (PIC) method and will see how our FEEC discretization fits into a larger system. First, we review some of the basic equations governing plasmas and then discuss the PIC method, followed by several examples.

In this section, we will use the canonical isomorphism between 1-forms and tangent vectors on a Riemannian manifold to interchange between 1-forms and vectors. We use $\langle\ ,\ \rangle$ to denote the metric on 1-forms and equivalently the metric on tangent vectors.

Maxwell-Vlasov System

There are two broad approaches in describing the dynamics of a plasma.

The approach of magnetohydrodynamics is to describe the plasma as a fluid, subject to a mass, momentum, and energy equation which incorporates the effect of electromagnetic fields (the Navier-Stokes system coupled to Maxwell's equations). However, since we are treating the plasma as a continuum, we lose some interesting effects of particle interactions with the fields.

We instead take the other approach, the kinetic description of a plasma, where the plasma is described by a distribution function $f(r,p,t)$ which gives the density of particles at each point in phase space, $(r,p) \in T^*M$, at time t. Here, p refers to the kinetic momentum of the particles. The starting point for the kinetic theory is the Boltzmann equation, which states that the total time derivative of the distribution function is equal to the collilsion rate in the plasma,

$$\frac{d}{dt} f(r,p,t) = \Big(\frac{\partial f}{\partial t}\Big)_{collision}.$$

For example, for small but non-negligible collisions in a plasma, $(\partial f/\partial t)_{coll} = -\partial(f\langle \Delta p_i\rangle)/\partial p_i + \frac{1}{2}\partial^2(f\langle \Delta p_i \Delta p_j\rangle)/\partial p_i \partial p_j$ which gives a Fokker-Planck equation to describe the plasma. However, for many plasmas, we can assume collisions occur on a time-scale much shorter than the time-scale of the plasma oscillations, $\langle \Delta p_i\rangle \approx 0$, and neglect second order effects $\mathcal{O}(\langle \Delta p_i \Delta p_j\rangle)$. Thus, we will ignore the collision rate and the plasma is then governed by the Vlasov equation,

$$0 = \frac{d}{dt} f(r,p,t) = \frac{\partial f}{\partial t} + \langle \dot{r}, \frac{\partial f}{\partial r}\rangle + \langle \dot{p}, \frac{\partial f}{\partial p}\rangle, \tag{3.2.1}$$

where we used the chain-rule to expand the total derivative. To complete this equation, we use the velocity $\dot{r} = p/m$ (assuming non-relativistic motion) and from the Lorentz force, $\dot{p} = q(E + p \times B/m)$. Of course, the electromagnetic field is coupled to the plasma; since the particles are charged, they generate an

electromagnetic field. This coupling is given by Maxwell's source equations

$$\nabla \cdot E(r,t) = \rho(r,t),$$
$$\nabla \times B(r,t) - \frac{\partial}{\partial t} E(r,t) = J(r,t),$$

where the charge and current densities are given by

$$\rho(r,t) = q \int_{T_r^* M} vol_p \ f(r,p,t),$$
$$J(r,t) = q \int_{T_r^* M} vol_p \ \frac{p}{m} f(r,p,t),$$

where q is the charge of the particle and m is the mass of the particle. These source equations can equivalently be characterized by an action, with scalar potential ϕ and potential one form $\mathcal{A}$,

$$S_f[\phi, \mathcal{A}] = \int dt \int_M \Big[\frac{1}{2}(\frac{\partial}{\partial t}\mathcal{A} + d\phi) \wedge \star (\frac{\partial}{\partial t}\mathcal{A} + d\phi) - \frac{1}{2} d\mathcal{A} \wedge \star d\mathcal{A} + \mathcal{A} \wedge \star J - \phi \wedge \star \rho\Big], \tag{3.2.2}$$

where the subscript f denotes that the action depends on the distribution function but is not a functional of the distribution function. As mentioned before, $E = -d\phi - \partial_t \mathcal{A}$ and $B = d\mathcal{A}$. Thus, the dynamical equations for the coupled Maxwell-Vlasov system are

$$\begin{aligned} 0 &= \frac{\partial f}{\partial t} + \langle \frac{p}{m}, \frac{\partial f}{\partial r} \rangle + q \langle E + \frac{p}{m} \times B, \frac{\partial f}{\partial p} \rangle, \\ 0 &= \frac{\delta S_f[\phi, \mathcal{A}]}{\delta \phi}, \\ 0 &= \frac{\delta S_f[\phi, \mathcal{A}]}{\delta \mathcal{A}}. \end{aligned} \tag{3.2.3}$$

Particle-In-Cell Method

One can think of the evolution of the distribution function in kinetic theory as the evolution of an infinite amount of particles, each occupying a single point in phase-space. In this picture, the α^{th} particle at (r_α, p_α) contributes $\delta(r - r_\alpha(t))\delta(p - p_\alpha(t))$ to the distribution $f(r,p,t)$. Each of these particles follows the characteristics of the Vlasov equation 3.2.1.

