The geometric theory of charge conservation
in particle-in-cell simulations

Alexander S. Glasser\(^1\)(*) , and Hong Qin\(^1\)

\(^1\)Department of Astrophysical Sciences, Princeton University, Princeton, New Jersey 08540

In recent years, much effort has been devoted to gauge-symmetric particle-in-cell (PIC) methods whose simulations of particles and electromagnetic fields are exactly charge-conserving. While it is rightly observed that these methods’ gauge symmetry gives rise to their charge conservation, this causal relationship has generally been described in ad hoc derivations of the associated conservation laws. In the following work, we develop a comprehensive theoretical grounding for charge conservation in PIC methods, and demonstrate the systematic derivation of charge conservation laws from the gauge symmetry of both Lagrangian and Hamiltonian algorithms. For variational Lagrangian PIC schemes, we apply Noether’s Second Theorem to demonstrate that gauge symmetry gives rise to a local charge conservation law as an off-shell identity. For Hamiltonian splitting methods, we define gauge-compatible splitting, a classification that determines a sufficient condition for the exact preservation of the momentum map even after time discretization, and which affords splitting schemes a decided advantage over other Hamiltonian integrators. We further apply our theoretical results to define a novel, gauge-compatible, explicit-time-advance, canonical splitting PIC method, whose momentum map yields an exact local charge conservation law. Additionally, we clarify the symplectic reduction and the appropriate initial conditions of such schemes.

1. Introduction

Particle-in-cell (PIC) methods have long been an indispensable tool in studies of theoretical plasma physics, with many algorithmic efforts tailored toward specific applications. (Dawson 1983; Hockney & Eastwood 1988; Birdsall & Langdon 1991; Okuda 1972; Cohen et al. 1982; Langdon et al. 1983; Lee 1983; Cohen et al. 1989; Liewer & Decyk 1993; Friedman et al. 1991; Eastwood 1991; Cary & Decyk 1993; Parker et al. 1993; Grote et al. 1998; Decyk 1995; Qin et al. 2000a,b; Qiang et al. 2000; Chen & Parker 2003; Qin et al. 2001; Vay et al. 2002; Nieter & Cary 2004; Huang et al. 2006) The literature counts several examples, in particular, of PIC methods that have been engineered to exactly conserve charge—(to machine precision)—by the use of various sophisticated numerical techniques. (Villasenor & Buneman 1992; Esirkepov 2001; Chen et al. 2011; Pukhov 2016)

In recent years, elegant PIC methods have been developed that preserve the gauge symmetry of the plasmas they simulate. Such methods exactly conserve charge, not as a result of bespoke numerical methods but as a natural consequence of preserving their systems’ geometric structure. It was Squire et al. (2012) that first derived an exactly-charge-conserving variational PIC scheme by imposing gauge symmetry on a discrete action. Several gauge-symmetric algorithms have since followed, especially in the form of symplectic Hamiltonian PIC schemes. (Xiao et al. 2015; He et al. 2015, 2016; Qin et al. 2016; Kraus et al. 2017; Xiao et al. 2018)

(*) Email address for correspondence: asg5@princeton.edu
Many of these references note that the gauge symmetry of their PIC schemes guarantees exact charge conservation, but this fact is often unproven; the associated conservation laws are not always stated, let alone systematically derived. The absence of such derivations encourages the development of a theoretical understanding of algorithmic conservation laws. In the present paper, we study the theoretical basis for the conservation of charge in Lagrangian variational algorithms and Hamiltonian splitting methods, and derive conservation laws from first principles. In so doing, we elucidate the requirements for gauge-symmetric codes to be charge-conserving, and provide a template for the general derivation of conservation laws in gauge-symmetric Lagrangian and Hamiltonian algorithms.

Our work will be divided between two principal efforts. First, we demonstrate the systematic derivation of an exact charge conservation law for the variational Lagrangian PIC method of Squire et al. (2012). By applying the versatile formalism of Hydon & Mansfield (2011), we demonstrate that its discrete conservation law arises as an off-shell identity as a consequence of Noether’s Second Theorem (N2T). Our effort draws upon the tools of discrete exterior calculus (Desbrun et al. 2005) (DEC), and emphasizes some of the challenges in deriving conservation laws for locally symmetric Lagrangian systems.

Second, we discuss the preservation of the momentum map (Souriau 1970; Marsden & Ratiu 1999)—\( \dot{\mu} = \{\mu, H\} = 0 \)—in gauge-symmetric Hamiltonian PIC methods, and we derive the conservation law that immediately follows from this preservation. We further consider the preservation of \( \mu \) under various discrete time integrators, and classify \textit{gauge-compatible splitting methods}, which guarantee the exact preservation of \( \mu \) and its associated conservation laws. By rigorously demonstrating the exact conservation laws of gauge-compatible splitting methods—even after time-discretization—we highlight a significant advantage of such methods over alternative Hamiltonian integrators.

The remainder of this paper is organized as follows: In Section 2, we follow Hydon & Mansfield (2011) and review the constructive derivation of N2T’s differential identities for a locally symmetric Lagrangian system. In Section 3.1, we apply this construction to the continuous Vlasov-Maxwell system, and in Section 3.2 we reapply it to the variational PIC method defined in Squire et al. (2012). In Section 4, we review the Hamiltonian formulation of the Vlasov-Maxwell system, its momentum map and symplectic reduction. (Marsden & Weinstein 1974, 1982) In Section 5, we demonstrate gauge-compatibility as a sufficient condition for the preservation of momentum maps in Hamiltonian splitting methods. In Section 6, we present a novel, gauge-compatible splitting PIC algorithm, and apply our results to derive its conservation law and its symplectic reduction. In Section 7, we summarize our results and conclude.

2. A Constructive Review of Noether’s Second Theorem

Noether’s First Theorem (N1T) famously establishes a one-to-one correspondence between the symmetries of a Lagrangian density \( L \) and the on-shell conservation laws of its Euler-Lagrange equations. However, for Lagrangians with local gauge symmetry—(i.e., with an infinite-dimensional group of transformations that independently transform each point of spacetime)—such conservation laws are often trivial (Olver 1986), and capture no meaningful information. Noether’s Second Theorem (N2T) addresses such gauge-symmetric Lagrangian systems. In particular, it establishes a one-to-one correspondence between the local gauge symmetries of a Lagrangian and off-shell differential identities of its Euler-Lagrange equations. Such identities may at first appear to be of similarly little use. However, we will show that in variational PIC codes, the local charge conservation law \( \partial_t \rho + \nabla \cdot J = 0 \) is just such an off-shell identity. Applying N2T, we will
systematically derive this charge conservation law from the local gauge symmetry of a discrete Lagrangian.

Local gauge symmetries can be understood to arise from a Lagrangian system’s redundancy, which, as N2T shows, manifests in its equations of motion (EOM) as well. In particular, N2T claims that a Lagrangian system admits a local gauge symmetry if and only if its equations of motion satisfy a differential identity:

\[ D^\alpha E^\alpha_1(L) + \cdots + D^\alpha_q E^\alpha_q(L) = 0 \]  

for some \( \{D^\alpha_i\} \). Here, \( E^\alpha_i(L) \) denotes the EOM of the \( \alpha_i \)th variable (e.g., Maxwell’s equation for \( A_\nu: E^\nu_\alpha(L) = \partial_\mu F^\mu_\nu + J^\nu \) and \( D^\alpha_i \) represents a differential operator (e.g., the Klein-Gordon operator: \( \partial^2 - m^2 \)).

Such an identity as Eq. (2.1) holds off-shell, which is to say that it does not require the EOM to be satisfied in order to be true. Although such differential identities may appear to be of little use—(as any mathematical identity, they are reasonably understood to be without physical content)—they nonetheless reveal valuable information for some Lagrangian systems. It might be said that N1T discovers conservation laws that hold dynamically (on-shell), while N2T discovers differential identities that hold kinematically (off-shell). For discrete systems, whose kinematics are sometimes less apparent or less studied, these differential identities can be especially enlightening.

In the following section, we introduce the reader to the formalism of Hydon & Mansfield (2011) to provide a proof by construction of N2T’s “only if” direction, which readily derives differential identities from the local gauge symmetries of a Lagrangian system. As we shall see, this formalism is extensible to both continuous and discrete systems.

To begin, let us recall the variation of an arbitrary action \( S = \int d^4x L[u, \partial_a u, \ldots] \) for a field \( u \) in flat spacetime with coordinates \( x^\alpha \):

\[ \delta S = \int d^4x \left[ \delta u \frac{\partial L}{\partial u} + \delta(\partial_a u) \frac{\partial L}{\partial(\partial_a u)} + \cdots \right] \]

\[ = \int d^4x \left[ \delta u E_u(L) + D_a \left( \delta u \frac{\partial L}{\partial(\partial_a u)} \right) + \cdots \right]. \]

In the above, we have defined

\[ E_u := \sum_J (-1)^J \frac{\partial}{\partial(\partial_J u)} \]

\[ = \frac{\partial}{\partial u} - D_a \frac{\partial}{\partial(\partial_a u)} + D_{ab} \frac{\partial}{\partial(\partial_{ab} u)} - \cdots \]

as the Euler operator (Olver 1986), which—as shown in Eq. (2.2)—discovers EOM by effectively implementing an integration by parts in the variation of an action. The sum in Eq. (2.3) is taken over all multi-indices \( J \) of spacetime variables—e.g., \( J \in \{ \varnothing, t, xx, yzz, \ldots \} \)—and \( D_{ab} \equiv D_a D_b \), where \( D_a \equiv \frac{d}{dx^a} = \partial_a + u_a \partial_a \) denotes a total derivative. (The notations \( u_a \equiv \partial_a u \equiv \partial u/\partial x^a \) will be used interchangeably.) For a Lagrangian with only first-order derivatives, the EOM of the field \( u \) is thus given by its familiar form:

\[ 0 = E_u(L) = \frac{\partial L}{\partial u} - D_a \left( \frac{\partial L}{\partial u_a} \right). \]

We now allow \( L[u^\alpha, u^\alpha_a, \ldots] \) to depend on multiple fields \( \{u^\alpha(x)\} \) and their derivatives. We suppose that \( L \) is invariant under an infinite group of local gauge transformations, each labeled by an arbitrary smooth function \( g(x) \). We denote the infinitesimal generator
of such a symmetry as a vector field

\[ \mathbf{v}_g = \sum_{\alpha} Q^\alpha[g] \partial_{u^\alpha} \]  

(2.5)

where \( Q^\alpha[g] \) are the so-called characteristics of \( \mathbf{v}_g \), which depend on \( g(x) \) and its derivatives. (We emphasize that the freedom to independently choose \( g(x) \) at each point in spacetime is what makes this symmetry group local. A global symmetry, by contrast, would transform the fields at each point of spacetime identically.)

Because the derivatives \( u_\alpha^J \) must transform in a consistent manner with \( u^\alpha \), \( \mathbf{v}_g \) acts in general via its prolongation (Olver 1986):

\[ \text{pr} \left[ \mathbf{v}_g \right] = \sum_{\alpha,J} \left( D_J Q^\alpha[g] \right) \frac{\partial}{\partial u^J} \]  

(2.6)

Therefore, a Lagrangian is locally gauge-invariant if and only if

\[ \text{pr} \left[ \mathbf{v}_g \right] (\mathcal{L}) = 0 \]  

(2.7)

—that is, if and only if it is infinitesimally invariant under the flow of the vector field generating the transformation.

