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

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In recent years, several gauge-symmetric particle-in-cell (PIC) methods have been developed whose simulations of particles and electromagnetic fields exactly conserve charge. While it is rightly observed that these methods' gauge symmetry gives rise to their charge conservation, this causal relationship has generally been asserted via *ad hoc* derivations of the associated conservation laws. In this work, we develop a comprehensive theoretical grounding for charge conservation in gauge-symmetric Lagrangian and Hamiltonian PIC algorithms. For Lagrangian variational PIC methods, 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 show that the momentum map establishes their charge conservation laws. We define a new class of algorithms – gauge-compatible splitting methods – that exactly preserve the momentum map associated with a Hamiltonian system's gauge symmetry – even after time discretization. This class of algorithms affords splitting schemes a decided advantage over alternative Hamiltonian integrators. We apply this general technique to design a novel, explicit, symplectic, gauge-compatible splitting PIC method, whose momentum map yields an exact local charge conservation law. Our study clarifies the appropriate initial conditions for such schemes and examines their symplectic reduction.

Key words: plasma simulation

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 (Okuda 1972; Cohen, Langdon & Friedman 1982; Dawson 1983; Langdon, Cohen & Friedman 1983; Lee 1983; Hockney & Eastwood 1988; Cohen *et al.* 1989; Liewer & Decyk 1989; Birdsall & Langdon 1991; Eastwood 1991; Friedman *et al.* 1991; Cary & Doxas 1993; Parker, Lee & Santoro 1993; Decyk 1995; Grote *et al.* 1998; Qiang *et al.* 2000; Qin, Davidson & Lee 2000*a*,*b*; Qin *et al.* 2001; Vay *et al.* 2002; Chen & Parker 2003; Nieter & Cary 2004; Huang *et al.* 2006).

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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, Chacón & Barnes 2011; Pukhov 2016).

In recent years, elegant PIC methods have been developed that preserve the gauge symmetry of the plasmas they simulate. Such gauge-symmetric methods exactly conserve charge, not as the result of bespoke numerical methods, but as a natural consequence of preserving their systems' geometric structure. It was Squire, Qin & Tang (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 Hamiltonian PIC schemes (He *et al.* 2015, 2016; Xiao *et al.* 2015; Qin *et al.* 2016; Kraus *et al.* 2017; Xiao, Qin & Liu 2018; Xiao & Qin 2019).

Many of these references note that the gauge symmetry of their algorithms 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 motivates a rigorous study of algorithmic conservation laws in PIC methods. In the present paper, we study Lagrangian variational and Hamiltonian splitting algorithms and derive their charge conservation laws from first principles. In so doing, we elucidate the requirements for gauge-symmetric codes to be charge conserving, and provide a general template for the derivation of conservation laws from the gauge symmetry of Lagrangian and Hamiltonian algorithms.

Our study of Hamiltonian systems, in particular, identifies a new and quite general class of algorithms – gauge-compatible splitting methods – which guarantee the exact preservation of the momentum map associated with gauge symmetries in Hamiltonian systems – even after time discretization. We leverage this general classification in our present study and construct a novel gauge-compatible splitting PIC method. Our effort highlights the practical importance of solving for the momentum map in Hamiltonian algorithms, especially in determining the correct specification of their initial conditions.

This paper is presented in two parts (§§ 2–3 and 4–6, respectively), each of which may be read independently. In §§ 2–3, we demonstrate the systematic derivation of an exact charge conservation law for the Lagrangian variational PIC method of Squire *et al.* (2012). We discover this conservation law from the system's local gauge symmetry using Noether's second theorem (N2T) in a discrete setting, leveraging the formalism of Hydon & Mansfield (2011). Our effort draws upon the tools of discrete exterior calculus (DEC) (Hirani 2003; Desbrun *et al.* 2005), and studies the subtleties involved in deriving conservation laws for degenerate Lagrangian systems.

In §§ 4–6, we study the Hamiltonian formulation of the Vlasov–Maxwell system, its momentum map and its Poisson reduction (Marsden & Weinstein 1974, 1982; Marsden & Ratiu 1986). We provide an introduction (Souriau 1970; Marsden & Ratiu 1999) to the momentum map μ that arises from the gauge symmetry of the Vlasov–Maxwell system, and we demonstrate how $\dot{\mu} = \{\mu, H\} = 0$ defines a continuous-time charge conservation law. We then define the class of gauge-compatible splitting methods, demonstrating their exact conservation laws in discrete time via the momentum map. In so doing, we highlight a significant advantage of such methods over alternative Hamiltonian integrators. We apply this general classification to design a new, explicit, symplectic, gauge-compatible splitting PIC algorithm for

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the Vlasov–Maxwell system, whose exact charge conservation law, initial conditions and symplectic reduction are systematically derived.

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 and conservation laws satisfied by its Euler–Lagrange equations. However, in instances of degenerate Lagrangians (specifically, Lagrangians whose equations of motion are underdetermined) this correspondence, while true, is nevertheless weakened. In particular, in underdetermined systems there is no guarantee that non-trivial symmetries are in one-to-one correspondence with non-trivial conservation laws (Olver 1986). Such degenerate Lagrangians may be investigated using N2T, which describes the interdependence of equations of motion in Lagrangian systems with local gauge symmetry.

For present purposes, we regard a trivial conservation law as a conservation law that holds whether or not the equations of motion (EOM) are satisfied. Such a conservation law is said to hold off-shell. (A dynamical field is said to be on-shell when it obeys the equations of motion defining a system of interest; it is said to be off-shell otherwise. A conservation law is said to hold on-shell if it is satisfied when restricted to on-shell fields; it is said to hold off-shell if satisfied even by off-shell fields.) In this way, trivial conservation laws are mathematical identities; they hold true regardless of any particular system dynamics.

N2T establishes a one-to-one correspondence between local gauge symmetries of a degenerate Lagrangian and off-shell differential identities of its Euler–Lagrange equations. Off-shell identities may at first appear to capture little information. Nevertheless, we will show that in variational PIC methods, the local charge conservation law $\partial_t \rho + \boldsymbol{\nabla} \cdot \boldsymbol{J} = 0$ is just such an identity – a trivial conservation law that is independent of the dynamics of ρ and $\boldsymbol{J}$. Applying N2T, we will systematically derive this charge conservation law from the local gauge symmetry of a discrete Lagrangian.