The particle-in-cell method uses this insight to numerically simulate the system 3.2.3. As opposed to tracking an infinite amount of particles each with zero width (computationally impossible), the PIC method tracks a finite number of computational particles which occupy some small but non-vanishing bandwidth in phase space (see figure 3.3). It is interesting to note that our Hamiltonian framework for discretizing a field theory worked on similar principles.

For every time step, we perform the following steps. First, use the fields from the previous time step to update the position and momentum of each particle.

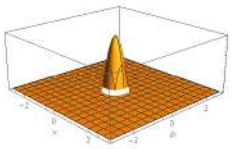

Figure 3.3: Computational particle in $1+1$ dimensional phase space

Then, use the updated computational particles to compute the distribution function, by summing over the phase-space bandwidths of each computational particle. This allows us to compute the charge density and current density. We then use our FEEC field solver to calculate $\mathcal{A}, \phi$ (and then E, B) from these densities. Reiterate. Below, we elaborate on the steps of this process.

Initialization

To initialize the PIC process, the initial positions and momenta of the particles and the initial field configurations must be determined. Assume that we have chosen an initial distribution function $f(r, p, 0)$.

Since our evolution equations involve time derivatives of ϕ and $\mathcal{A}$, we need the initial field configurations. There are several choices for initial configurations. One choice would be to impose external fields $\phi(r, 0)$ and $\mathcal{A}(r, 0)$, for example if the plasma was initially radiated by an electromagnetic wave. Another option would be to use the field solver to determine $\phi(r, 0)$ from the electrostatic equation $\Delta^0\phi = \rho_0(r)$ and $\mathcal{A}(r, 0)$ from the magnetostatic equation $\Delta^1\mathcal{A} = J_0(r)$, where $\rho_0(r) = q\int_{T^*_rM} vol_p f(r, p, 0)$ and $J_0(r) = q\int_{T^*_rM} vol_p \frac{p}{m} f(r, p, 0)$.

Furthermore, the distribution must be sampled in order to determine the initial positions and momenta of N computational particles, i.e. the α^{th} sample of $f(r, p, 0)$ determines $(r_\alpha(0), p_\alpha(0))$, $\alpha \in \{1, .., N\}$. We use the rejection method to sample the distribution: To sample an arbitrary distribution function f, instead sample from a distribution function g which we already know how to sample from (e.g. a box function), satisfying $\text{supp(g)} \supseteq \text{supp(f)}$ and $\sup(f/g) \leq L$. Upon sampling a point x from g, sample a random number from $r \in [0, 1]$ and if $r \leq f(x)/Lg(x)$, accept the sampled value x; otherwise, reject it and resample. An example is shown in figure 3.4.

Updating position and momentum

Recall that the particles follow the characteristics of the equation governing the distribution function, the first equation of 3.2.3. By setting $f = f(r_\alpha(t), p_\alpha(t), t)$ and computing the characteristics the of corresponding equation, the α^{th} particle obeys

$$\begin{aligned}\dot{r}_\alpha &= p_\alpha/m,\\ \dot{p}_\alpha &= q(E + p_\alpha \times B/m).\end{aligned}$$

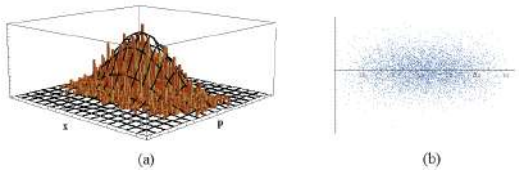

Figure 3.4: Example of the rejection method for $f(r,p,0) = sin^2(r)e^{-p^2}$ on $[0,\pi] \times [-3,3]$ for $N = 10,000$ particles. (a) Histogram of sampled values with f outlined in black. (b) Corresponding phase space plot

The updated positions and momenta are obtained by integrating these equations to get r^{n+1} and p^{n+1} from the n^{th} step. There are of course many possible ways to integrate these equations of motion. In our case, we utilize the Hamiltonian structure of the dynamics to symplectically integrate the equations of motion. One benefit of this approach is that the integration preserves the symplectic form $dz_i \wedge dr^i$, where z is the momenta conjugate to r (not necessarily the kinetic momentum p),

$$(dz^n)_i \wedge (dr^n)^i = (dz^{n+1})_i \wedge (dr^{n+1})^i, \tag{3.2.4}$$

which can be visualized as the conservation of phase space volume. Along with preserving the symplectic form, these integrators have the interesting property that they conserve a modified Hamiltonian which is quantifiably close to the exact Hamiltonian.