We now aim to derive N2T from the local gauge invariance condition expressed in Eq. (2.7). We first use the Euler operator of Eq. (2.3) to integrate \( \text{pr} \left[ \mathbf{v}_g \right] (\mathcal{L}) \) by parts. The resulting expression may be explicitly derived (see Olver (1986), Proposition 5.98), but for our purposes it will be sufficient to note that

\[ \text{pr} \left[ \mathbf{v}_g \right] (\mathcal{L}) = \sum_{\alpha} Q^\alpha[g] \mathbf{E}_{u^\alpha}(\mathcal{L}) + \text{Div}A \]  

(2.8)

for some \( A \equiv (A^t, A^x, A^y, A^z) \), where \( \text{Div}A \equiv \sum_a D_a A^a \) denotes a divergence. Combining Eqs. (2.7)-(2.8), we have:

\[ \sum_{\alpha} Q^\alpha[g] \mathbf{E}_{u^\alpha}(\mathcal{L}) = \text{Div}(-A). \]  

(2.9)

This relation is merely a consequence of our Lagrangian’s local gauge symmetry.

Specializing to characteristics \( Q^\alpha[g] \) that are linear in \( g \) and its derivatives, we are now poised to derive the N2T differential identity satisfied by our equations of motion. (Our symmetries will have linear characteristics in this paper, so we proceed with this assumption; the general nonlinear case follows straightforwardly.) We recall that a divergence vanishes under an Euler operator, (in much the same way that a divergence added to a Lagrangian does not alter its equations of motion). That is:

\[ \mathbf{E}_u \circ \text{Div} \equiv 0 \]  

(2.10)

\( \forall \ u \).

We therefore apply the Euler operator \( \mathbf{E}_g \) to Eq. (2.9) to find:

\[ \mathbf{E}_g \left[ \sum_{\alpha} Q^\alpha[g] \mathbf{E}_{u^\alpha}(\mathcal{L}) \right] = 0. \]  

(2.11)

Because \( Q^\alpha[g] \mathbf{E}_{u^\alpha}(\mathcal{L}) \) is assumed linear in \( g \) and its derivatives, this expression is independent of \( g \). It is an off-shell differential identity of the equations of motion; (nowhere
in this derivation has a dynamical equation \( E_{\nu} (\mathcal{L}) = 0 \) been enforced.) Thus concludes the constructive proof of N2T; using the characteristics of a Lagrangian’s local gauge symmetry, the off-shell differential identity of Eq. (2.11) is easily constructed.

Before applying this method to the Vlasov-Maxwell system of interest in Section 3, we make the preceding formalism more concrete with a brief example from the vacuum Maxwell action:

\[
S = \int d^4x \mathcal{L} = - \int d^4x \frac{1}{4} F_{\mu\nu} F^{\mu\nu}. \tag{2.12}
\]

where \( F_{\mu\nu} \equiv \partial_{\mu} A_{\nu} - \partial_{\nu} A_{\mu} \). This action yields the familiar EOM:

\[
0 = E_{A_{\nu}} (\mathcal{L}) = \partial_{\nu} F^{\tau\sigma}. \tag{2.13}
\]

The gauge symmetry of \( A_{\mu} \) is given by:

\[
v_{\lambda} = - (\partial_{\mu} \lambda) \partial_{A_{\mu}}, \tag{2.14}
\]

where \( Q^{A_{\mu}} = - \partial_{\mu} \lambda \). The flow generated by \( v_{\lambda} \) results in the familiar transformation of \( A_{\mu} \):

\[
\exp [v_{\lambda}] A_{\mu} = [1 + \epsilon v_{\lambda} + \cdots] A_{\mu} = A_{\mu} - \epsilon \partial_{\mu} \lambda. \tag{2.15}
\]

Moreover, using Eq. (2.6), the prolongation of this vector field is given by

\[
pr [v_{\lambda}] = - (\partial_{\mu} \lambda) \partial_{A_{\mu}} - (\partial_{\nu} \partial_{\mu} \lambda) \partial_{(\partial_{\nu} A_{\mu})} + \cdots, \tag{2.16}
\]

so it is readily checked that \( \mathcal{L} \) is gauge-invariant, i.e. \( pr [v_{\lambda}] (\mathcal{L}) = 0 \).

Given our EOM in Eq. (2.13) and our symmetry characteristics in Eq. (2.14), we plug in for \( E_{\alpha} (\mathcal{L}) \) and \( Q^{\alpha}[\lambda] \) in Eq. (2.11) to derive our N2T differential identity:

\[
0 = E_{\lambda} \left[ - (\partial_{\sigma} \lambda) \partial_{\tau} F^{\tau\sigma} \right] = \partial_{\sigma} \partial_{\tau} F^{\tau\sigma}. \tag{2.17}
\]

Due to the antisymmetry of \( F^{\mu\nu} \), this N2T identity is rather trivial, and conveys the appropriate sense that N2T generally produces identities lacking in physical content. Nonetheless, we will find in the next section that this procedure can be used to derive the local charge conservation law of the Vlasov-Maxwell system.

3. Noether’s Second Theorem for Vlasov-Maxwell Systems

3.1. The Continuous Klimontovich-Maxwell Model

We now use N2T to derive charge conservation for the continuous Klimontovich-Maxwell system, governed by the following Lagrangian density:

\[
\mathcal{L}[\phi, A, X_i] = \frac{1}{2} (\nabla \phi + \partial_{t} A)^2 - \frac{1}{2} (\nabla \times A)^2 + \sum_{j=1}^{N} \delta_{j} \cdot \left( \frac{1}{2} m_j \dot{X}_j^2 - q_j \phi + q_j A \cdot \dot{X}_j \right). \tag{3.1}
\]

Here, \( A = A(t, x) \) is the vector potential, \( \phi = \phi(t, x) \) is the electric potential, \( X_i = X_i(t) \) are particle positions, and particle mass and charge are denoted by \( m_i \) and \( q_i \), respectively. We have also used the following shorthand for the delta function:

\[
\delta_{j} := \delta^{(3)}(x - X_j(t)). \tag{3.2}
\]
We apply Euler operators to derive the Euler-Lagrange equations of each field:

\[
\begin{align*}
E_\phi(\mathcal{L}) &= \nabla \cdot E - \rho \\
E_A(\mathcal{L}) &= \partial_t E - \nabla \times B + J \\
E_{\mathbf{X}_i}(\mathcal{L}) &= \delta_i \cdot \left[ -m_i \ddot{\mathbf{X}}_i + q_i (E + \ddot{\mathbf{X}}_i \times B) \right]
\end{align*}
\] (3.3)

where we have used the distributional derivative

\[
\int f(\eta) \delta'(\eta) d\eta = -\int f'(\eta) \delta(\eta) d\eta
\] (3.4)

\[\forall \eta \in \{t, x\}\] and where

\[
\begin{align*}
E(t, x) &:= -\nabla \phi(t, x) - \partial_t A(t, x) \\
B(t, x) &:= \nabla \times A(t, x) \\
\rho(t, x) &:= \sum_{j=1}^{N} q_j \delta_j \\
J(t, x) &:= \sum_{j=1}^{N} q_j \dot{\mathbf{X}}_j(t) \delta_j.
\end{align*}
\] (3.5)

As noted above, the Euler operator \(E\) is essentially defined to allow the integration by parts of Eq. (3.4). In particular, total derivatives—such as \((f\delta)'\), or \(\text{Div}A\) above—that contribute to boundary terms of the action integral \(S = \int \mathcal{L} d^4x\)—such as \(f\delta|_{-\infty}^{\infty}\)—lie in the kernel of \(E\).

We now apply the gauge transformation, equivalent to Eq. (2.15),

\[
\begin{align*}
\phi &\rightarrow \phi' = \phi + \partial_t \lambda \\
A &\rightarrow A' = A - \nabla \lambda
\end{align*}
\] (3.6)

for an arbitrary smooth function \(\lambda(x)\). We thus employ the construction of Eq. (2.11) to derive the corresponding differential identity of N2T:

\[
Q^\alpha[\lambda]E_\alpha(\mathcal{L}) = \delta \phi[\lambda] \cdot E_\phi(\mathcal{L}) + \delta A[\lambda] \cdot E_A(\mathcal{L}) = (\partial_t \lambda) [\nabla \cdot E - \rho] - \nabla \lambda \cdot [\partial_t E - \nabla \times B + J]
\] (3.7)

such that

\[
\begin{align*}
0 &= E_\lambda \left[ Q^\alpha[\lambda]E_\alpha(\mathcal{L}) \right] \\
&= -\partial_t [\nabla \cdot E - \rho] + \nabla \cdot [\partial_t E - \nabla \times B + J] \\
&= \partial_t \rho + \nabla \cdot J.
\end{align*}
\] (3.8)

From this derivation, we see that the differential identity of the gauge symmetry of the Klimontovich-Maxwell Lagrangian is the charge conservation law itself.

This derivation reveals that the charge conservation law for point particles holds off-shell and identically; in particular, Eq. (3.8) does not require the equations of motion in order to hold true. It is therefore said to be a strong conservation law. This often-overlooked fact is immediately verified upon examining the definitions of \(\rho\) and \(J\) in Eq. (3.5). In this sense, the distinction between a differential identity and a conservation law is blurred in the VM system.
3.2. The Geometric PIC Method of Squire et al. (2012)

We now study an analogous conservation law derivation for a discrete, gauge-symmetric PIC method defined by Squire et al. (2012). In this PIC scheme, spacetime is discretized by constructing a $d$-dimensional spatial simplicial complex whose structure is constant throughout a uniformly discretized time. The time dimension may be envisaged as forming temporal edges that extend orthogonally from the spatial simplices, as in a triangular prism. We denote this $(d+1)$-dimensional primal complex by $P_C$. We employ DEC (Desbrun et al. 2005) on $P_C$ to define fields that are single-valued on simplices of the complex (or their circumcentric duals). In the present paper, we shall assume a spatial dimensionality $d = 3$.

Because it will be useful to distinguish the spatial edges from the temporal edges of $P_C$, we denote a vertex of $P_C$ by $[i^n]$, where $i$ is the spatial index of the vertex, and $n$ its temporal index. A discrete 0-form $\alpha$ is then defined by its values at each vertex, and a discrete 1-form $\beta$ by its values on each edge:

$$\alpha = \sum_{[i^n]} \alpha_i^n \Delta_i^n,$$
$$\beta = \sum_{i,n} \beta_{i}^{\frac{n-1}{2}} \Delta_{i}^{\frac{n}{2}} + \sum_{[ij],n} \beta_{ij}^{n} \Delta_{ij}^{n}. \quad (3.9)$$

Here we have expressed the discrete forms (equivalently, cochains) $\alpha$ and $\beta$ in terms of their cochain bases where, for example, $\Delta_i^n$ is an element of the 0-cochain basis that maps $[i^n]$ to 1 and all other vertices to 0. $\Delta_{ij}^n$ is similarly an element of the 1-cochain basis that maps the oriented edge $[ij]$ to 1 and all others to 0. (*) Discrete $k$-forms of higher degree may be constructed with cochain bases in essentially the same way. The formalism of cochains will prove useful when we consider variations of dynamical fields defined on $P_C$—that is, when we define an Euler operator for DEC.

The DEC exterior derivative on $k$-forms may be defined (Elcott & Schröder 2005; Desbrun et al. 2006) by a matrix multiplication in the cochain basis, for example:

$$d\beta = d (\beta_e \Delta_e) = \beta_e d\Delta_e = \beta_e W^e_f \Delta_f \quad (3.10)$$

where the matrix entry $W^e_f$ stores the weight—$\{\pm 1, 0\}$—of the 1-cochain $\Delta_e$ in the 2-cochain $\Delta_f$. (***) We denote by $\{v\}$ the set of all vertices, by $\{e\} = \{e_s\} \sqcup \{e_t\}$ the set of spatial and temporal edges, and by $\{f\} = \{f_s\} \sqcup \{f_t\}$ the set of spatial and ‘spatiotemporal’ faces. We adopt the Einstein convention in Eq. (3.10) and hereafter that any such repeated indices are summed over.