N2T demonstrates that the redundancy of physical variables in a degenerate Lagrangian manifests in the interdependence of its EOM. In particular, N2T states that a general Lagrangian system admits a local gauge symmetry if and only if its EOM satisfy a differential identity of the form

$$\mathcal{D}^1 E_{\alpha_1}(\mathcal{L}) + \cdots + \mathcal{D}^q E_{\alpha_q}(\mathcal{L}) = 0. \tag{2.1}$$

Here, $\mathcal{D}^i$ represents an arbitrary differential operator (e.g. the Klein–Gordon operator: $\mathcal{D}^i = \partial^2 - m^2$), and $E_{\alpha_i}(\mathcal{L})$ denotes the Euler–Lagrange equation for the variable α_i (e.g. Maxwell's equation for A_ν: $E_{A_\nu}(\mathcal{L}) = \partial_\mu F^{\mu\nu} + J^\nu$).

N1T can discover conservation laws that hold dynamically (on-shell), while N2T discovers differential identities that hold kinematically (off-shell). Although (2.1) is an off-shell identity, it may nonetheless reveal valuable information for some Lagrangian systems. For discrete systems in particular, whose kinematics are sometimes less apparent or less studied, these differential identities can be especially enlightening.

In the following section, we briefly describe the formalism of Hydon & Mansfield (2011), which derives N2T's differential identities in the form of (2.1) from the local gauge symmetries of a general Lagrangian system. As we shall see, this formalism is extensible to both continuous and discrete systems.

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To begin, we recall the variation of an arbitrary action $S = \int \mathrm{d}^4x\, \mathcal{L}[\phi, \partial_\mu\phi, \ldots]$ for a field ϕ in flat space–time with coordinates x^μ

$$\begin{aligned}\delta S &= \int \mathrm{d}^4x \left[\delta\phi \frac{\partial \mathcal{L}}{\partial \phi} + \delta(\partial_\mu\phi)\frac{\partial \mathcal{L}}{\partial(\partial_\mu\phi)} + \cdots\right] \\ &= \int \mathrm{d}^4x \left[\delta\phi E_\phi(\mathcal{L}) + D_\mu\left(\delta\phi \frac{\partial \mathcal{L}}{\partial(\partial_\mu\phi)}\right) + \cdots\right].\end{aligned} \tag{2.2}$$

In the above, we have employed the Euler operator (Olver 1986)

$$\begin{aligned}E_\phi &:= \sum_J (-D)_J \frac{\partial}{\partial(\partial_J\phi)} \\ &= \left(\frac{\partial}{\partial\phi} - D_\mu\frac{\partial}{\partial(\partial_\mu\phi)} + D_{\mu\nu}\frac{\partial}{\partial(\partial_{\mu\nu}\phi)} - \cdots\right),\end{aligned} \tag{2.3}$$

which discovers a Lagrangian's EOM by implementing a variational derivative with respect to a dynamical variable. The sum in (2.3) is taken over all multi-indices J of space–time variables – e.g. $J \in \{\varnothing, x, tt, yzz, \ldots\}$ – and $D_{\mu\nu} \equiv D_\mu D_\nu$, where $D_\mu \equiv \mathrm{d}/\mathrm{d}x^\mu = \partial_\mu + \phi_\mu\partial_\phi + \phi_{\mu\nu}\partial_{\phi_\nu} + \cdots$ denotes a total derivative. (The notations $\phi_\mu \equiv \partial_\mu\phi \equiv \partial\phi/\partial x^\mu$, $\phi_{\mu\nu} \equiv \partial_{\mu\nu}\phi \equiv \partial^2\phi/\partial x^\mu\partial x^\nu$, etc. are to be used interchangeably.) For a Lagrangian with only first-order derivatives, the EOM of the field ϕ is thus given by its familiar form

$$0 = E_\phi(\mathcal{L}) = \frac{\partial \mathcal{L}}{\partial\phi} - D_\mu\left(\frac{\partial \mathcal{L}}{\partial\phi_\mu}\right). \tag{2.4}$$

We now consider a Lagrangian $\mathcal{L}[u^\alpha, u^\alpha_\mu, \ldots]$ that depends on multiple fields $\{u^\alpha(x)\}$ and their derivatives. We suppose that $S = \int \mathrm{d}^4x\, \mathcal{L}$ is invariant under an (infinite) group of local gauge transformations, each labelled by an arbitrary smooth function $g(x)$ over space–time. Such a gauge transformation may be envisioned as parametrizing a Lie group action on dynamical variables at each point of space–time individually, with the local transformation at each point determined by $g(x)$. (In the $U(1)$ gauge theory of electromagnetism, for example, the function $g(x) = \theta(x)$ may be associated with the local phase rotation of a matter field, $\phi(x) \to \mathrm{e}^{\mathrm{i}\theta(x)}\phi(x)$ at each point $x \in \mathbb{R}^4$.)

We next define the infinitesimal generator $\boldsymbol{v}_g$ of a gauge symmetry as a vector field on the product manifold $X \times U = \{(x^\mu, u^\alpha)\}$ (where X represents space–time and U the space of dynamical fields). Such a vector field may be realized as a differential operator

$$\boldsymbol{v}_g = \sum_\alpha Q^\alpha[g]\partial_{u^\alpha}. \tag{2.5}$$

Here, $Q^\alpha[g]$ are the so-called characteristics of $\boldsymbol{v}_g$, which generally depend on $\{g(x), \partial_\mu g(x), \ldots\}$ and are defined for each dynamical variable u^α. The symbol ∂_{u^α} defines a vector field on $X \times U$, which acts as a partial derivative with respect to u^α on functions of x^μ and u^α. (We will clarify this with a concrete example momentarily.) We emphasize that the freedom to independently specify $g(x)$ at each point in space–time is what makes $\boldsymbol{v}_g$ a local symmetry. A global symmetry, by contrast, would transform the fields at each point of space–time identically, such that $g(x) = \text{const}$.