To utilize the Hamiltonian structure, introduce the canonical momentum $z = p + qA$ (kinetic momentum plus a contribution from the vector potential). At each timestep, we will assume the fields obtained from the field solver are fixed, as to eliminate the time dependency. The Hamiltonian for the system is

$$H(r,z) = \frac{1}{2m}(z - qA(r))^2 + q\phi(r), \tag{3.2.5}$$

(we saw essentially the same Hamiltonian for the Maxwell-Schrödinger system in the equation $i\partial_t\psi = H\psi$) and the equations of motion are given by Hamilton's equations,

$$\dot{z} = -\nabla_r H(r,z),$$
$$\dot{r} = \nabla_z H(r,z),$$

which are equivalent to the previous equations of motion upon substituting $z = p + qA$, $E = -\nabla\phi - \partial_t A$, $B = \nabla \times A$. To integrate, we will use a relatively straight-forward method, a symplectic Euler method,

$$z^{n+1} = z^n - \Delta t \nabla_r H(r^n, z^{n+1}),$$
$$r^{n+1} = r^n + \Delta t \nabla_z H(r^n, z^{n+1}),$$

which can be shown to satisfy the symplectic map condition 3.2.4. In general, this system is implicit in the momentum z^{n+1}. However, for our specific Hamiltonian 3.2.5, $\nabla_r H(r^n, z^{n+1})$ is linear in z^{n+1} and hence, the system becomes linear in z^{n+1}. Using $p = z - qA$, this system provides a map $(r_\alpha^n, p_\alpha^n) \mapsto (r_\alpha^{n+1}, p_\alpha^{n+1})$ to update the position and momentum for each particle.

Quantities involving the distribution function

As mentioned before, each computational particle contributes a small bandwidth of phase space to the distribution function. For computation, we represent particles by shape functions which have similar properties to a delta function (has an area of 1, is maximum at the origin, and falls off to zero rapidly). Choosing one such function $S(r)$ for positions and $\tilde{S}(p)$ for momenta,

$$f(r,p,t) = \sum_{\alpha=1}^{N} S(r - r_\alpha(t))\tilde{S}(p - p_\alpha(t)). \tag{3.2.6}$$

Subsequently, the charge and current densities are given by

$$\begin{aligned}
\rho(r,t) &= q\int_{T_r^*M} vol_p f(r,p,t) = q\int_{T_r^*M} vol_p \sum_{\alpha=1}^{N} S(r - r_\alpha(t))\tilde{S}(p - p_\alpha(t)) \\
&= q\sum_{\alpha=1}^{N} S(r - r_\alpha(t)) \int_{T_r^*M} vol_p \tilde{S}(p - p_\alpha(t)) = q\sum_{\alpha=1}^{N} S(r - r_\alpha(t)), \\
J(r,t) &= q\int_{T_r^*M} vol_p \frac{p}{m} f(r,p,t) = q\int_{T_r^*M} vol_p \frac{p}{m} \sum_{\alpha=1}^{N} S(r - r_\alpha(t))\tilde{S}(p - p_\alpha(t)) \\
&= q\sum_{\alpha=1}^{N} S(r - r_\alpha(t)) \int_{T_r^*M} vol_p \frac{p}{m} \tilde{S}(p - p_\alpha(t)).
\end{aligned}$$