Duals to primal $k$-forms are defined in the usual sense of DEC, and the map between primal $k$-forms and dual $(4-k)$-forms is effected via the metric-dependent Hodge star operator, $\star$. We adopt a $(-+++)$ convention for our Lorentzian metric $\eta$ with index (Abraham et al. 1988) $\text{Ind}(\eta) = 1$, such that given some arbitrary chain $\sigma$ of dimension $k$, (alternatively written $\sigma^k$):

$$\langle \star \alpha, \star \sigma \rangle = \epsilon(\sigma) \frac{|\star \sigma|}{|\sigma|} \langle \alpha, \sigma \rangle, \quad (3.11)$$

(*) A temporal edge is understood to be oriented in the positive time direction, and its cochain is notated by $\Delta_i^{n-\frac{1}{2}}$.

(**) Note, the boundary operator $\partial$ is determined by $W^f_e = (W^e_f)^T$. 


where

\[ \epsilon(\sigma) = \begin{cases} +1 & \text{if } \sigma \text{ is entirely spacelike} \\ -1 & \text{otherwise.} \end{cases} \]  

(3.12)

Here, \(|\sigma^k|\) is the \(k\)-volume of \(\sigma^k\) (where \(|\sigma^0| = 1\) for a single vertex), and \(\langle \cdot, \cdot \rangle\) denotes a \(k\)-cochain evaluated on a \(k\)-chain.

The electromagnetic gauge field \(A\)—a discrete 1-form defined on all edges of \(P_C\)—neatly splits in the primal complex into an electric potential \(\phi^i_{n-\frac{1}{2}} := -A^i_{n-\frac{1}{2}}\) and a vector potential(*) \(A^{ij}_{n} := A^{ij}_{n}\), as follows:

\[ A = -\sum_{i,n} \phi^i_{n-\frac{1}{2}} \Delta^i_{n-\frac{1}{2}} + \sum_{[ij],n} A^{ij}_{n} \Delta^i_{n} \]  

(3.13)

We now restate the discrete action of Squire et al. (2012) on \(P_C\):

\[ S = \sum_{V_{\sigma^2}} \frac{1}{2} dA \wedge \star dA + \sum_{p,n} \left\{ \frac{h}{2} m_p \left[ \frac{X^p_{n+\frac{1}{2}} - X^p_{n-\frac{1}{2}}}{h} \right]^2 \right\} \]

\[ - q_p \sum_i \phi^i_{n-\frac{1}{2}} \varphi_i \left( \frac{X^p_{n-\frac{1}{2}}}{h} \right) \]

\[ + q_p \left( \frac{X^p_{n+\frac{1}{2}} - X^p_{n-\frac{1}{2}}}{h} \right) \cdot \sum_{[ij]} A^{ij}_{n} \int_{n-\frac{1}{2}}^{n+\frac{1}{2}} dt \varphi_{ij}(X^p(t)) \} \].

(3.14)

In Eq. (3.14), we have denoted a sum over support volumes \(V_{\sigma^2}\) for the primal-dual 4-form \(dA \wedge \star dA\). \(V_{\sigma^2}\) represents the convex hull of the 2-chain \(\sigma^2\) and its dual \(\star \sigma^2\) on which \(\langle dA, \sigma^2 \rangle\) and \(\langle \star dA, \sigma^2 \rangle\) are respectively defined. (Desbrun et al. 2005) The symbol \(h\) denotes the time-step, \(n\) the time index and \(p\) the particle index. \(X^p(t)\) is defined as the constant velocity path between the particle’s staggered-time positions \(X^p_{n-\frac{1}{2}}\) and \(X^p_{n+\frac{1}{2}}\). In particular, particle paths are chosen to have straight line trajectories between the staggered times \(t \in [(n - \frac{1}{2})h, (n + \frac{1}{2})h]\), \(\forall \ n \in \mathbb{Z}\).

The Whitney 0-form \(\varphi_i(x)\) and 1-form \(\varphi_{ij}(x)\) interpolate \(\phi\) and \(A\) to an arbitrary point \(x \in P_C\). (Bossavit 1988) In effect, the Whitney forms \(\varphi\) complete the spatial components of the cochain bases \(\Delta\) adopted in Eq. (3.9) by extending DEC forms to the convex hull of \(P_C\). In the continuous spacetime of the Klimontovich-Maxwell system, the everywhere-defined gauge fields \(\phi(t, x)\) and \(A(t, x)\) were ‘attached’ to point particles by the delta function. In the primal complex \(P_C\), Whitney forms play this role by interpolating the gauge fields to the locations of point particles. Likewise, while we continue to avoid ascribing any geometric notion to point particles themselves, we see that Whitney forms on \(P_C\) attach geometry to the charge densities and currents of the particles, as did the delta function in Eq. (3.5).

To assist our derivation of the EOM from the action of Eq. (3.14), it is helpful to introduce some additional formalism. We note that integration by parts may be facilitated on \(P_C\) via the coderivative operator, \(\delta\). Up to boundary contributions, \(\delta\) is a formal adjoint

(*) We emphasize that there are no components of the single-valued simplicial vector potential \(A\), and its bold notation is only suggestive. On the other hand, its Whitney interpolant coordinatizes \(\mathbb{R}^3\), and thereby extends \(A\) to a 3-component vector field, as we shall see.
to $d$, that is:

$$(d\alpha, \beta)\mu = (\alpha, \delta\beta)\mu + d(\alpha \wedge \ast \beta)$$  \hfill (3.15)$$

for $\mu$ the volume top form. (Arnold et al. 2006) When acting on a $k$-form defined on a general pseudo-Riemannian $n$-dimensional complex, $\delta$ is given by (Desbrun et al. 2006; Abraham et al. 1988):

$$\delta = (-1)^{n(k-1)+1+\text{Ind}(\eta)} \ast d \ast .$$  \hfill (3.16)$$

The Hodge star is defined such that the symmetric inner product $(\cdot, \cdot)$ of Eq. (3.15) satisfies

$$(\omega, \nu)\mu = \omega \wedge \ast \nu$$  \hfill (3.17)$$

for primal $k$-cochains $\omega$ and $\nu$, from which it can be shown:

$$\ast (\ast \omega) = (-1)^{k(n-k)+\text{Ind}(\eta)} \omega.$$  \hfill (3.18)$$

In what follows, we will take the boundary term of Eq. (3.15) to vanish, since any such term is excluded from the variational derivative. (This choice mirrors our treatment of the distributional derivative in the Klimontovich-Maxwell system of Eq. (3.3).) We further leverage Eqs. (3.15) and (3.17) to re-express wedge products where desirable.

For an action $S$ defined on $P_C$, let us suppose that a form $\alpha$ is defined on a face corresponding to a cochain basis element $\Delta_i$ of arbitrary dimension. Then the Euler operator $E_{\alpha_i}$ of $\alpha$ on $\Delta_i$ is defined simply by:

$$E_{\alpha_i} := \frac{\partial S}{\partial \alpha_i} = \frac{\partial}{\partial \alpha_i} \sum L.$$  \hfill (3.19)$$

As usual we assume that all fields have compact support, such that any divergence term in $L$—that contributes to $\sum L$ only at the boundary—vanishes under $E_{\alpha_i}$. This Euler operator is the DEC counterpart of the continuous operator defined in Eq. (2.3).

As a final observation, we note that we can express $dA$ as:

$$dA = d(-\phi_{e_t} \Delta_{e_t} + A_{e_s} \Delta_{e_s})$$

$$= -\phi_{e_t} d\Delta_{e_t} + A_{e_s} d\Delta_{e_s}$$

$$= \left( -\phi_{e_t} W_{f_t}^{e_t} + A_{e_s} W_{f_s}^{e_s} \right) \Delta_{f_t} + A_{e_s} W_{f_s}^{e_s} \Delta_{f_s}$$

$$= E \wedge dt + B$$

$$= F$$  \hfill (3.20)$$

where we have made use of the 1-form $dt := \sum_{e_t} \Delta_{e_t}$ and implicitly defined the spatial 1- and 2-forms $E$ and $B$, respectively, and the Faraday 2-form $F$. (Stern et al. 2015)

Applying Eqs. (3.15)-(3.20), we thus derive the gauge field EOM from the action of Eq. (3.14):

$$E_{\phi_{e_t}} = \Delta_{e_t} \wedge d \ast dA - \rho_{e_t}$$  \hfill (3.21a)$$

$$E_{A_{e_s}} = -\Delta_{e_s} \wedge d \ast dA + J_{e_s}$$  \hfill (3.21b)$$
where
\[
\rho_{e_t} := \sum_p q_p \varphi(t) \left( X^p_{t(e_t)} \right) \\
J_{e_s} := \sum_p q_p \left( \frac{X^p_{t_f(e_s)} - X^p_{t_i(e_s)}}{h} \right) \cdot \int_{t_i(e_s)}^{t_f(e_s)} dt \varphi_{e_s}(X^p(t)) .
\]

(3.22)

Above, \(X^p_{t(e_t)}\) denotes the position of particle \(p\) at the time coincident with the staggered midpoint \(\left[ i \cdot \frac{n}{2} \right]\) of \(e_t\), and \(X^p_{t_i(e_s)}\) and \(X^p_{t_f(e_s)}\) denote the particle position coincident with the staggered midpoints \(\left[ i \cdot \frac{n}{2} \right]\) and \(\left[ i \cdot \frac{n+1}{2} \right]\), before and after the \(t = n\) time slice containing \(e_s\), respectively. As in the above discussion of integration by parts, we have substituted \(\alpha \wedge \beta \delta \beta\) for \(d \alpha \wedge \beta \beta\) where appropriate in the derivations of these EOM.

Before deriving a charge conservation law from the above EOM, it is worth pausing to interpret them. We first observe that the primal-dual wedge product in Eq. (3.21a) is only nonvanishing on the spatial \(*\Delta e_t\) component of \(d * dA\). This follows from the definition of the primal-dual wedge product, which is only nonzero on the convex hulls of a cell and its dual: \(CH(\sigma, *\sigma)\). Reading off from Eq. (3.20), therefore, Eq. (3.21a) becomes
\[
dD \wedge \Delta e_t = \Delta e_t \wedge d * (E \wedge dt) = \rho_{e_t} \tag{3.23}
\]
—Gauss’s law for the electric displacement dual 2-form \(D\), as expected. An analogous interpretation of Eq. (3.21b) yields a simplicial Ampère-Maxwell EOM.

We have omitted the \(E_{X^p}\) EOM for particle trajectories, as they will not be necessary for the derivation of charge conservation via N2T—just as they were unnecessary in Eq. (3.8). These implicit-time-step particle EOM are derived in Squire et al. (2012).

At last, we examine a local gauge transformation of the form \(A \rightarrow A - df\) defined by:
\[
\phi^i_n + \frac{1}{2} \rightarrow \phi^i_n + \frac{1}{2} + \delta \phi^i_n + \frac{1}{2} = \phi^i_n + \frac{1}{2} + \left( f^i_{n+1} - f^i_n \right) \\
A^i_n \rightarrow A^i_n + \delta A^i_n = A^i_n - \left( f^i_n - f^i_n \right) .
\]

(3.24)

where \(f\) is an arbitrary primal 0-form on \(P_C\).