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Referring the reader to Hydon & Mansfield (2011) for greater detail, we have now assembled the minimal formalism necessary to construct N2T's differential identity from a system's local gauge symmetry. Given an action $S[u^\alpha, u^\alpha_\mu, \ldots] = \int \mathrm{d}^4x\, \mathcal{L}$ that is invariant under the symmetry generator $\boldsymbol{v}_g$ of (2.5), N2T guarantees the following differential identity of its EOM:

$$E_g\left[\sum_\alpha Q^\alpha[g] E_{u^\alpha}(\mathcal{L})\right] = 0. \tag{2.6}$$

In this equation, $g(x)$ is treated as a dynamical variable, and its Euler operator E_g is applied to an expression involving each dynamical variable's EOM – $E_{u^\alpha}(\mathcal{L})$ – and its corresponding characteristic in $\boldsymbol{v}_g$ – $Q^\alpha[g]$.

Assuming that the characteristics $Q^\alpha[g]$ of $\boldsymbol{v}_g$ are linear in g and its derivatives, the final expression of (2.6) is independent of g (as we soon show by example), and correspondingly takes the form of (2.1). Equation (2.6) is therefore an off-shell differential identity of the equations of motion; nowhere in this construction is the dynamical equation $E_{u^\alpha}(\mathcal{L}) = 0$ enforced. Accordingly, using the characteristics of a Lagrangian system's local gauge symmetry, N2T's off-shell differential identity is easily discovered via (2.6).

Before applying this method to the Vlasov–Maxwell system of interest in § 3, we make the preceding N2T formalism more concrete with a brief example from the vacuum Maxwell action

$$S = \int \mathrm{d}^4x \mathcal{L} = -\frac{1}{4}\int \mathrm{d}^4x\, F_{\mu\nu}F^{\mu\nu}, \tag{2.7}$$

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

$$0 = E_{A_\sigma}(\mathcal{L}) = \left[\frac{\partial}{\partial A_\sigma} - D_\tau \frac{\partial}{\partial(\partial_\tau A_\sigma)} + \cdots\right]\mathcal{L} = \partial_\tau F^{\tau\sigma}. \tag{2.8}$$

We now observe that, for arbitrary smooth $\lambda(x)$, S is invariant under the local gauge transformation $A_\mu(x) \to A_\mu(x) - \partial_\mu\lambda(x)$. The infinitesimal generator of this gauge transformation is given by the following vector field with characteristics $Q^{A_\mu}[\lambda] = -\partial_\mu\lambda$:

$$\boldsymbol{v}_\lambda = -(\partial_\mu\lambda)\partial_{A_\mu}. \tag{2.9}$$

Here, as above, the Einstein summation convention over μ is implicit. To see that this vector field is correct, note that the flow generated by $\boldsymbol{v}_\lambda$ on the product manifold $X \times \{A_\mu\}$ transforms A_μ appropriately

$$\begin{aligned}\exp[\boldsymbol{v}_\lambda](x^\rho, A_\sigma) &= \left[\mathbb{1} + \boldsymbol{v}_\lambda + \frac{1}{2!}\boldsymbol{v}_\lambda^2 + \cdots\right](x^\rho, A_\sigma)\\ &= \left[\mathbb{1} - (\partial_\mu\lambda)\partial_{A_\mu} + \frac{1}{2!}(\partial_\mu\lambda)^2\partial_{A_\mu}^2 + \cdots\right](x^\rho, A_\sigma)\\ &= (x^\rho, A_\sigma - \partial_\sigma\lambda).\end{aligned} \tag{2.10}$$

(We note that ∂_{A_μ} acts as a partial derivative, as expected. The space–time X itself is invariant under such an 'internal' gauge transformation, since $\boldsymbol{v}_\lambda$ – like $\boldsymbol{v}_g$ in (2.5) – has no components of the form ∂_{x^μ}. This is in contrast to a space–time translation ∂_t or rotation $y\partial_x - x\partial_y$, for example.)

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Given the EOM in (2.8) and the symmetry characteristics in (2.9), we now simply plug in for $E_{u^\alpha}(\mathcal{L})$ and $Q^\alpha[\lambda]$ in (2.6) to derive this system's N2T differential identity

$$\begin{aligned} 0 &= E_\lambda[-(\partial_\sigma\lambda)\partial_\tau F^{\tau\sigma}] \\ &= \partial_\sigma\partial_\tau F^{\tau\sigma}. \end{aligned} \tag{2.11}$$

As expected, because of the linearity of $\lambda(x)$ in $Q^{A_\mu}[\lambda]$, $\lambda(x)$ vanishes from (2.11).

Equation (2.11) is the resultant N2T differential identity. Due to the antisymmetry of $F^{\mu\nu}$, this identity appears rather trivial, and conveys the appropriate sense that N2T produces off-shell identities independent of a system's dynamics. Nevertheless, merely from the gauge symmetry of S, the above N2T procedure sheds light on the kinematics of the Maxwell action. In the next section, we will find that the same procedure derives the local charge conservation law of the Vlasov–Maxwell system.