It may be the case that we are only interested in the particles and not the distribution function (after all, the distribution function is supposed to represent the particles). In this case, we can take the momentum shape function to be a delta function, $\tilde{S} \equiv \delta$, and the formula for the current simplifies to

$$J(r,t) = \frac{q}{m}\sum_{\alpha=1}^{N} p_\alpha(t) S(r - r_\alpha(t)).$$

Lastly, another quantity of interest is the total kinetic energy of the particles,

$$T(t) = \int_M vol_r \int_{T_r^*M} vol_p \frac{p^2}{2m} f(r,p,t) = \sum_{\alpha=1}^{N} \frac{p_\alpha^2(t)}{2m}, \tag{3.2.7}$$

where again we use $\tilde{S} = \delta$. The kinetic energy will allow us to measure how the energy of the particles is transferred to or from the electromagnetic field energy,

$$U(t) = \frac{1}{2}\int_M vol_r\Big(E^2(r,t) + B^2(r,t)\Big). \tag{3.2.8}$$

Field Solver

The field solver for finding the potentials (and hence the electric and magnetic fields) is analogous to the previous discussion of the Maxwell-Schrödinger system. Applying the semi-discrete Euler-Lagrange equation 2.5.6 to the action 3.2.2 and expanding in terms of basis functions,

$$\begin{aligned}\frac{dA_k}{dt}(\varphi_1^k, d\varphi_0^j) + \phi_k(d\varphi_0^k, d\varphi_0^j) &= (\rho, \phi_0^j),\\ A_k(d\varphi_1^k, d\varphi_1^j) + \frac{d^2A_k}{dt^2}(\varphi_1^k, \varphi_1^j) + \frac{d\phi_k}{dt}(d\varphi_0^k, \varphi_1^j) &= (J, \phi_1^j).\end{aligned}$$

As before, we use the Hamiltonian formulation of the semi-discrete equation.

$$\begin{aligned}M'_{kj}\frac{dA_k}{dt} &= M'_{kj}\pi_k - S^T_{kj}\phi_k,\\ -M'_{kj}\frac{d\pi_k}{dt} &= K'_{kj}A_k - (J, \varphi_1^j),\\ M_{kj}\frac{d\phi_k}{dt} &= 0,\\ 0 = -M_{kj}\frac{d\theta_k}{dt} &= (\rho, \varphi_0^j) - S_{kj}\pi_k,\end{aligned}$$

where the matrices M, M', K', and S are defined in the previous example. Subsequently, discretize in time via a symplectic method. With all of the elements of the PIC method in place, we can examine a few examples.

Example: 1D 1V System

In this example, we will explore a plasma in one spatial dimension and one momentum dimension (two dimensional phase space). Although there are ways of defining magnetic fields in one dimension, we will assume there is no magnetic field and as a result, only an electric field interacts with the plasma.

For one-dimensional plasmas (plasmas longitudinally oscillating along one direction), an interesting damping mechanism occurs known as Landau damping. The oscillations of the particles in the plasma generate oscillations in the electric field. As these field oscillations propagate, they resonate with particles moving with the same velocity (since, in the comoving frame of the particles, the electric field can do work on these particles). Of course, as with any real resonance phenomena, there is some bandwidth to the velocities in which the particles can resonate (see figure 3.5). For particles moving slightly slower than the electric field, the electric field will accelerate the particles and give energy

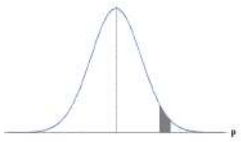

Figure 3.5: Resonance in distribution function monotone in $|p|$

to these particles; likewise, for particles moving slightly faster, the electric field will decelerate the particles and gain energy from the particles. If the initial distribution function is monotone decreasing in $|p|$ (the magnitude of the kinetic momentum), more particles will be accelerated by the field and hence gain energy; as a result, we expect the electric field energy to dissipate. This damping occurs until nonlinearities arise which keep the electric field from dissipating completely. Hence, this process is usually referred to as linear Landau damping.

Of course, the initial distribution function may not be monotone decreasing in $|p|$ (see figure 3.6). In this case, if the electric field travels at a velocity in which the distribution function is increasing, the electric field instead gains energy from the particles, producing an instability. If the function is mostly decreasing, then as the dynamics of the system progresses, the electric field will mostly be damped with occasional instabilities. This is referred to as the bump-on-tail instability due to the shape of the initial distribution function.

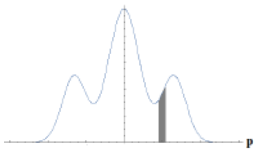

Figure 3.6: Resonance in non-monotone distribution function

For a more rigorous explanation of these damping phenomena and instabilities in plasmas, see e.g. [17].