Following the N2T construction of Eq. (2.11), then:
\[
Q^\alpha[f] E_{\alpha} = \delta \phi_{e_t}[f] : E_{\phi_{e_t}} + \delta A_{e_s}[f] : E_{A_{e_s}} \\
= \left( d_{e_t} f \right) \cdot \left( \Delta e_t \wedge d * dA - \rho_{e_t} \right) \\
+ \left( -d_{e_s} f \right) \cdot \left( - \Delta e_s \wedge d * dA + J_{e_s} \right) \tag{3.25}
\]

where \(d_{e_t} f\) denotes the oriented difference of the 0-form \(f = f_v \Delta e\) across edge \(e\). We now observe that
\[
(d_{e_t} f) \Delta e = d(f_v \Delta e) , \tag{3.26}
\]
so applying the Euler operator for $f_v$ at vertex $v = [i]$ to Eq. (3.25) yields:

$$0 = E_{f_v} \left[ Q^\alpha [f] E_\alpha \right]$$

$$= \Delta_v \land \star \delta \land \mathbf{d} \land \mathbf{d} A + \left( \rho_{n+\frac{1}{2}}^i - \rho_{n-\frac{1}{2}}^i \right) + \sum_j J_{[ij]}$$

$$= \left( \rho_{n+\frac{1}{2}}^i - \rho_{n-\frac{1}{2}}^i \right) + \sum_j J_{[ij]} .$$

(3.27)

The last equality of Eq. (3.27) yields the desired charge conservation law on $P_C$. As a result of N2T, this conservation law is guaranteed to be an off-shell differential identity, as was Eq. (3.8). We readily verify this fact as follows.

First, we restrict our sources $\rho$ and $J$ to a particle of charge $q$ whose path over one timestep remains within a single spatial tetrahedron; the general case follows without significant alteration. We then recall that the Whitney 0-form $\varphi_i$ interpolates from vertex $i$ via barycentric coordinates such that, over the tetrahedron $[ijk\ell]$,

$$\varphi_i + \varphi_j + \varphi_k + \varphi_\ell = 1 .$$

(3.28)

In vector form, the 1-form $\varphi_{ij}$ is then defined by:

$$\varphi_{ij} = \varphi_i \nabla \varphi_j - \varphi_j \nabla \varphi_i .$$

(3.29)

Summing over three spatial edges terminating on vertex $i$ of the tetrahedron containing the particle, therefore:

$$\sum_{j \neq i} \varphi_{ij} = \varphi_i \nabla \left( \sum_{j \neq i} \varphi_j \right) - \left( \sum_{j \neq i} \varphi_j \right) \nabla \varphi_i$$

$$= \varphi_i \nabla (1 - \varphi_i) - (1 - \varphi_i) \nabla \varphi_i$$

$$= -\nabla \varphi_i .$$

(3.30)

It follows, then, that:

$$\sum_j J_{[ij]} = q \left( \frac{X_f - X_i}{h} \right) \cdot \int_{t_i}^{t_f} \mathbf{d} \sum_j \varphi_{ij} (\mathbf{X}(t))$$

$$= -q \left( \frac{X_f - X_i}{h} \right) \cdot \int_{t_i}^{t_f} \mathbf{d} \nabla \varphi_i (\mathbf{X}(t))$$

$$= -q \int_{t_i}^{t_f} \mathbf{v} \cdot \mathbf{d} \varphi_i$$

$$= -q [\varphi_i (X_f) - \varphi_i (X_i)]$$

(3.31)

where $\mathbf{v} \cdot \mathbf{d} \varphi_i$ is the interior product of the exact form $\mathbf{d} \varphi_i$ with respect to the velocity $\mathbf{v} := \frac{1}{h}(X_f - X_i)$, which is constant over a single timestep of the particle. Upon comparison with the definition for $\rho$ in Eq. (3.22), it is clear that Eq. (3.27) holds off-shell, as desired. The N2T formalism of Hydon & Mansfield (2011) has succeeded in deriving the intended off-shell, discrete conservation law.
4. The Momentum Map and Symplectic Reduction of the Vlasov-Maxwell System

Having derived the charge conservation laws of continuous and discrete Vlasov-Maxwell Lagrangian systems in the formalism of N2T, we now turn to the canonical derivation of conservation laws from the gauge symmetry of Hamiltonian PIC systems. To proceed, we first review the symplectic structure of the Vlasov-Maxwell system, first discovered in Morrison (1980) and corrected thereafter in Marsden & Weinstein (1982). Closely following this latter reference, we review the Marsden-Weinstein symplectic reduction (Marsden & Weinstein 1974) of the Vlasov-Maxwell system, which ‘spends’ the system’s gauge symmetries in order to eliminate their associated redundant (gauge) degrees of freedom. In so doing, the local charge conservation law of this Hamiltonian system is revealed via the momentum map, as we will discuss at length. The following section is intended to be a concise pedagogical summary of Marsden & Weinstein (1982), with additional discussion relevant to the more recent plasma physics literature.

4.1. The Symplectic Structure of the Vlasov-Maxwell System

We first recall the Poisson bracket of Marsden & Weinstein (1982) of the (unreduced) Vlasov-Maxwell system,

$$\{\{F,G\}\}[f, A, Y] = \int dxdp f \left\{ \frac{\delta F}{\delta f}, \frac{\delta G}{\delta f} \right\}_{xp} \times p + \int dx \left( \frac{\delta F}{\delta A} \cdot \frac{\delta G}{\delta Y} - \frac{\delta G}{\delta A} \cdot \frac{\delta F}{\delta Y} \right)$$

(4.1)

with time evolution defined by the Hamiltonian

$$H[f, A, Y] = \frac{1}{2} \int f \cdot |p - A|^2 dxdp + \frac{1}{2} \int \left[ |Y|^2 + |\nabla \times A|^2 \right] dx.$$  

(4.2)

Above, \(F\) and \(G\) represent arbitrary functionals of the distribution function \(f(x, p)\), the 3-component vector potential \(A(x)\) and its conjugate momentum \(Y(x)\). We will see that the covector \(Y\) will be readily identified as negative the electric field strength—\((Y = -E)\)—by deriving Hamilton’s equations of motion from Eqns. (4.1)-(4.2). We note that our fields are rendered in the temporal gauge, wherein the electric potential satisfies \(\phi(x) = 0\).

The \(\int dxdp f\{\delta f, \delta f\}_{xp}\) operator in the first line of Eq. (4.1) is a Lie-Poisson bracket (Marsden & Weinstein 1982; Marsden & Ratiu 1999), which defines a Poisson structure for functions on a dual Lie algebra \(g^*\), as we now describe.

The Lie-Poisson bracket on a general dual Lie algebra \(g^*\) is defined to inherit the bracket \([\cdot, \cdot]\) of its underlying Lie algebra \(g\) as follows:

$$\{F,G\}(\alpha) := - \left\langle \alpha, \left[ \frac{\delta F}{\delta \alpha}, \frac{\delta G}{\delta \alpha} \right] \right\rangle.$$  

(4.3)

The bracket of Eq. (4.3) is defined \(\forall F, G \in \mathcal{C}^\infty (g^*)\) with respect to some fixed \(\alpha \in g^*\), where \(\langle \cdot, \cdot \rangle\) represents the linear pairing of elements of \(g^*\) and \(g\). The functional derivative \(\delta F/\delta \alpha \in g^{**}\) can be seen to define a linear function on \(g^*\), in that it acts akin to a tangent
map $T_\alpha F$ for the functional $F$ at the "point" $\alpha$. In particular, for arbitrary $\beta \in g^*$:

$$\langle \beta, \frac{\delta F}{\delta \alpha} \rangle = T_\alpha F \cdot \beta. \quad (4.4)$$

(In understanding $\beta \in g^*$ in this way, we have loosely identified the vector space $g^*$ with its own tangent space. Our definition is equivalent to a Fréchet derivative.) Since $g^{**} \cong g$, the functional derivative is interpreted as an element of the Lie algebra. This construction of the Lie-Poisson structure is nondegenerate, and can be shown to be equivalent to the Kostant-Kirillov canonical symplectic form (Silva 2001; Marsden & Weinstein 1982) on the coadjoint orbits of $g^*$.

In the present context, the Lie algebra $g$ corresponds to infinitesimal canonical transformations of $(x, p) \cong \mathbb{R}^6$, the position-momentum phase space. Such transformations can be regarded as Hamiltonian vector fields on $\mathbb{R}^6$, which map via anti-homomorphism to their corresponding generating functions, i.e.

$$[X_h, X_k] = \{-h, k\}_{xp}. \quad (4.5)$$

The bracket $\{\cdot, \cdot\}_{xp}$ therefore serves as a Lie bracket, defined pointwise on $\mathbb{R}^6$:

$$\{h, k\}_{xp} := \left( \partial_x h \cdot \partial_p k - \partial_x k \cdot \partial_p h \right). \quad (4.6)$$

The dual Lie algebra $g^*$ is then identified by distribution densities on $\mathbb{R}^6$, which pair linearly to Hamiltonian functions via integration:

$$\langle f, h \rangle := \int f \cdot h \, dx dp \quad (4.7)$$

for $f \in g^*, h \in g$.

In this way, the operator $\int dx dp \, f \{\delta f, \delta f\}_{xp}$ comprising the first term of Eq. (4.1) is seen to be a Lie-Poisson bracket of the form in Eq. (4.3). We note that the negative sign of Eq. (4.3) cancels with the negative sign of the anti-homomorphism of Eq. (4.5) to produce this first term.

The second term of Eq. (4.1) represents the electromagnetic "sector" of our symplectic structure, and derives from the canonical Poisson structure on the cotangent space—$T^*Q = \{(A, Y)\}$—of the configuration space $Q = \{A\}$. As a result, the dynamical setting of the unreduced Vlasov-Maxwell system is a symplectic manifold, given by:

$$M = g^* \times T^*Q. \quad (4.8)$$

We now consider dynamics on the symplectic manifold $M$. To derive our Hamiltonian EOM, it is convenient to define functionals:

$$F(u) := \int du' F(u') \delta(u - u') \quad (4.9)$$

for $F \in \{f, A, Y\}$ as in Kraus et al. (2017), where $u = (x, p)$ or $u = x$, as appropriate. Plugging such functionals into Eqs. (4.1)-(4.2), we find:

$$\dot{f}(x, p) = \{\{f, H\}\} = -\left[ \partial_x f + \partial_p f \cdot (\nabla A) \right] \cdot (p - A)$$

$$\dot{A}(x) = \{\{A, H\}\} = Y$$

$$\dot{Y}(x) = \{\{Y, H\}\} = \int f \cdot (p - A) \, dp - \nabla \times \nabla \times A. \quad (4.10)$$

For convenience, we note that the familiar form of the Vlasov equation may be
recovered from the first line of Eq. (4.10) by defining a distribution density \( \tilde{f} \) on \( (x, v) \) space where \( v = p - A \), i.e.

\[
f(x, p) = \tilde{f}(x, p - A) = \tilde{f}(x, v),
\]

(4.11)
such that \( \partial_x f = \partial_x \tilde{f} - (\nabla A) \cdot \partial_v \tilde{f} \); \( \partial_p f = \partial_p \tilde{f} \); and \( \dot{f} = \partial_t \tilde{f} - \dot{A} \cdot \partial_v \tilde{f} \). Here, we use \( \nabla \equiv \partial_x \) interchangeably, and adopt the dyad convention

\[
v \cdot AB \cdot w = v_i A_i B_j w_j
\]

(4.12)
in Einstein notation.