3. Noether's second theorem for Vlasov–Maxwell systems

3.1. *The continuous space–time Klimontovich–Maxwell model*

We now use the preceding N2T procedure to systematically derive a charge conservation law for the continuous space–time Klimontovich–Maxwell system. This system specializes a Vlasov–Maxwell system to the following distribution function defined by N point particles

$$f(t,\boldsymbol{x},\boldsymbol{v}) = \sum_{j=1}^{N} \delta^{(3)}(\boldsymbol{x}-\boldsymbol{X}_j(t))\delta^{(3)}(\boldsymbol{v}-\dot{\boldsymbol{X}}_j(t)). \tag{3.1}$$

The Klimontovich–Maxwell system is accordingly described by the following action:

$$\begin{aligned} S = \int \mathrm{d}^4x\ \mathcal{L}[\phi,\boldsymbol{A},\boldsymbol{X}_i] \ = \ \int \mathrm{d}^4x \Bigg[&\frac{1}{2}(\nabla\phi+\partial_t\boldsymbol{A})^2 - \frac{1}{2}(\nabla\times\boldsymbol{A})^2 \\ &+ \sum_{j=1}^{N} \delta_j \cdot \left(\frac{1}{2}m_j\dot{\boldsymbol{X}}_j^2 - q_j\phi + q_j\boldsymbol{A}\cdot\dot{\boldsymbol{X}}_j\right)\Bigg]. \end{aligned} \tag{3.2}$$

Here, $\boldsymbol{A}=\boldsymbol{A}(t,\boldsymbol{x})$ is the vector potential, $\phi=\phi(t,\boldsymbol{x})$ is the electric potential, $\boldsymbol{X}_i=\boldsymbol{X}_i(t)$ 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:

$$\delta_j := \delta^{(3)}(\boldsymbol{x}-\boldsymbol{X}_j(t)). \tag{3.3}$$

We apply Euler operators to derive the Euler–Lagrange equations of each field

$$\left.\begin{aligned} E_\phi(\mathcal{L}) &= \nabla\cdot\boldsymbol{E}-\rho, \\ E_{\boldsymbol{A}}(\mathcal{L}) &= \partial_t\boldsymbol{E}-\nabla\times\boldsymbol{B}+\boldsymbol{J}, \\ E_{\boldsymbol{X}_i}(\mathcal{L}) &= \delta_i\cdot[-m_i\ddot{\boldsymbol{X}}_i + q_i(\boldsymbol{E}+\dot{\boldsymbol{X}}_i\times\boldsymbol{B})], \end{aligned}\right\} \tag{3.4}$$

where we have used the distributional derivative

$$\int f(\eta)\delta'(\eta)\,\mathrm{d}\eta = -\int f'(\eta)\delta(\eta)\,\mathrm{d}\eta, \tag{3.5}$$

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with $\eta \in \{t, \boldsymbol{x}\}$, and where

$$\left.\begin{aligned} \boldsymbol{E}(t,\boldsymbol{x}) &:= -\nabla\phi(t,\boldsymbol{x}) - \partial_t \boldsymbol{A}(t,\boldsymbol{x}), \\ \boldsymbol{B}(t,\boldsymbol{x}) &:= \nabla \times \boldsymbol{A}(t,\boldsymbol{x}), \\ \rho(t,\boldsymbol{x}) &:= \sum_{j=1}^{N} q_j \delta_j, \\ \boldsymbol{J}(t,\boldsymbol{x}) &:= \sum_{j=1}^{N} q_j \dot{\boldsymbol{X}}_j(t) \delta_j. \end{aligned}\right\} \tag{3.6}$$

As noted in (2.2), an Euler operator E_u for an arbitrary field u is essentially defined to accommodate integration by parts, such as that in (3.5). In particular, total derivatives in $\mathcal{L}$ – e.g. $(f\delta)'$ – that contribute to boundary terms of the action integral $S = \int \mathcal{L}\, \mathrm{d}^4x$ – e.g. $f\delta|_{-\infty}^{\infty}$ – lie in the kernel of E_u, such that $E_u(\mathcal{L} + \mathrm{Div}\,\gamma) = E_u(\mathcal{L})$. Indeed, the operator relation $E_u \circ \mathrm{Div} = 0$ always holds (see the 'variational complex' of Olver (1986)), where Div denotes a divergence.

We now note that the action of (3.2) is invariant under the following gauge transformation:

$$\left.\begin{aligned} \phi &\to \phi' = \phi + \partial_t \lambda, \\ \boldsymbol{A} &\to \boldsymbol{A}' = \boldsymbol{A} - \nabla\lambda. \end{aligned}\right\} \tag{3.7}$$

In particular, the electromagnetic terms of the Lagrangian are invariant, while the coupled particle terms pick up a divergence – namely, $\mathcal{L} \to \mathcal{L} + \partial_\mu \gamma^\mu$, where $\gamma^\mu = -\sum_j q_j \delta_j \lambda \cdot (1, \dot{\boldsymbol{X}}_j)$ – that vanishes on the boundary of S. The vector field corresponding to this transformation – equivalent to (2.9) – is given by

$$\boldsymbol{v}_\lambda = \sum_\alpha Q^\alpha[\lambda]\partial_{u^\alpha} = (\partial_t\lambda)\partial_\phi - (\nabla\lambda)\cdot\partial_{\boldsymbol{A}} \tag{3.8}$$

for an arbitrary smooth function $\lambda(x)$.

Finally, given EOM in (3.4) and the characteristics of our gauge symmetry in (3.8), we may derive the differential identity of N2T using the construction of (2.6)

$$\begin{aligned} \sum_\alpha Q^\alpha[\lambda] E_{u^\alpha}(\mathcal{L}) &= Q^\phi[\lambda]\cdot E_\phi(\mathcal{L}) + Q^{\boldsymbol{A}}[\lambda]\cdot E_{\boldsymbol{A}}(\mathcal{L}) \\ &= (\partial_t\lambda)[\nabla\cdot\boldsymbol{E} - \rho] - \nabla\lambda\cdot[\partial_t\boldsymbol{E} - \nabla\times\boldsymbol{B} + \boldsymbol{J}] \end{aligned} \tag{3.9}$$

such that

$$\begin{aligned} 0 &= E_\lambda\left[\sum_\alpha Q^\alpha[\lambda] E_{u^\alpha}(\mathcal{L})\right] \\ &= -\partial_t[\nabla\cdot\boldsymbol{E} - \rho] + \nabla\cdot[\partial_t\boldsymbol{E} - \nabla\times\boldsymbol{B} + \boldsymbol{J}] \\ &= \partial_t\rho + \nabla\cdot\boldsymbol{J}. \end{aligned} \tag{3.10}$$

In the final line, we have noted the equality of mixed partials and the vanishing divergence of the curl.