To test these damping and instability mechanisms, we employ the PIC method outlined above for a one dimensional plasma. The following tests further motivate the choice of a symplectic integrator, since we can attribute dissipation or instability that we see in the system to the physical processes occuring, not to numerical dissipation or instability in the integrator. Other than the initial distribution $f(x, p, 0)$, the parameters relevant to both tests are the same (e.g. number of particles, time-step, etc.). For both tests, the spatial domain is the interval $[0, 10]$ with periodic boundary conditions, or $\mathbb{R}/10\mathbb{Z}$.

Landau Damping To model a system under Landau damping, we initialize the distribution function $f(x, p, 0) = (1 + cos(2(x - 2)))e^{-p^2}$ which is monotone decreasing in $|p|$ and oscillatory in x. Snapshots of the evolution of this system is shown in figure 3.7. As can be seen from the energy plots in figure 3.8, the

electric field is damped exponentially and the particles gain energy. Furthermore, figure 3.8(c) shows that the total energy $E = U + T$ is approximately constant (with the deviation occurring during the damping), which tells us the energy is being transferred from the electric field to the particles.

Bump-on-tail Instability To model the bump-on-tail instability, we initialize $f(x, p, 0) = (1 + cos(2(x - 2)))e^{-p^2} + 0.85e^{-5(p-1.3)^2} + 0.85e^{-5(p+1.3)^2}$, which is the distribution function from the previous test with two additional terms (two streams of energetic particles), making the function not monotone in $|p|$. The evolution of the system is shown in 3.9. From the energy plots in figure 3.10, the electric field is no longer damped exponentially and there are instabilities which occur throughout the resonance process.

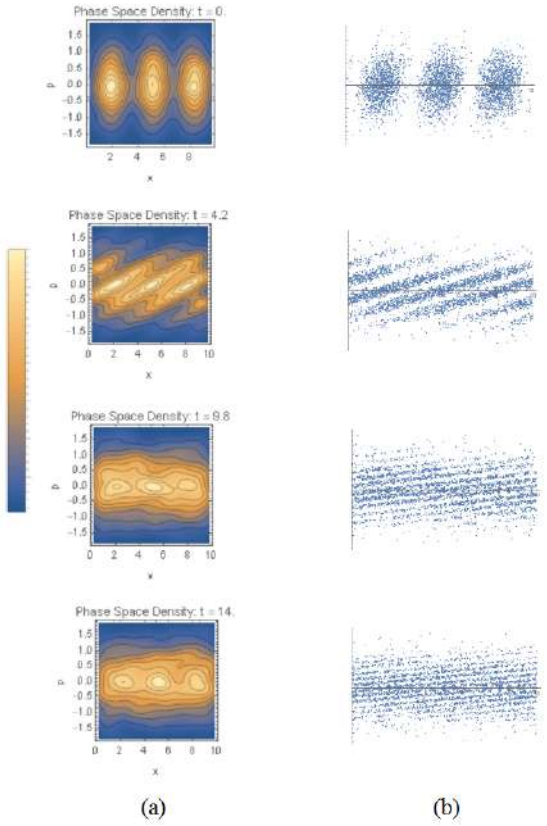

Figure 3.7: **Landau Damping**: (a) Evolution of Distribution Function. (b) Corresponding evolution of particles in phase space

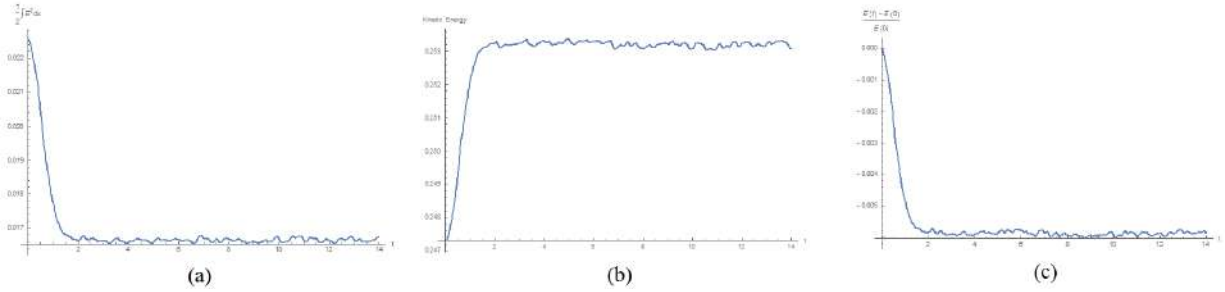

Figure 3.8: **Landau Damping**: (a) Electric Field Energy $U(t)$ (equation 3.2.8). (b) Kinetic Energy $T(t)$ (equation 3.2.7). (c) Fractional Energy Error