### 4.2. Gauge Symmetry and the Momentum Map

With our symplectic and Hamiltonian structures in hand, we now examine the gauge symmetry of the Vlasov-Maxwell system. Continuing to follow Marsden & Weinstein (1982), we define a group action \( \Phi_\psi : M \to M \) on our symplectic manifold \( M = g^* \times T^*Q \) of the form:

\[
\Phi_\psi : (f, A, Y) \mapsto \left(f \circ \tau_\psi, \ A - \nabla \psi, \ Y\right),
\]

(4.13)

where

\[
\tau_\psi(x, p) := (x, p + \nabla \psi).
\]

(4.14)

We emphasize that \( \Phi_\psi \) transforms \( f \), and not \( p \) itself. It is straightforward to check that \( \Phi_\psi \) is a canonical transformation, i.e. that the Poisson bracket is preserved by its pullback: \( \Phi_\psi^* \{\{F, G\}\} = \{\{\Phi_\psi^* F, \Phi_\psi^* G\}\} \).

We define such an arbitrary function \( \psi \in F \) as belonging to the group \( F := C^\infty(\mathbb{R}^3) \) of smooth functions on \( \mathbb{R}^3 \), with a group composition law of addition. Its Lie algebra \( \mathfrak{f} \) is also identifiable as the smooth functions on \( \mathbb{R}^3 \), while its dual \( \mathfrak{f}^* \) is the set of densities over \( \mathbb{R}^3 \) that pair to elements of \( \mathfrak{f} \) via integration over \( \mathbb{R}^3 \), analogous to the \( \mathbb{R}^6 \) integration of Eq. (4.7).

We therefore seek a momentum map for the group action of Eq. (4.13). We denote by \( \phi \in \mathfrak{f} \) the Lie algebra generator of an arbitrary group element \( \psi \in F \). To any such \( \phi \), we may associate a corresponding vector field \( \phi_M \) on \( M \), namely:

\[
\phi_M := \frac{d}{d\epsilon} \bigg|_{\epsilon=0} \Phi_{\exp(\epsilon\phi)}.
\]

(4.15)

\( \phi_M \) is, therefore, the infinitesimal generator of the group action on \( M \) corresponding to \( \phi \).

The momentum map \( \mu : M \to \mathfrak{f}^* \) of our group action is then defined such that, \( \forall \phi \in \mathfrak{f}, \) the function

\[
\mu_\phi : M \to \mathbb{R}
\]

\[
m \mapsto \langle \mu(m), \phi \rangle
\]

(4.16)
satisfies

\[
\{\{F, \mu_\phi\}\} = \phi_M(F)
\]

(4.17)
\( \forall \ m \in M \text{ and } F \in C^\infty(M) \). That is, \( \mu \) assigns an element of \( \mathfrak{f}^* \) to each point of \( M \), such that, when everywhere paired with an element \( \phi \in \mathfrak{f} \) of the Lie algebra, the resulting function \( \mu_\phi \) on \( M \) is a generating function of the associated vector field \( \phi_M \). We comment that a single point \( m \in M \) specifies \( (f, A, Y) \) over the entire \( (x, p) \) phase space.
Given the group action defined in Eqs. (4.13)-(4.14), we may express $\phi_M$ as the following infinitesimal operator on $M$ corresponding to $\phi(x) \in \mathfrak{f}$:

$$\left\{\cdot, \mu^\phi\right\} = \int dx dp \ \nabla \phi \cdot \frac{\partial f}{\partial p} \delta \frac{\delta f}{\delta A} - \int dx \ \nabla \phi \cdot \frac{\delta}{\delta A}$$  \hspace{1cm} (4.18)

Upon inspection, it is evident that to generate the operator of Eq. (4.18), the Poisson bracket of Eq. (4.1) requires that $\mu^\phi$ be given by

$$\mu^\phi(m) := (\mu(m), \phi)$$

$$= \int dx \left[ \int dp \ f(x, p) + \nabla \cdot Y \right] \phi(x).$$  \hspace{1cm} (4.19)

Therefore, the linear momentum map in $\mathfrak{f}^*$ must be given by:

$$\mu(m) = \int dp \ f(x, p) + \nabla \cdot Y$$

$$:= \rho + \nabla \cdot Y,$$  \hspace{1cm} (4.20)

where $\rho := \int f \ dp$. We note that $\mu^\phi : M \rightarrow \mathbb{R}$ is real-valued while $\mu(m) \in \mathfrak{f}^*$ is a density on $\mathbb{R}^3$, as desired.

As a final comment, we note that $\mu$ is group-equivariant:

$$\mu \circ \Phi_{\psi} = \text{Ad}_{\psi^{-1}}^* \circ \mu,$$  \hspace{1cm} (4.21)

where $\text{Ad}_{\psi^{-1}}^*$ represents the coadjoint action (Marsden & Ratiu 1999) of $\psi \in \mathcal{F}$ on an element of $\mathfrak{f}^*$. In particular, it is clear by inspection of Eq. (4.20) that $\mu$ is invariant under $\mathcal{F}$ transformations.

### 4.3. Deriving the Conservation Law

The momentum map canonically derives our conservation law. To show this, we first note that $\Phi_{\psi}$ leaves the Hamiltonian invariant: $\Phi_{\psi}^* H = H$. By differentiating this expression with respect to $\psi$ as in Eq. (4.15), it is seen that, infinitesimally:

$$0 = \phi_M(H) = \left\{\{H, \mu^\phi\}\right\} = -\left\{\mu^\phi, H\right\} = -\dot{\mu}^\phi.$$  \hspace{1cm} (4.22)

Each linearly independent $\phi \in \mathfrak{f}$ therefore determines a unique first integral of the system—i.e., $\mu^\phi$.

We can make a stronger observation as well. Since $\dot{\mu}^\phi = 0$ holds for arbitrary $\phi \in \mathfrak{f}$, the entire momentum map is invariant under the flow of $H$—that is:

$$\dot{\mu} = \left\{\mu, H\right\} = 0.$$  \hspace{1cm} (4.23)

This follows rigorously from the fundamental lemma of variational calculus applied to $\dot{\mu}^\phi$ via Eq. (4.19). As a result, we apply the definition of Eq. (4.20) to derive:

$$0 = \dot{\mu} = \dot{\rho} + \nabla \cdot \dot{Y}.$$  \hspace{1cm} (4.24)

This completes the canonical derivation of the Vlasov-Maxwell local conservation law—$\dot{\mu} = 0$—in the continuous Hamiltonian formalism. We note that, recognizing $Y$ as negative the electric field, Eq. (4.24) is a time evolution of Gauss’s law.

With an additional substitution to Eq. (4.24) from the EOM for $\dot{Y}$ in Eq. (4.10), we find the familiar form of the local charge conservation law:

$$0 = \dot{\rho} + \nabla \cdot J,$$  \hspace{1cm} (4.25)

where $J := \int f \cdot (p - A) dp$. Here $\rho$ and $J$ are (scalar and vector) densities over $\mathbb{R}^3$ and...
functionals in the sense of Eq. (4.9). This conservation law may be immediately checked by substituting the expression for \( \dot{f} \) from Eq. (4.10). In the present Hamiltonian context, it is evident that Eq. (4.25) can no longer be regarded as an off-shell identity. (After all, time evolution itself is only ‘dynamically defined’, so to speak, by the Hamiltonian.)

4.4. Symplectic Reduction of the Vlasov-Maxwell System

Finally, with the momentum map specified, we undertake the Marsden-Weinstein symplectic reduction of the Vlasov-Maxwell system. We first consider the preimage of any \( \alpha \in \mathfrak{f}^* \) under \( \mu \), that is: \( \mu^{-1}(\alpha) \subset M \). We then take equivalence classes of this preimage under the full action of \( \Phi_\psi \forall \psi \in \mathcal{F} \). That is, we reduce our symplectic manifold \( M \) to the quotient manifold \( M^{-1}(\alpha)/\mathcal{F} \), and thereby take a “slice” of the orbit of \( \mu^{-1}(\alpha) \) under the action of \( \mathcal{F} \). Because \( \mu \) is equivariant in the sense of Eq. (4.21), this quotient is well-defined. As is proven in Marsden & Weinstein (1974), the reduced manifold \( M^{-1}(\alpha)/\mathcal{F} \) is again symplectic.

Let us consider the particular case \( \alpha = 0 \), and define \( M_0 := \mu^{-1}(0) \). By Eq. (4.20), \( M_0 \) then corresponds to the submanifold of \( M \) on which \( \rho = -\nabla \cdot \mathbf{Y} \). We now take equivalence classes of \( M_0 \) under the orbit of \( \mathcal{F} \) by defining new phase space coordinates that are invariant under the action of Eq. (4.13), namely:

\[
\tilde{f}(x, v) = f(x, p = v + A) \\
\mathbf{B} = \nabla \times \mathbf{A} \\
\mathbf{E} = -\mathbf{Y}.
\] (4.26)

We therefore identify the manifold of equivalence classes \( \tilde{M}_0 := M_0/\mathcal{F} \) with the manifold \((\tilde{f}, \mathbf{B}, \mathbf{E})\) of densities \( \tilde{f} \) defined on \((x, v)\) space, vector fields \( \mathbf{B} \) that satisfy \( \nabla \cdot \mathbf{B} = 0 \), and vector fields \( \mathbf{E} \) that satisfy \( \bar{\mathbf{E}} = \nabla \cdot \mathbf{E} \), where now \( \bar{\mathbf{E}} := \int \tilde{f} \, dv \). (We note that the choice to constrain \( M \) to \( \mu \)'s preimage of 0, in particular, evidently corresponds to the physical case in which no ‘external’ charges are present in the system—a choice that has consequences for our system’s initial conditions, as we shall see.) Our reduction map may therefore be summarized by:

\[
\pi_{\text{red}} : \quad M \rightarrow \tilde{M}_0 := \mu^{-1}(0)/\mathcal{F} \\
(f(x, p), A, Y) \quad \rightarrow \quad (\tilde{f}(x, v), B, E).
\] (4.27)

As calculated in Marsden & Weinstein (1982) Sec. 7, the substitution of Eq. (4.26) into the bracket of Eq. (4.1) yields the symplectic, reduced bracket on \( \tilde{M}_0 \):

\[
\{\{F, G\}\}^{\text{red}}[\tilde{f}, \mathbf{B}, \mathbf{E}] = \int dx dv \left[ \tilde{f} \left\{ \frac{\delta F}{\delta f}, \frac{\delta G}{\delta f} \right\}_{xv} + \right.
\]

\[
\tilde{f} \mathbf{B} \cdot \left( \frac{\partial}{\partial v} \frac{\delta F}{\delta f} \times \frac{\partial}{\partial v} \frac{\delta G}{\delta f} \right) + \left( \frac{\delta F}{\delta \mathbf{E}} \cdot \nabla \times \frac{\delta G}{\delta \mathbf{f}} - \frac{\delta G}{\delta \mathbf{E}} \cdot \nabla \times \frac{\delta F}{\delta \mathbf{f}} \right) \] (4.28)

\[
+ \int dx \left( \frac{\delta F}{\delta \mathbf{E}} \cdot \nabla \times \frac{\delta G}{\delta \mathbf{B}} - \frac{\delta G}{\delta \mathbf{E}} \cdot \nabla \times \frac{\delta F}{\delta \mathbf{B}} \right).
\]

We note that symplectic reduction always preserves the \( \dot{\mu} = 0 \) conservation law derived from an unreduced symplectic system. After all, symplectic reduction restricts an unreduced symplectic manifold to (quotients of) a submanifold on which \( \mu \) is constant—in particular, preimages of a single value of \( \mu \). In our case, the conservation law of Eq. (4.24) is clearly respected by symplectic reduction, and may simply be re-expressed in the phase...
space variables of the reduced manifold $\tilde{M}_0$, along with its continuity form in Eq. (4.25):

$$0 = \dot{\bar{\mu}} = \dot{\bar{\rho}} - \nabla \cdot \dot{E}$$

$$= \dot{\bar{\rho}} + \nabla \cdot \dot{J},$$

(4.29)

where

$$\bar{\mu} = \int d\mathbf{v} \tilde{f}(\mathbf{x}, \mathbf{v}) - \nabla \cdot \mathbf{E}$$

$$= \bar{\rho} - \nabla \cdot \mathbf{E},$$

(4.30)

and where $\bar{\rho} := \int \tilde{f} \, d\mathbf{v}$ and $\bar{J} := \int \tilde{f} \mathbf{v} \, d\mathbf{v}$.