The N2T differential identity arising from the Klimontovich–Maxwell Lagrangian's local gauge symmetry evidently discovers the charge conservation law itself. By construction, this conservation law must hold off-shell and identically; in particular, equation (3.10) does not require the equations of motion in order to hold true. It is a trivial conservation law – also referred to as a 'strong' or 'improper' conservation

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law (Brading & Brown 2000) – an often-overlooked fact that is immediately verified upon examining the definitions of ρ and $\boldsymbol{J}$ in (3.6).

3.2. *The geometric PIC method of Squire et al. (2012)*

We now derive an analogous charge conservation law for the discrete, gauge-symmetric Vlasov–Maxwell PIC method defined by Squire *et al.* (2012). In this PIC scheme, space–time is discretized by a d-dimensional spatial simplicial complex (comprised of triangles in two dimensions or tetrahedra in three dimensions) whose structure is held 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 prismal complex P_C. We use DEC (Desbrun *et al.* 2005) to define fields on P_C that are single valued on its k-cells (or their circumcentric duals) for $0 \leqslant k \leqslant d+1$. In the present paper, we shall assume a spatial dimensionality $d = 3$, such that P_C is four-dimensional, with three-dimensional spatial tetrahedra comprising each time slice.

We first review some elements of DEC formalism that are necessary in the present study. It will be useful to distinguish the spatial edges from the temporal edges of P_C, so we denote a vertex of P_C by $\left[\begin{smallmatrix} i \\ n \end{smallmatrix}\right]$, where i is the spatial index of the vertex and n is its temporal index. A discrete 0-form α is then defined by its values at each vertex, and a discrete 1-form β by its values on each edge

$$\left.\begin{aligned} \alpha &= \sum_{\left[\begin{smallmatrix} i \\ n \end{smallmatrix}\right]} \alpha^i_n \Delta^i_n, \\ \beta &= \sum_{i,n} \beta^i_{n-1/2} \Delta^i_{n-1/2} + \sum_{[ij],n} \beta^{ij}_n \Delta^{ij}_n. \end{aligned}\right\} \tag{3.11}$$

Here, we have expressed the discrete forms (equivalently, cochains) α and β in terms of their cochain bases, where Δ^i_n is an element of the 0-cochain basis that maps $\left[\begin{smallmatrix} i \\ n \end{smallmatrix}\right]$ to 1 and all other vertices to 0; Δ^{ij}_n is similarly an element of the 1-cochain basis that maps the oriented edge $[ij]$ to 1 and all others to 0. (A temporal edge is understood to be oriented in the positive time direction, and its cochain is denoted $\Delta^i_{n-1/2}$.) Discrete k-forms of higher degree may be constructed with cochain bases in essentially the same way. The formalism of cochain bases will prove especially useful when we derive EOM for the dynamical fields on P_C – that is, when we define a DEC Euler operator.

Let us denote the set of all vertices in P_C by $\{v\}$, the set of spatial and temporal edges by $\{e\} = \{e_s\} \sqcup \{e_t\}$, and the set of spatial and 'spatio-temporal' faces by $\{f\} = \{f_s\} \sqcup \{f_t\}$. The DEC exterior derivative d, satisfying $\mathrm{d}^2 = 0$, may be defined (Elcott & Schröder 2005; Desbrun, Kanso & Tong 2006) by a matrix multiplication in the cochain basis. For a 1-form β, we see this as follows:

$$\mathrm{d}\beta = \mathrm{d}(\beta_e \Delta^e) = \beta_e \, \mathrm{d}\Delta^e = \beta_e W^e_f \Delta^f, \tag{3.12}$$

where the matrix entry W^e_f stores the weight – $\{\pm 1, 0\}$ – of the 1-cochain Δ^e in the 2-cochain Δ^f. (We recall that the boundary operator on chains – ∂ – is similarly determined by $W^f_e = (W^e_f)^T$.) We adopt the Einstein summation convention in (3.12) and hereafter for prismal complex indices: $\{v\}$, $\{e\}$, and $\{f\}$.

For example, the electromagnetic gauge field A – a discrete 1-form defined on all edges of P_C – neatly splits in into an electric potential $\phi^i_{n-1/2} := -A^i_{n-1/2}$ and a vector

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potential $\boldsymbol{A}_n^{ij} := A_n^{ij}$, as follows:

$$\begin{aligned} A &= -\sum_{i,n} \phi^i_{n-1/2} \Delta^i_{n-1/2} + \sum_{[ij],n} \boldsymbol{A}^{ij}_n \Delta^{ij}_n \\ &= -\phi_{e_t} \Delta^{e_t} + \boldsymbol{A}_{e_s} \Delta^{e_s}. \end{aligned} \tag{3.13}$$

Using (3.12), we may correspondingly express $\mathrm{d}A$ as

$$\begin{aligned} \mathrm{d}A &= -\phi_{e_t}\, \mathrm{d}\Delta^{e_t} + \boldsymbol{A}_{e_s}\, \mathrm{d}\Delta^{e_s}, \\ &= (-\phi_{e_t} W^{e_t}_{f_t} + \boldsymbol{A}_{e_s} W^{e_s}_{f_t}) \Delta^{f_t} + \boldsymbol{A}_{e_s} W^{e_s}_{f_s} \Delta^{f_s} \\ &= E \wedge \mathrm{d}t + B \\ &= F, \end{aligned} \tag{3.14}$$

where we have made use of the 1-form $\mathrm{d}t := \sum_{e_t} \Delta^{e_t}$ and wedge product to implicitly define the spatial 1- and 2-forms E and B, respectively, and the Faraday 2-form F (Stern *et al.* 2015). (As a note of caution, we emphasize that the preceding vector potential $\boldsymbol{A}$ is a single number on each spatial edge, and its bold notation is only suggestive. On the other hand, the Whitney interpolant of $\boldsymbol{A}$ will coordinatize $\mathbb{R}^3$ and thereby extend the single valued $\boldsymbol{A}$ from the spatial edges of P_C to a 3-component vector field, as we shall see.)