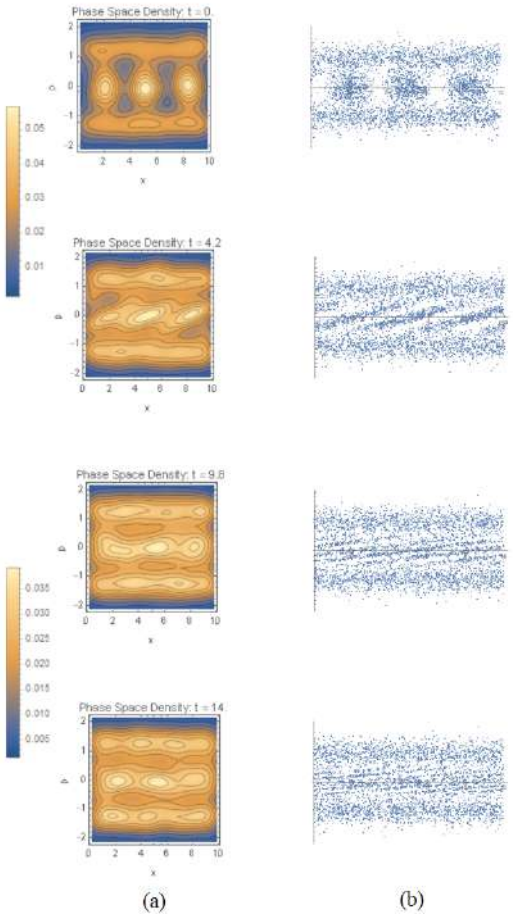

Figure 3.9: **Bump-on-tail Instability**: (a) Evolution of Distribution Function, (b) Corresponding evolution of particles in phase space

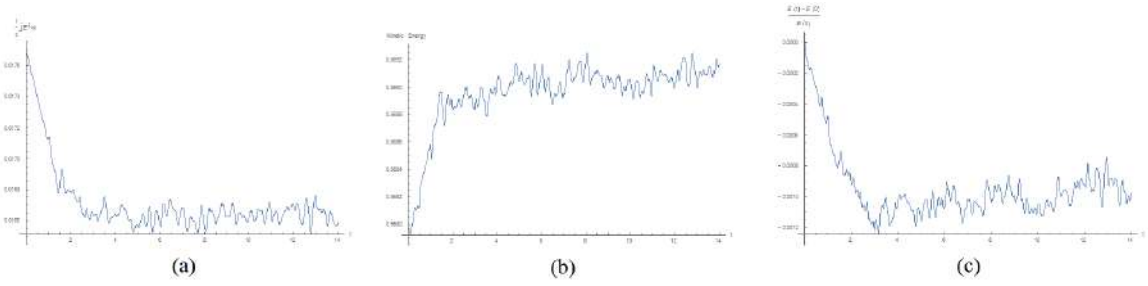

Figure 3.10: **Bump-on-tail Instability**: (a) Electric Field Energy $U(t)$ (equation 3.2.8). (b) Kinetic Energy $T(t)$ (equation 3.2.7). (c) Fractional Energy Error

Example: 2D 2V System

In this example, we consider a plasma in two spatial dimensions with coordinates (x, y) and the corresponding momenta with coordinates (p_x, p_y). The spatial domain is a rectangular interval $[0, 5] \times [0, 2]$ with periodic boundary conditions, or $\mathbb{R}^2/(5\mathbb{Z} \times 2\mathbb{Z})$. In this case, by dimensional reduction, a magnetic field can exist normal to the spatial manifold (meaning the vector potential can only have x and y components, not a normal component).

In particular, due to the introduction of a magnetic field, the interaction between the particles and the fields is now fully electromagnetic and time dependent. This leads to different instabilities than interaction with a pure electric field. For example, if the initial distribution is anisotropic in momentum space (more specifically, not Maxwellian of the form $exp(-\alpha\vec{p}^2)$), an instability arises: a magnetic field is generated which restores the isotropy of the momentum space distribution. This magnetic field generation causes the electromagnetic field energy to become unstable (grow exponentially) until the isotropy of the system is restored. This mechanism is known as the Weibel instability, which for example is responsible for the generation of magnetic fields in astrophysical systems.