We note that the reduced bracket of Eq. (4.28) is symplectic—and nondegenerate—specifically on the quotient submanifold $\tilde{M}_0$. Some of the plasma physics literature (e.g. Morrison 1982, 2013; Kraus et al. 2017) refers to Eq. (4.28) as a degenerate bracket, however, so we pause to elucidate the source of this contrast.

In particular, we note that the bracket of Eq. (4.28) becomes degenerate if we define the Maxwell-Vlasov system on an augmented manifold that includes all unconstrained vector fields $\mathbf{E}, \mathbf{B} \in \mathbb{R}^3$:

$$\tilde{M}_0^+ := \tilde{M}_0 \cup \{ \mathbf{E}, \mathbf{B} \mid \nabla \cdot \mathbf{E} \neq \bar{\rho}, \nabla \cdot \mathbf{B} \neq 0 \}. \quad (4.31)$$

This degeneracy on $\tilde{M}_0^+$ appears in the form of two new Casimirs:

$$\{\cdot, \mu\} = \{\cdot, \bar{\rho} - \nabla \cdot \mathbf{E}\} = 0$$

$$\{\cdot, \nabla \cdot \mathbf{B}\} = 0.$$

(4.32)

This is not mere coincidence; it can be viewed as a consequence of discarding the $\bar{\mu} = \bar{\rho} - \nabla \cdot \mathbf{E} = 0$ constraint and redefining the divergenceless $\mathbf{B}$ coordinates that constructed the manifold $\tilde{M}_0 = \bar{\mu}^{-1}(0)/\mathcal{F}$ in Eq. (4.26). From this viewpoint, the degeneracy in Eq. (4.32) is analogous to defining a symplectic structure on $\mathbb{R}^2 = \{(x, y)\}$, and noting that the $z$ coordinate becomes a Casimir when the system is embedded in $\mathbb{R}^3$.

We further recall that when the bracket of Eq. (4.28) is defined on $\tilde{M}_0^+$ and not on $\tilde{M}_0$, it no longer everywhere obeys the Jacobi identity (Morrison 1982; Chandre et al. 2013); in particular, the Jacobi identity is satisfied on $\tilde{M}_0^+$ only when $\nabla \cdot \mathbf{B} = 0$. Indeed, the constraint $\nabla \cdot \mathbf{B} = 0$ appears as an exogenous defect that must be satisfied for $(\tilde{M}_0^+, \{\cdot, \cdot\}_{\text{red}})$ to be considered a Poisson manifold.

However, we adopt the point of view that it is more natural to consider the bracket of Eq. (4.28) as symplectic on the submanifold of physical interest—$\tilde{M}_0$—rather than a degenerate and defected bracket on the larger manifold including arbitrary vector fields $\mathbf{E}$ and $\mathbf{B}$. In a sense, it is merely a lack of economical notation that leads us to coordinatize $\tilde{M}_0$ with vector symbols $\mathbf{E}$ and $\mathbf{B}$ that are more commonly defined in $\mathbb{R}^3$. We emphasize that Eq. (4.28) is nondegenerate and obeys the Jacobi identity on $\tilde{M}_0$. In these ways, the symplectic manifold $\tilde{M}_0$—which is systematically derived by symplectic reduction—is the appropriate setting for the reduced bracket of Eq. (4.28).

It is clear from this discussion, however, that care must be taken in any numerical implementation of the reduced Vlasov-Maxwell bracket. One’s fields must be constrained to the phase space of $\tilde{M}_0$, and generic, unconstrained vector fields $\mathbf{E}, \mathbf{B} \in \mathbb{R}^3$ must be avoided.
5. The Momentum Map in Hamiltonian Splitting Methods

We now reconsider the momentum map—and its associated conservation laws—in the context of Hamiltonian splitting algorithms. Due to their ease of computation, splitting methods offer an appealing algorithmic implementation of many Hamiltonian systems. (He et al. 2016) In effect, a splitting method splits a system’s Hamiltonian $H$ into some finite number of ‘sub-Hamiltonians’ $\{H_i\}$ such that:

$$H = \sum_{i=1}^{N} H_i.$$  \hspace{1cm} (5.1)

The system’s dynamical variables $u$ are then evolved by each subsystem individually, arranged in a sequence chosen to minimize discretization error, e.g.:

$$u(t + \Delta t) = \exp\left(\Delta t H\right) u(t) 
\approx \exp\left(\frac{\Delta t}{2} H_1\right) \exp\left(\Delta t H_2\right) \exp\left(\frac{\Delta t}{2} H_1\right) u(t),$$ \hspace{1cm} (5.2)

where we have schematically represented two subsystems, $H = H_1 + H_2$, arranged in a second-order Strang splitting. (Hairer et al. 2006)

The advantage afforded by this subdivision of the Hamiltonian is that its subsystems $\{H_i\}$ are often much more easily integrated individually than the full system $H$. In fact, each sub-Hamiltonian $H_i$ can often be made sufficiently simple to allow its exact integration, without any discrete approximation. We will see examples of this exact evolution in the Vlasov-Maxwell splitting methods detailed in Section 6.

Our interest concerns the status of the momentum map $\mu$ in such algorithms. A sufficient condition for the exact preservation of $\mu$ in splitting methods is, in fact, quite straightforward to state. In particular, let us suppose that each sub-Hamiltonian is gauge-invariant—that is, invariant under the group action of some group $G$:

$$\Phi_g^* H_i = H_i \quad \forall \ i \text{ and } g \in G.$$ \hspace{1cm} (5.3)

Then, differentiating with respect to $g$, we find by the same argument of Eqs. (4.22)-(4.23) that $\dot{\mu} = 0$ in each Hamiltonian subsystem, where $\mu$ is the total system’s momentum map. This result follows simply from the observation that $\mu$ is an object defined kinematically by its symplectic manifold $(M, \omega)$, separate and apart from the dynamics defined via some Hamiltonian on that manifold (see Salmon & Ewing-DeRemer 1993). It is therefore preserved by the exact evolution of any gauge-invariant Hamiltonian. Indeed, if each Hamiltonian subsystem is gauge-invariant and exactly integrated, then the momentum map is exactly preserved after each discrete timestep. We summarize this result as a theorem.

**Theorem.** Let $\Phi$ be a symplectic action of $G$ on $(M, \omega)$ with momentum map $\mu$, and let $H : M \rightarrow \mathbb{R}$ satisfy $\Phi_g^* H = H, \ \forall \ g \in G$. Suppose a splitting method $H = \sum_{i=1}^{N} H_i$ satisfies:

1. $\Phi_g^* H_i = H_i, \ \forall \ i \text{ and } g \in G$
2. subsystem $H_i$ is solved exactly $\forall \ i$.

Then $\mu$ is exactly preserved by the splitting method—that is, $\dot{\mu} = 0$.

We refer to such an algorithm as a *gauge-compatible splitting method*. Gauge-compatible splitting methods have a distinct advantage over other time-discretizations of Hamiltonian systems, in that they preserve the geometric structure of the systems they
simulate—(in particular, the momentum map)—and therefore obey exact conservation laws.

6. Conservation Laws in Hamiltonian PIC Splitting Methods

6.1. A ‘Symplectically Unreduced’ Hamiltonian PIC Method

With the formalism we have developed, we proceed to explore PIC methods in the Hamiltonian setting, by considering a PIC splitting method adapted from Xiao et al. (2015) and Qin et al. (2016) The latter of these references implements a symplectic-Euler integrator for the the unreduced Poisson bracket of Eq. (4.1), while the former implements a splitting method for the reduced bracket of Eq. (4.28). We shall synthesize the two, defining a gauge-compatible splitting method for the unreduced bracket of Eq. (4.1), and thereby demonstrate the merit of this new class of splitting methods. The result is an explicit-time-advance, canonical, symplectic, locally-charge-conserving PIC method, whose conservation law we shall systematically derive.

In Qin et al. (2016), a Klimontovich-Maxwell PIC method is derived from the unreduced bracket of Eq. (4.1) by specifying the following form for the distribution function \( f(x, p) \):

\[
f(x, p) = \sum_{i=1}^{L} \delta(x - X_i)\delta(p - P_i)
\]

where \((X_i, P_i)\) denote the time-varying particle coordinates of \(L\) particles on phase space; we emphasize that \((X_i, P_i)\) are coordinates, and not functionals. The fields \(A\) and \(Y\) are also discretized on a (3-dimensional) spatial lattice, as \((A_n, Y_n)\). We shall further require the interpolation of \(A\):

\[
A(x) = \sum_{n=1}^{N} A_n W_{\sigma_1}(x - x_n)
\]

where \(n\) is an index over all lattice sites and \(W_{\sigma_1}\) is some interpolation function for the 1-form \(A\).

To define a Poisson bracket for our discrete system, we simply note the canonical symplectic structure of our variables. In particular, we define a symplectic manifold

\[
M_d = T^*X \times T^*Q,
\]

where \(X = \mathbb{R}^{3L}\) is the space of particle position coordinates and \(Q = \mathbb{R}^{3N}\) is the space of vector potentials on the grid, such that \(T^*X = \{(X_i, P_i)\}\) and \(T^*Q = \{(A_n, Y_n)\}\). A point \(m \in M_d\) correspondingly specifies \((X_i, P_i, A_n, Y_n)\) \(\forall\ i, n\).

The Poisson bracket for this symplectic manifold therefore takes its usual canonical (Darboux-coordinate) form:

\[
\{\{F, G\}\}_d[X_i, P_i, A_n, Y_n] = \sum_{i=1}^{L} \left( \frac{\partial F}{\partial X_i} \cdot \frac{\partial G}{\partial P_i} - \frac{\partial G}{\partial X_i} \cdot \frac{\partial F}{\partial P_i} \right) + \sum_{n=1}^{N} \left( \frac{\partial F}{\partial A_n} \cdot \frac{\partial G}{\partial Y_n} - \frac{\partial G}{\partial A_n} \cdot \frac{\partial F}{\partial Y_n} \right).
\]

As in \(M_d\), we let the subscript \(d\) denote discretization.

The discrete Hamiltonian of Qin et al. (2016) is derived from Eq. (4.2) by substituting
the Klimontovich distribution of Eq. (6.1) and expanding terms of the form $|P_i - A(X_i)|^2$ using Eq. (6.2):

$$H_d[X_i, P_i, A_n, Y_n] = \frac{1}{2} \sum_{i=1}^{L} \left[ P_i^2 - 2P_i \cdot \sum_{n=1}^{N} A_n W_{\sigma_1}(X_i - x_n) \right]$$

$$+ \sum_{m,n=1}^{N} A_m \cdot A_n W_{\sigma_1}(X_i - x_m) W_{\sigma_1}(X_i - x_n)$$

$$+ \frac{1}{2} \sum_{n=1}^{N} [Y_n^2 + |\nabla_d^+ \times A_n|^2].$$

(6.5)

Here the operator $(\nabla_d^+ \times \cdot)_n$ represents a discrete curl, defined by:

$$\left(\nabla_d^+ \times A\right)_n := \pm \left( \begin{array}{c} \frac{A_{i,j+1,k}^3 - A_{i,j,k}^3}{\Delta y} - \frac{A_{i,j,k}^3 - A_{i,j,k+1}^3}{\Delta z} \\ \frac{A_{i,j+1,k}^3 - A_{i,j,k}^3}{\Delta z} - \frac{A_{i,j,k}^3 - A_{i,j,k+1}^3}{\Delta x} \\ \frac{A_{i+1,j,k}^3 - A_{i,j,k}^3}{\Delta x} - \frac{A_{i,j,k}^3 - A_{i+1,j,k}^3}{\Delta y} \end{array} \right)$$

(6.6)

for $n = (i, j, k)$.