The map from primal k-forms to dual $(4-k)$-forms on P_C is effected via the metric-dependent Hodge star operator, $\star$. The Hodge star is defined (Abraham, Marsden & Ratiu 1988; Desbrun *et al.* 2005) such that the symmetric, metric-induced inner product $(\cdot, \cdot)$ on k-forms satisfies

$$(\omega, \nu)\mu = \omega \wedge \star\nu \tag{3.15}$$

for primal k-forms ω and ν and volume top form μ. For a k-form ω on an n-dimensional cell complex ($n = 4$ on P_C), it can therefore be shown that

$$\star\,(\star\omega) = (-1)^{k(n-k)+\mathrm{Ind}(g)}\omega. \tag{3.16}$$

Here, $\mathrm{Ind}(g) = \#\{\mathrm{eig}[g] < 0\}$ represents the index of the metric g. In the present context, we adopt a $(-+++)$ convention for our Lorentzian metric $g = \eta$, such that $\mathrm{Ind}(g) = 1$ on P_C. The dual $(4-k)$-form $\star\alpha$ is thus defined on a dual chain $(\star\sigma)^{4-k}$ as follows:

$$\langle \star\alpha, \star\sigma \rangle = \epsilon(\sigma) \frac{|\star\,\sigma|}{|\sigma|} \langle \alpha, \sigma \rangle, \tag{3.17}$$

where

$$\epsilon(\sigma) = \begin{cases} +1 & \text{if } \sigma \text{ is entirely spacelike} \\ -1 & \text{otherwise.} \end{cases} \tag{3.18}$$

Here, $|\sigma^k|$ denotes the k-volume of the k-dimensional σ^k (where $|\sigma^0| = 1$ for a single vertex), and $\langle \cdot, \cdot \rangle$ denotes a k-cochain evaluated on a k-chain in (3.17).

Integration by parts on P_C – which is necessary for the derivation of EOM, as in (2.2) – may be facilitated via the codifferential operator, δ. Up to boundary contributions, δ is a formal adjoint to d, that is

$$(\mathrm{d}\alpha, \beta)\mu = (\alpha, \delta\beta)\mu + \mathrm{d}(\alpha \wedge \star\beta). \tag{3.19}$$

When acting on a k-form defined on an n-dimensional complex, δ is given by (Abraham *et al.* 1988; Desbrun *et al.* 2005)

$$\delta = (-1)^{n(k-1)+1+\mathrm{Ind}(g)} \star\, \mathrm{d}\, \star. \tag{3.20}$$

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We observe that, whereas d maps a k-form to a $(k+1)$-form, δ reduces its degree to a $(k-1)$ form.

Having briefly reviewed relevant elements of DEC, we may now restate the discrete action of Squire *et al.* (2012), defined on P_C

$$S = \sum_{V_{\sigma^2}} -\frac{1}{2}\,\mathrm{d}A \wedge \star\,\mathrm{d}A + \sum_{p,n}\left\{\frac{h}{2}m_p\left|\frac{\boldsymbol{X}^p_{n+1/2}-\boldsymbol{X}^p_{n-1/2}}{h}\right|^2 - q_p\sum_i \phi^i_{n-1/2}\varphi^i(\boldsymbol{X}^p_{n-1/2})\right.$$
$$\left. + q_p\left(\frac{\boldsymbol{X}^p_{n+1/2}-\boldsymbol{X}^p_{n-1/2}}{h}\right)\cdot\sum_{[ij]}\boldsymbol{A}^{ij}_n\int_{t_{n-1/2}}^{t_{n+1/2}}\mathrm{d}t\,\varphi^{ij}(\boldsymbol{X}^p(t))\right\}. \tag{3.21}$$

In (3.21), we have denoted a sum over support volumes V_{σ^2} for the primal-dual 4-form $\mathrm{d}A \wedge \star\mathrm{d}A$, with A defined as in (3.13). V_{σ^2} represents the convex hull of the 2-chain σ^2 and its dual $\star\sigma^2$ on which $\langle \mathrm{d}A, \sigma^2\rangle$ and $\langle \star\mathrm{d}A, \star\sigma^2\rangle$ are respectively defined. The symbol h denotes the time step, n the time index and p the particle index. $\boldsymbol{X}^p(t)$ is defined as the constant velocity path between the particle's staggered-time positions $\boldsymbol{X}^p_{n-1/2}$ and $\boldsymbol{X}^p_{n+1/2}$. In particular, particle paths are chosen to have straight line trajectories between the staggered times $t \in [(n-1/2)h, (n+1/2)h]$, $\forall n \in \mathbb{Z}$.

The Whitney 0-form $\varphi^i(x)$ and 1-form $\varphi^{ij}(x)$ interpolate ϕ and $\boldsymbol{A}$ to an arbitrary point $x \in P_C$ (Bossavit 1988). In effect, φ^i and φ^{ij} complete the spatial components of the cochain bases Δ^i_n and Δ^{ij}_n adopted in (3.11) by extending DEC forms to the convex hull of P_C. In the continuous space–time of the Klimontovich–Maxwell system, the everywhere-defined gauge fields $\phi(t, \boldsymbol{x})$ and $\boldsymbol{A}(t, \boldsymbol{x})$ were 'attached' to point particles by the delta function, $\delta^{(3)}(\boldsymbol{x} - \boldsymbol{X}_j(t))$. In the prismal 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 (3.6). For example, the spatial dot product in (3.21) composes $\boldsymbol{X}^p_{n+1/2}$ with the Whitney-interpolated 3-component vector field $\boldsymbol{A}^{ij}_n\varphi^{ij}(\boldsymbol{X}^p(t))$, (where $\boldsymbol{A}^{ij}_n$ represents a single number and φ^{ij} a 3-component vector).

We now follow the continuous space–time N2T procedure of (3.4)–(3.10) by examining the equations of motion and gauge symmetry of S in (3.21). As we have already seen, the differential structure of space–time has been replaced in the discrete setting by the prismal complex P_C, its DEC operators and Whitney forms. To derive the Euler–Lagrange equations of S, therefore, we must define an Euler operator for fields defined on this discrete structure. By analogy with (2.3), such an operator must implement a variational derivative on the space of fields defined on P_C.