To test the Weibel instability, we take an initial distribution function $f(x, y, p_x, p_y, 0) = (1 + cos(2x))exp(-p_x^2 - 0.9p_y^2)$ which is slightly perturbed from an isotropic momentum distribution. The evolution of this system is shown in 3.11. The corresponding instability in the electromagnetic field energy is shown in figure 3.12.

Animations of the evolution of the 1D and 2D systems can be found at Maxwell Vlasov GIFs.

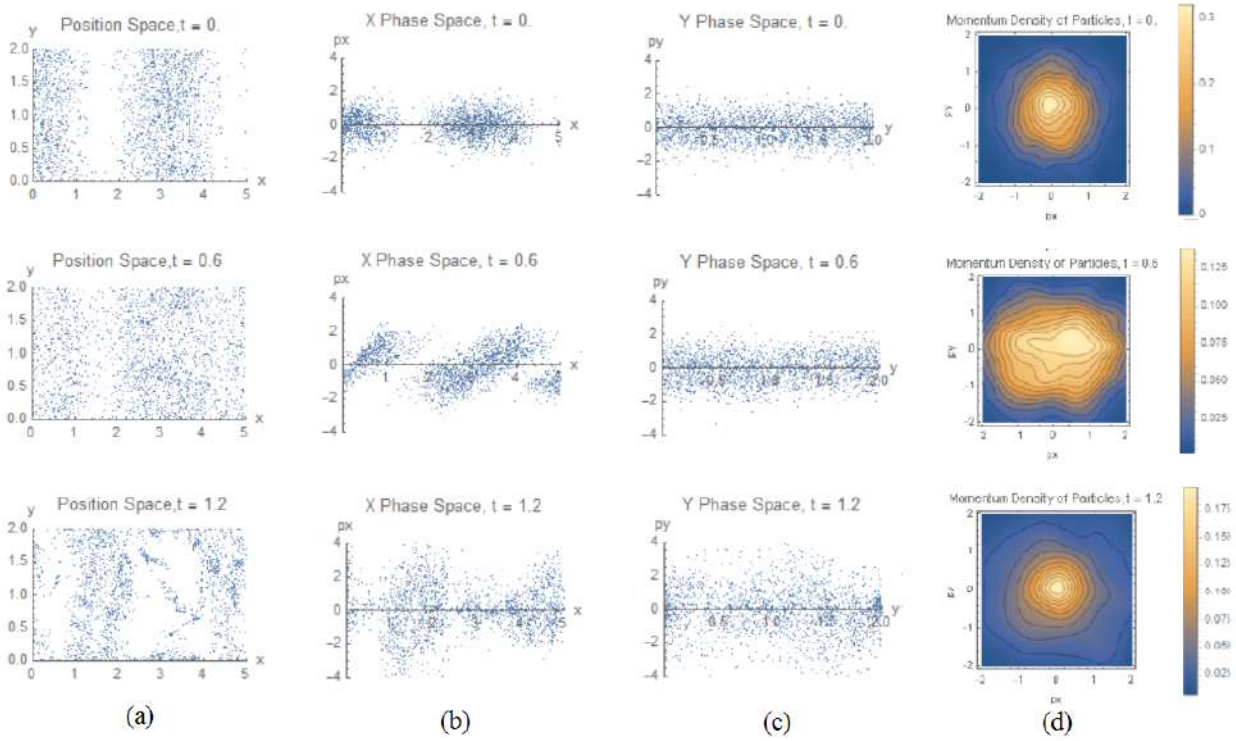

Figure 3.11: **Weibel Instability**: (a) Evolution of particle positions. (b) Evolution in (x, p_x) phase space. (c) Evolution in (y, p_y) phase space. (d) Evolution of momenta density; note the initial anisotropy versus the final isotropy

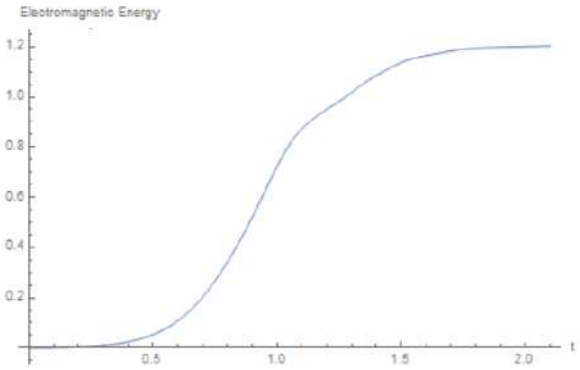

Figure 3.12: **Weibel Instability**: Instability in Electromagnetic Field Energy (equation 3.2.8)

A | Appendix: Lie Groups, Algebras

We briefly review concepts from Lie groups, algebras, and their representations to supplement the material presented in the main paper.