We now describe the gauge symmetry of this discrete Hamiltonian system. A group action $\Phi_f$ on $M_d$ may be defined by analogy with Eq. (4.13):

$$\Phi_f(X_i, P_i, A_n, Y_n) = \left( X_i, \left[ P_i - \nabla_d^+ f(X_i) \right], \left[ A_n - (\nabla_d^+ f)_n \right], Y_n \right),$$

(6.7)

where

$$\nabla_d^+ f(x) = \sum_{n=1}^{N} (\nabla_d^+ f)_n W_{\sigma_1}(x - x_n)$$

(6.8)

and where $(\nabla_d^+ : \cdot)_n$ is a discrete gradient defined by:

$$\left(\nabla_d^+ f\right)_n := \pm \left( \begin{array}{c} \frac{f_{i+1,j,k} - f_{i,j,k}}{\Delta x} \\ \frac{f_{i,j+1,k} - f_{i,j,k}}{\Delta y} \\ \frac{f_{i,j,k+1} - f_{i,j,k}}{\Delta z} \end{array} \right).$$

(6.9)

We note that $\nabla_d^+ \times \nabla_d^+ = 0$ as an operator. (If the ± signs agree, this relation holds identically; if they disagree, it holds only after summation $\sum_n$ over grid points.) We also note that—in contrast with Eqs. (4.13)-(4.14)—$P_i$ and $A_n$ are shifted in the same direction in Eq. (6.7), reflecting the fact that $p$ and $P_i$ have opposite signs in Eq. (6.1) when we reinterpret the transformation of Eq. (4.14) as a transformation of $P_i$.

The function $f$ appearing in the group action of Eq. (6.7) is to be understood as a scalar function defined only on the grid points. In particular, $f \in \mathcal{F}_d$ is a group element of the set $\mathcal{F}_d$ of discrete scalar functions with a composition law of addition. Its Lie algebra $f_d$ is also the set of discrete scalar functions on the grid, while its dual $f_d^*$ is the set of densities, which pair to elements of $f_d$ by summing over pointwise products:

$$\langle \phi, \alpha \rangle := \sum_{n=1}^{N} \phi_n \alpha_n, \ \forall \phi \in f_d, \ \alpha \in f_d^*.$$

(6.10)
We must verify that the group action is canonical, a task most easily approached infinitesimally. In particular, we investigate whether the following infinitesimal form of $$\{\{\Phi^*F,\Phi^*G\}\}$$ holds:

$$\left\{ \left\{ -\nabla^d\phi(X_i) \cdot \frac{\partial F}{\partial P_i} - \nabla^d\phi_n \cdot \frac{\partial F}{\partial A_n}, G \right\} \right\} = -\nabla^d\phi(X_i) \cdot \frac{\partial \{\{F,G\}\}}{\partial P_i} - \nabla^d\phi_n \cdot \frac{\partial \{\{F,G\}\}}{\partial A_n},$$

(6.11)

where summation over repeated indices is implicit. After applying Eq. (6.4) to evaluate each bracket, Eq. (6.11) is seen to be true only when $$\nabla \times \nabla^d\phi(X_i) = 0$$. This requires the operator relation:

$$\nabla \times \nabla^d = 0.$$  

(6.12)

Here, $$\nabla = \partial X_i$$ is a continuous spatial gradient.

Eq. (6.12) therefore necessitates the following condition on the interpolation function $$W_{\sigma_1}$$:

$$\sum_{n=1}^{N} (\nabla^d\phi)n W_{\sigma_1}(x - x_n) = \nabla \sum_{n=1}^{N} \phi_n W_{\sigma_0}(x - x_n)$$

(6.13)

for some interpolation function $$W_{\sigma_0}$$ on 0-forms. This condition was already discovered in the context of a reduced Hamiltonian system in Xiao et al. (2015), and is closely analogous to a property of the simplicial Whitney forms described earlier. (Bossavit 1988) Our discussion of this condition in the present context merely contributes that, in a Hamiltonian setting, the motivation for the constraint in Eq. (6.13) is the canonicality of the group action.

We now solve for $$\mu_d$$—the momentum map on $$M_d$$—using the symplectic structure of Eq. (6.4) and the group action defined by Eq. (6.7). We first find the infinitesimal generator of our group action on $$M_d$$—$$\phi_{M_d}$$—defined analogously to Eq. (4.15). Given the group action of Eq. (6.7) we expect $$\phi_{M_d}$$ to take the form (already implicitly used in Eq. (6.11)):

$$\{\cdot, \mu^\phi_d\} = -\sum_{i=1}^{L} \nabla^d\phi(X_i) \cdot \frac{\partial}{\partial P_i} - \sum_{n=1}^{N} (\nabla^d\phi)n \cdot \frac{\partial}{\partial A_n},$$

(6.14)

where we denote the pairing of the momentum map with $$\phi$$ by $$\mu^\phi_d$$. The Poisson bracket of Eq. (6.4) therefore requires that $$\mu^\phi_d$$ be given by:

$$\mu^\phi_d(m) = \sum_{n=1}^{N} (\nabla^d\phi)n \cdot \left[ \sum_{i=1}^{L} \int_{-\infty}^{X_i} \right] dX_i W_{\sigma_1}(X_i' - x_n) - Y_n$$

(6.15)

where we have summed by parts (Hydon & Mansfield 2011) using the discrete divergence operator:

$$\nabla^d \cdot v_n := \pm \sum_{\alpha=1}^{3} \frac{v_{n+\alpha}^\alpha - v_n^\alpha}{\Delta x^\alpha}.$$  

(6.16)
Note that \( dX'_i \) in Eq. (6.15) is treated as a vector, with each component integrated individually.

Given the pairing defined in Eq. (6.10), the momentum map \( \mu_d \) must therefore be:

\[
\left( \mu_d(m) \right)_n = -\nabla_d^{-} \cdot \sum_{i=1}^{L} \int_{-\infty}^{X'_i} dX'W_{\sigma_1}(X'_i - x_n) + \nabla_d^{-} \cdot Y_n \tag{6.17}
\]

defined at each \( n \in [1, N] \). Due to the gauge invariance of \( H_d \)—that is, \( \Phi_f^*H_d = H_d \)—the full system evolved in continuous time by \( H_d \) obeys the conservation law

\[
\dot{\mu}_d = 0, \tag{6.18}
\]
as in the continuous case. Eqs. (6.17)-(6.18) define the conservation law of our discrete Hamiltonian system in continuous time, systematically derived via the momentum map.

Following the analysis of Eqs. (4.24)-(4.25), we may re-express this conservation law by deriving the continuous-time EOM of the full Hamiltonian \( H_d \), as follows:

\[
\begin{align*}
\dot{X}_i &= \{\{X_i, H_d\}\}_d = P_i - \sum_{m=1}^{N} A_m W_{\sigma_1}(X_i - x_m) \\
\dot{P}_i &= \{\{P_i, H_d\}\}_d = \sum_{m=1}^{N} \left( \dot{X}_i \cdot A_m \right) \nabla W_{\sigma_1}(X_i - x_m) \\
\dot{A}_n &= \{\{A_n, H_d\}\}_d = Y_n \\
\dot{Y}_n &= \{\{Y_n, H_d\}\}_d = \sum_{i=1}^{L} \dot{X}_i W_{\sigma_1}(X_i - x_n) - \left( \nabla_d^{-} \times \nabla_d^{+} \times A \right)_n.
\end{align*}
\tag{6.19}
\]

Substituting \( \dot{Y}_n \) into Eqs. (6.17)-(6.18), we note that

\[
0 = \dot{\rho}_n + \nabla_d^{-} \cdot J_n \tag{6.20}
\]

where

\[
\begin{align*}
\rho_n &:= -\nabla_d^{-} \cdot \sum_{i=1}^{L} \int_{-\infty}^{X'_i} dX'W_{\sigma_1}(X'_i - x_n) \\
J_n &:= \sum_{i=1}^{L} \dot{X}_i W_{\sigma_1}(X_i - x_n).
\end{align*}
\tag{6.21}
\]

This is the local charge conservation law for the continuous-time evolution of the Hamiltonian system of Qin et al. (2016). (We observe that, unlike its counterpart in Eq. (4.25), it is an off-shell identity.)

The form of \( \rho_n \) in Eq. (6.21) is easily justified by a 1-D example in which \( W_{\sigma_1}(x) = 1 \) on \( 0 \leq x < \Delta x \) and 0 otherwise. For a single particle at \( X_i = 0.2 \), we have:

\[
\begin{align*}
\rho_n = -\nabla_d^{-} \cdot \int_{-\infty}^{0.2} dX'W_{\sigma_1}(X'_i - x_n) &= \begin{cases} 
0.8/\Delta x & n = 0 \\
0.2/\Delta x & n = 1 \\
0 & n \neq 0, 1.
\end{cases}
\end{align*}
\tag{6.22}
\]

This result demonstrates the appropriateness of the momentum map’s systematically-derived charge density.

We now define an algorithmic solution of this Hamiltonian system via a splitting method, and examine the preservation of \( \mu_d \). To algorithmically evolve this system in
discrete time, we define a gauge-compatible splitting method, inspired by He et al. (2015, 2016), as follows. We define Hamiltonian subsystems:

\[ H = \sum_{\alpha=1}^{3} H_{\text{Klim}}^{\alpha} + H_{A} + H_{Y} \]  \hspace{1cm} (6.23)

where

\[ H_{\text{Klim}}^{\alpha} := \frac{1}{2} \sum_{i=1}^{L} \left( P_{i}^{\alpha} - A_{i}^{\alpha}(X_{i}) \right)^{2} \]

\[ H_{A} := \frac{1}{2} \sum_{n=1}^{N} \left( \nabla_{d} \times A_{n} \right)^{2} \]  \hspace{1cm} (6.24)

\[ H_{Y} := \frac{1}{2} \sum_{n=1}^{N} Y_{n}^{2}. \]

We note that these subsystems are all gauge-invariant for the group action of Eq. (6.7)—\( \Phi_{f}^{*} H_{i} = H_{i} \forall f \in \mathcal{F}_{d} \)—and will therefore comprise a gauge-compatible splitting—and preserve \( \mu_{d} \)—if they can be exactly solved.