Consider, for example, a k-form α defined by its expansion in k-cochain basis elements: $\alpha = \sum_\sigma \alpha_\sigma \Delta^\sigma$, where σ ranges over all k-cells on P_C. Since each component α_σ of α can be varied independently, the variational derivative of α_σ takes the simple form of a partial derivative. We therefore define the Euler operator E_{α_σ} on the action S as follows:

$$E_{\alpha_\sigma}(S) := \frac{\partial S}{\partial \alpha_\sigma} = \frac{\partial}{\partial \alpha_\sigma}\sum L. \tag{3.22}$$

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(We note that in a discrete setting, variational derivatives are made to act on the entire action S, rather than on the Lagrangian, because discrete Lagrangians are necessarily non-local.) As usual we will assume that all fields and their variations have compact support, such that any divergence term in L – which contributes to $S = \sum L$ only at the boundary – vanishes under E_{α_σ}. Equation (3.22) is the DEC counterpart to the continuous Euler operator defined in (2.3), and is now applied to derive our EOM.

To calculate $E_{\phi_{e_t}}(S)$ and $E_{A_{e_s}}(S)$, we first re-express $\mathrm{d}A \wedge \star \mathrm{d}A$ in S using (3.15)–(3.20) and the invariance of S under the addition of a divergence ($L \to L + \mathrm{d}\gamma$)

$$\begin{aligned} \mathrm{d}A \wedge \star \mathrm{d}A &\overset{(3.15)}{=} (\mathrm{d}A, \mathrm{d}A)\mu \overset{(3.19)}{\approx} (A, \delta\, \mathrm{d}A)\mu \\ &\overset{(3.15)}{=} A \wedge \star\delta\, \mathrm{d}A \overset{(3.20)}{=} A \wedge \star\star\, \mathrm{d} \star \mathrm{d}A \overset{(3.16)}{=} A \wedge \mathrm{d} \star \mathrm{d}A, \end{aligned} \tag{3.23}$$

where $\approx$ indicates equality up to an (ignorable) divergence. Then, using (3.13) and noting the symmetry of the intermediate expression $(\mathrm{d}A, \mathrm{d}A)\mu$ above, we apply the Euler operator of (3.22) to derive the EOM for A as follows:

$$0 = E_{\phi_{e_t}}(S) = \Delta^{e_t} \wedge \mathrm{d} \star \mathrm{d}A - \rho^{e_t}, \tag{3.24a}$$

$$0 = E_{A_{e_s}}(S) = -\Delta^{e_s} \wedge \mathrm{d} \star \mathrm{d}A + J^{e_s}, \tag{3.24b}$$

where

$$\rho^{e_t} := \sum_p q_p \varphi^i(\boldsymbol{X}^p_{t(e_t)}), \tag{3.25a}$$

$$J^{e_s} := \sum_p q_p \left(\frac{\boldsymbol{X}^p_{t_f(e_s)} - \boldsymbol{X}^p_{t_i(e_s)}}{h} \right) \cdot \int_{t_i(e_s)}^{t_f(e_s)} \mathrm{d}t\, \varphi^{e_s}(\boldsymbol{X}^p(t)). \tag{3.25b}$$

In (3.25*a*), i denotes the spatial vertex associated with e_t, and $\boldsymbol{X}^p_{t(e_t)}$ denotes the position of particle p at the time coincident with the midpoint $\left[{}^{i}_{n-\frac{1}{2}}\right]$ of e_t. In (3.25*b*), $\boldsymbol{X}^p_{t_i(e_s)}$ and $\boldsymbol{X}^p_{t_f(e_s)}$ denote the initial and final particle positions, respectively, coincident with the midpoints $\left[{}^{i}_{n-\frac{1}{2}}\right]$ and $\left[{}^{i}_{n+\frac{1}{2}}\right]$ that bookend the $t = n$ time slice containing e_s.

It is worth pausing to interpret these EOM. We first observe that the primal-dual wedge product in (3.24*a*) is only non-vanishing on the spatial ($\star\Delta^{e_t}$) component of $\mathrm{d} \star \mathrm{d}A$. This follows from the definition of the primal-dual wedge product, which is only non-zero on the convex hulls of a cell and its dual: $CH(\sigma, \star\sigma)$. Reading off from (3.14), therefore, equation (3.24*a*) becomes

$$\rho^{e_t} = \Delta^{e_t} \wedge \mathrm{d} \star (E \wedge \mathrm{d}t) = \mathrm{d}D \wedge \Delta^{e_t}, \tag{3.26}$$

Gauss's law for the electric displacement dual 2-form D, as expected. An analogous interpretation of (3.24*b*) yields a discrete Ampère–Maxwell law. We have omitted the $E_{\boldsymbol{X}^p}(S)$ EOM for particle trajectories, as they will not be necessary for the derivation of charge conservation via N2T – just as they were unnecessary in (3.9)–(3.10). These implicit time-step particle EOM are derived in Squire *et al.* (2012).

Having derived our field equations of motion, we must now examine the gauge symmetry of the action S in (3.21). In particular, S is invariant under the local gauge transformation $A \to A - \mathrm{d}f$, defined by

$$\left.\begin{aligned} \phi^i_{n+1/2} \to \phi^i_{n+1/2} + \delta\phi^i_{n+1/2} = \phi^i_{n+1/2} + (f^i_{n+1} - f^i_n), \\ \boldsymbol{A}^{ij}_n \to \boldsymbol{A}^{ij}_n + \delta\boldsymbol{A}^{ij}_n = \boldsymbol{A}^{ij}_n - (f^j_n - f^i_n), \end{aligned}\right\} \tag{3.27}$$

where $f = f_v \Delta^v$ is an arbitrary primal 0-form on P_C.