Definition A.0.1 *A **Lie Group** is a group G which has the structure of a differentiable manifold with a differentiable group structure i.e. the maps $(g, g') \mapsto gg'$ and $g \mapsto g^{-1}$ are differentiable for all $g, g' \in G$.*

Let G be a Lie Group with identity e. Consider left translation on by $g \in G$,

$$L_g(g') := gg' \ \forall \ g' \in G.$$

Clearly, by the differentiable group structure on G, L_g is a differentiable map. Furthermore, since $(L_g)^{-1} = L_{g^{-1}}$ is also a differentiable map, L_g is a diffeomorphism from G to itself. We say that a vector field $Z \in \Gamma(TG)$ is left-invariant if $L_{h*}Z|_g = Z|_{hg} \ \forall \ h, g \in G$, where L_{h*} denotes the tangent mapping induced by L_h. Clearly, a linear combination of left-invariant vector fields is left-invariant. Furthermore, the Lie bracket of left-invariant vector fields is left-invariant, where we define the Lie bracket on its action for functions $f \in C^\infty M$,

$$[X, Y]f = X(Y(f)) - Y(X(f)),$$

which is bilinear, anticommutative, and satisfies the Jacobi identiy $[X, [Y, Z]] + [Z, [X, Y]] + [Y, [Z, X]] = 0$. The space of left-invariant vector fields on G, equipped with the Lie bracket, forms the **Lie Algebra** of G, denoted $\mathfrak{g}$. Since the values of left-invariant vector fields are uniquely determined by their value at the identity, $Z|_g = L_{g*}Z|_e$, the Lie algebra structure of $\mathfrak{g}$ is isomorphic to the Lie algebra structure of T_eG, equipped with the bracket

$$[\eta|_e, \zeta|_e] = [\eta, \zeta]_e \ \forall \ \eta, \zeta \in \Gamma(TG).$$

Thus, we can think of the Lie Algebra $\mathfrak{g}$ as T_eG equipped with the above Lie bracket.

As needed in our discussion of Yang-Mills theory, we can equip the Lie Algebra with an inner product. Consider the adjoint representation of $X \in \mathfrak{g}$, ad_X, defined by

$$ad_X(Y) = [X, Y].$$

Then, the **Killing Form** tr' is a map $\mathfrak{g} \times \mathfrak{g} \to \mathbb{R}$ (or more generally a field $\mathbb{K}$ which the Lie algebra is defined over), given by

$$tr'(X, Y) := tr(ad_X \circ ad_Y).$$

Since $tr(AB) = tr(BA)$ and ad is linear, the Killing Form is symmetric and bilinear. Furthermore, if $\mathfrak{g}$ is the Lie algebra of a compact semisimple Lie group, then tr' is negative definite and thus $-tr'$ defines an inner product on $\mathfrak{g}$.

A.1 Representations

One application of the theory of Lie groups is their action on other spaces, i.e. their representations.

Let G be a Lie group and M be a manifold. Then, we say that M carries a **representation** of G if there is a differentiable map

$$\begin{aligned}\rho : G \times M &\to M, \\ G &\to \text{Diff}(M, M),\end{aligned}$$

which is a group homomorphism from G into the group of self-diffeomorphisms of M. Of particular importance for our purposes is a linear representation of G on a vector space V, where ρ is a group homomorphism from G into the general linear group of V, $GL(V)$. Similarly, a representation of the Lie algebra is a group homomorphism $\theta : \mathfrak{g} \to \mathfrak{gl}(V)$. Note that given a Lie group representation ρ on a vector space V, there is an induced Lie algebra representation from the tangent map $\theta = \rho^*$.

Now consider a vector bundle (E, π, M) where the fiber $\pi^{-1}(x)$ carries a representation ρ_x of G for each $x \in M$. We define a **gauge transformation** as a smooth map $\phi : M \to G$. Under a gauge transformation, a field $\Psi \in \Gamma(E)$ transforms as

$$\Psi(x) \overset{\phi}{\mapsto} \rho_x(\phi(x))\Psi(x).$$

The set of gauge transformations forms a group under pointwise multiplication, which we call the **gauge group** of E. Often, as in the main chapters, we do not explicitly write the representation and write the transformation as $\phi(x)\Psi(x)$.

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