Let us examine the EOM for each subsystem \( H_{i} \) in turn:

\[
\begin{aligned}
\dot{X}_{i}^{\beta} &= \delta_{\alpha}^{\beta} \left[ P_{i}^{\alpha} - \sum_{m=1}^{N} A_{m}^{\alpha} W_{\sigma_{1}}(X_{i} - x_{m}) \right] \\
\dot{P}_{i}^{\beta} &= X_{i}^{\alpha} \sum_{m=1}^{N} A_{m}^{\alpha} \partial_{\beta} W_{\sigma_{1}}(X_{i} - x_{m}) \\
\dot{A}_{n}^{\beta} &= 0 \\
\dot{Y}_{n}^{\beta} &= \delta_{\alpha}^{\beta} \sum_{i=1}^{L} \dot{X}_{i}^{\alpha} W_{\sigma_{1}}(X_{i} - x_{n})
\end{aligned}
\]  \hspace{1cm} (6.25)

\[
\begin{aligned}
\dot{X}_{i} &= 0 \\
\dot{P}_{i} &= 0 \\
\dot{A}_{n} &= 0 \\
\dot{Y}_{n} &= -\left( \nabla_{d} \times \nabla_{d}^{\perp} \times A_{n} \right)
\end{aligned}
\]  \hspace{1cm} (6.26)

\[
\begin{aligned}
\dot{X}_{i} &= 0 \\
\dot{P}_{i} &= 0 \\
\dot{A}_{n} &= Y_{n} \\
\dot{Y}_{n} &= 0
\end{aligned}
\]  \hspace{1cm} (6.27)

where \( \partial_{\beta} \equiv \partial/\partial X_{i}^{\beta} \). We note that \( \alpha \) is fixed, and is not summed over in the expressions for \( H_{\text{Klim}}^{\alpha}, H_{A} \) and \( H_{Y} \) are exactly solvable at a glance. Furthermore, \( H_{\text{Klim}}^{\alpha} \) is seen to be exactly solvable by noting that \( \ddot{X}_{i}^{\beta} = 0; \dot{X}_{i}^{\beta} \) is therefore a constant determined by a timestep’s initial conditions. The evolutions of \( \dot{P}_{i} \) and \( \dot{Y}_{n} \) in \( H_{\text{Klim}}^{\alpha} \) follow immediately from this analysis.

The exact time evolutions of \( H_{A}, H_{Y} \) and \( H_{\text{Klim}}^{\alpha} \) are therefore explicitly solved, defining by construction an explicit-time-advance splitting method that exactly preserves the momentum map, \( \dot{\mu}_{d} = 0 \), as desired. We also refer the reader to a brief discussion of the
appropriate initial conditions for the preceding algorithm, in the text following Eq. (6.30) below.

As a final note, the alternative form of the charge conservation law given in Eq. (6.20)—that is, \( \dot{\rho}_n + \nabla_d \cdot J_n = 0 \)—is also exactly preserved, because the substitution that led from Eq. (6.18) to Eq. (6.20)—that is, \( \nabla_d \cdot Y_n = \nabla_d \cdot J_n \)—holds for each Hamiltonian subsystem.

6.2. A ‘Symplectically Reduced’ Hamiltonian PIC Method

We now examine the PIC method of Xiao et al. (2015), which employs a splitting method equivalent to that of the preceding section for the reduced Vlasov-Maxwell bracket of Eq. (4.28).

We will mirror Xiao et al. (2015) and derive this PIC scheme by undertaking the symplectic reduction of the discrete bracket defined in Eq. (6.4). As in Section 4, we define a mapping to the reduced symplectic manifold \( \tilde{M}_{d0} = \frac{\mu_d^{-1}(0)}{\mathcal{F}_d} \), with coordinates given by

\[
\pi_{d, \text{red}} : \quad M_d \rightarrow \tilde{M}_{d0} \\
(X_i, P_i, A_n, Y_n) \mapsto (X_i, V_i, B_n, E_n),
\]

(6.28)

where

\[
\begin{align*}
X_i &= X_i \\
V_i &= P_i - A(X_i) \\
B_n &= (\nabla_d^+ \times A)_n \\
E_n &= -Y_n.
\end{align*}
\]

(6.29)

As discussed earlier, care must be taken to ensure that the discrete fields \( B_n \) and \( E_n \) of \( \tilde{M}_{d0} \) obey the reduced manifold constraints:

\[
\begin{align*}
(\nabla_d^+ \cdot B)_n &= 0 \\
(\nabla_d^- \cdot E)_n &= -\nabla_d^- \cdot \sum_{i=1}^L \int_{-\infty}^{X_i} dX'_i W_{\sigma_1}(X'_i - x_n).
\end{align*}
\]

(6.30)

These constraints must also be satisfied by any initial condition of the algorithm; we note that, if the latter condition is not satisfied, it will have the effect of adding fixed ‘external’ charges at the corresponding vertex \( n \). In particular, an incorrect initial condition will evolve the system along some other reduced manifold \( \tilde{M}_{d\alpha} = \frac{\mu_d^{-1}(\alpha)}{\mathcal{F}_d} \) with external charge density \( \alpha \). (We note that a similar initial condition must be determined for the unreduced algorithm of Section 6.1 as well. For example, for simulations without external charges, care should be taken so that the value of \( (\mu_d(m))_n \) in Eq. (6.17) is everywhere initialized to zero. On the other hand, the unreduced algorithm enforces the constraint \( (\nabla_d^+ \cdot B)_n = 0 \) automatically.)
We therefore substitute Eq. (6.29) into the bracket of Eq. (6.4) to find:

$$\{\{F, G\}\}_d^{\text{red}} [X_i, V_i, B_n, E_n] =$$

$$\sum_{i=1}^L \left( \frac{\partial F}{\partial X_i} \cdot \frac{\partial G}{\partial V_i} - \frac{\partial G}{\partial X_i} \cdot \frac{\partial F}{\partial V_i} + \left[ \frac{\partial F}{\partial V_i} \times \frac{\partial G}{\partial V_i} \right] \cdot \sum_{n=1}^N B_n W_{\sigma_2}(X_i - x_n) \right) +$$

$$\sum_{n=1}^N \left( \sum_{i=1}^L \frac{\partial F}{\partial V_i} W_{\sigma_1}(X_i - x_n) + \left( \nabla_d \times \frac{\partial F}{\partial B} \right)_n \cdot \frac{\partial G}{\partial E_n} \right) \cdot \frac{\partial F}{\partial E_n} \right).$$

(6.31)

To derive the $\partial_{V_i} F \times \partial_{V_i} G \cdot B(X_i)$ term in the bracket above, our interpolation functions were required to satisfy an additional constraint:

$$\nabla \times \sum_{n=1}^N A_n W_{\sigma_1}(x - x_n) = \sum_{n=1}^N (\nabla_d^+ \times A)_n W_{\sigma_2}(x - x_n)$$

(6.32)

for some interpolation function $W_{\sigma_2}$. As in Eq. (6.13), this is a cubical complex (and higher-dimensional) equivalent to the Whitney interpolant constraint on simplicial complexes (see Squire et al. 2012): $d((A)_{\text{interp}}) = (d_d A)_{\text{interp}}$.

Lastly, we re-express the Hamiltonian on $\tilde{M}_{d_0}$ as:

$$H_{d_0}^{\text{red}} [X_i, V_i, B_n, E_n] = \frac{1}{2} \sum_{i=1}^L V_i^2 + \frac{1}{2} \sum_{n=1}^N \left( E_n^2 + B_n^2 \right).$$

(6.33)

We have thus recovered the reduced Hamiltonian system of Xiao et al. (2015).

As discussed in Section 4 for continuous systems, this reduced Hamiltonian system is automatically guaranteed to preserve the momentum map of its parent, as long as its evolution is constrained to $\tilde{M}_{d_0}$. To see that this is the case, we may compute its evolution equations under the splitting scheme analogous to the unreduced case (He et al. 2015, 2016; Xiao et al. 2015):

$$H = \sum_{\alpha=1}^3 H_{V}^\alpha + H_B + H_E$$

(6.34)

where

$$H_{V}^\alpha := \frac{1}{2} \sum_{i=1}^L (V_i^\alpha)^2$$

$$H_B := \frac{1}{2} \sum_{n=1}^N B_n^2$$

$$H_E := \frac{1}{2} \sum_{n=1}^N E_n^2.$$

(6.35)
These subsystems generate the following EOM:

\[
H_{V}^\alpha \begin{cases}
\dot{X}^\beta_i = \delta^\beta_\alpha V^\alpha_i \\
\dot{V}^\beta_i = \epsilon_{\beta \alpha \gamma} V^\alpha_i \sum_{n=1}^{N} B_n^\gamma W_{\sigma_2} (X_i - x_n) \\
\dot{B}_n^\beta = 0 \\
\dot{E}_n^\beta = -\delta^\beta_\alpha \sum_{i=1}^{L} V^\alpha_i W_{\sigma_1} (X_i - x_n)
\end{cases}
\]  

(6.36)

\[
H_B \begin{cases}
\dot{X}_i = 0 \\
\dot{V}_i = 0 \\
\dot{B}_n = 0 \\
\dot{E}_n = (\nabla_d^- \times B)_n
\end{cases}
\]  

(6.37)

\[
H_E \begin{cases}
\dot{X}_i = 0 \\
\dot{V}_i = \sum_{n=1}^{N} E_n W_{\sigma_1} (X_i - x_n) \\
\dot{B}_n = -(\nabla_d^+ \times E)_n \\
\dot{E}_n = 0.
\end{cases}
\]  

(6.38)

We note again that \( \alpha \) is not summed over in \( H_{V}^\alpha \).

Upon inspection, it is evident that the \( \tilde{M}_{d0} \) constraints of Eq. (6.30) are obeyed in each subsystem when they are exactly solved. Consequently, the conservation law of the reduced system is systematically derived by simply expressing the unreduced momentum map of Eq. (6.17) in \( \tilde{M}_{d0} \) coordinates:

\[
(\tilde{\mu}_d)_n = -\nabla_d^- \cdot \sum_{i=1}^{L} \int_{-\infty}^{X_i} dX'_i W_{\sigma_1} (X'_i - x_n) - \nabla_d^- \cdot E_n
\]

\[
:= \rho_n - \nabla_d^- \cdot E_n
\]

\[
= 0,
\]

(6.39)

where we have noted that \( \tilde{\mu}_d \) vanishes by our choice of reduction to the preimage submanifold \( \tilde{\mu}_d^{-1}(0) \). This is Gauss’s law, for which we are by construction guaranteed:

\[
\dot{\tilde{\mu}}_d = 0,
\]

(6.40)

as desired. (An analogous observation was made for the reduced bracket in Kraus et al. (2017), wherein the momentum map was treated as a Casimir.) The local charge conservation law of Eq. (6.20)—whose expression is unmodified in the reduced submanifold—is furthermore satisfied, since \( \nabla_d^- \cdot \dot{E}_n = -\nabla_d^- \cdot J_n \) holds for each subsystem as well.

7. Conclusion

We have systematically derived conservation laws for both Lagrangian variational and Hamiltonian splitting PIC methods. Our approach for Lagrangian systems followed Noether’s Second Theorem, and for Hamiltonian systems we employed the momentum map. Our treatment of Hamiltonian methods additionally revealed the decided advantage of gauge-compatible splitting methods over other time-discretizations of Hamiltonian
systems; when the sub-Hamiltonians of a splitting method are chosen to be gauge-invariant and exactly solvable, such methods exactly preserve the momentum map and its conservation laws.

Our treatment of Hamiltonian methods additionally revealed the importance of deriving a discrete system’s momentum map in order to correctly specify its initial conditions. In the case of gauge-invariant PIC methods, the momentum map’s systematic definition of charge density enables the precise assignment (or avoidance) of ‘external’ fixed charges at each lattice site \( n \) as an initial condition.

The techniques we have defined are more generally applicable, and in principle provide a template for the derivation of exact conservation laws in any gauge-symmetric variational or gauge-compatible splitting algorithm. They can also be used to derive the conservation laws associated with more general gauge symmetries as well.

As a final note, our results convey an overall impression of the adaptability of gauge theories to the discrete structures of algorithms. Gauge symmetries, (as we define them), are characterized by the transformation of fields defined against the background of spacetime, and their geometric structure can therefore be maintained even after the algorithmic discretization of this background. The present effort demonstrates that much of the formalism that gauge theories employ in continuous spacetime is easily ported to discrete settings more suitable for computation.

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