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After all, the electromagnetic term of $S - \mathrm{d}A \wedge \star \mathrm{d}A -$ is clearly invariant under $A \to A - \mathrm{d}f$, since $\mathrm{d}^2 = 0$. Furthermore, as noted in Squire *et al.* (2012), the gauge invariance of the particle terms of S follows from a defining property of Whitney interpolation: $\mathrm{d}_c((\alpha)_{\text{interp}}) = (\mathrm{d}_d\alpha)_{\text{interp}}$, where d_c and d_d denote continuous and discrete exterior derivatives, respectively and $(\cdot)_{\text{interp}}$ denotes Whitney interpolation. Equation (3.27) therefore transforms $L \to L + \mathrm{d}_c\gamma$, adding a divergence term analogous to the transformation of (3.7) for the continuous space–time Vlasov–Maxwell system.

Following (3.8), the gauge transformation of (3.27) is seen to be generated by a vector field

$$\boldsymbol{v}_f = \sum_\alpha Q^\alpha[f]\partial_{u^\alpha} = \sum_{e_t}(\mathrm{d}_{e_t}f)\partial_{\phi_{e_t}} - \sum_{e_s}(\mathrm{d}_{e_s}f)\partial_{\boldsymbol{A}_{e_s}}, \tag{3.28}$$

where the coefficient $\mathrm{d}_e f = f_{v_2} - f_{v_1}$ corresponds to the oriented edge $e = [v_1 v_2]$, and where the sums are taken over all temporal and spatial edges, respectively.

We have thus gathered the necessary data to complete the N2T construction of (2.6) for our DEC system. As in (3.9), we note

$$\begin{aligned}\sum_\alpha Q^\alpha[f]E_{u^\alpha}(S) &= \sum_{e_t} Q^{\phi_{e_t}}[f]\cdot E_{\phi_{e_t}}(S) + \sum_{e_s} Q^{\boldsymbol{A}_{e_s}}[f]\cdot E_{\boldsymbol{A}_{e_s}}(S)\\ &= \sum_{e_t}(\mathrm{d}_{e_t}f)\cdot(\Delta^{e_t}\wedge \mathrm{d}\star\,\mathrm{d}A - \rho^{e_t})\\ &\quad + \sum_{e_s}(-\mathrm{d}_{e_s}f)\cdot(-\Delta^{e_s}\wedge \mathrm{d}\star\,\mathrm{d}A + J^{e_s}).\end{aligned} \tag{3.29}$$

We now observe that

$$(\mathrm{d}_e f)\Delta^e = \mathrm{d}(f_v\Delta^v) = \mathrm{d}f, \tag{3.30}$$

so applying the Euler operator for f_v at vertex $v = \left[\begin{smallmatrix} i \\ n \end{smallmatrix}\right]$ to (3.29) yields

$$\begin{aligned} 0 &= E_{f_v}\left[\sum_\alpha Q^\alpha[f]E_{u^\alpha}(S)\right]\\ &= E_{f_v}\left[\sum_{V_{\sigma 1}} \mathrm{d}f\wedge \mathrm{d}\star\,\mathrm{d}A - \sum_{e_t}\left(\mathrm{d}_{e_t}f\right)\cdot\rho^{e_t} - \sum_{e_s}(\mathrm{d}_{e_s}f)\cdot J^{e_s}\right]\\ &= \Delta^v\wedge\star\delta\star\,\mathrm{d}\star\,\mathrm{d}A + (\rho^i_{n+1/2} - \rho^i_{n-1/2}) + \sum_j J^{[ij]}\\ &= (\rho^i_{n+1/2} - \rho^i_{n-1/2}) + \sum_j J^{[ij]}\end{aligned} \tag{3.31}$$

since up to a sign, $(\delta\star\,\mathrm{d}) = (\star\,\mathrm{d}\star\star\,\mathrm{d}) = \star\mathrm{d}^2 = 0$. The sum of $J^{[ij]}$ over j captures all spatial edges that terminate on vertex $v = \left[\begin{smallmatrix} i \\ n \end{smallmatrix}\right]$. The last equality of (3.31) reveals the desired charge conservation law on P_C. By its very construction through N2T, this conservation law is guaranteed to be an off-shell differential identity, as was (3.10). We readily verify this fact as follows.

First, we restrict our sources ρ and J to a particle of charge q whose path over one time step remains within a single spatial tetrahedron; the general case follows without significant alteration. We then recall (Bossavit 1988) that the Whitney 0-form φ^i

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interpolates from vertex i via barycentric coordinates such that, over the tetrahedron $[ijk\ell]$,

$$\varphi^i + \varphi^j + \varphi^k + \varphi^\ell = 1. \tag{3.32}$$

In vector form, the 1-form φ^{ij} is then given by

$$\varphi^{ij} = \varphi^i \nabla \varphi^j - \varphi^j \nabla \varphi^i. \tag{3.33}$$

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

$$\begin{aligned} \sum_{j \neq i} \varphi^{ij} &= \varphi^i \nabla \left(\sum_{j \neq i} \varphi^j \right) - \left(\sum_{j \neq i} \varphi^j \right) \nabla \varphi^i \\ &= \varphi^i \nabla (1 - \varphi^i) - (1 - \varphi^i) \nabla \varphi^i \\ &= -\nabla \varphi^i. \end{aligned} \tag{3.34}$$

It follows, then, that

$$\begin{aligned} \sum_{j \neq i} J^{[ij]} &= q \left(\frac{\boldsymbol{X}_f - \boldsymbol{X}_i}{h} \right) \cdot \int_{t_i}^{t_f} \mathrm{d}t \sum_{j \neq i} \varphi^{ij}(\boldsymbol{X}(t)) \\ &= -q \left(\frac{\boldsymbol{X}_f - \boldsymbol{X}_i}{h} \right) \cdot \int_{t_i}^{t_f} \mathrm{d}t \, \nabla \varphi^i(\boldsymbol{X}(t)) \\ &= -q \int_i^f \boldsymbol{v} \lrcorner \, \mathrm{d}\varphi^i \\ &= -q[\varphi^i(\boldsymbol{X}_f) - \varphi^i(\boldsymbol{X}_i)], \end{aligned} \tag{3.35}$$

where $\boldsymbol{v} \lrcorner \, \mathrm{d}\varphi^i$ is the interior product of the exact form $\mathrm{d}\varphi^i$ with respect to the velocity $\boldsymbol{v} := (1/h)(\boldsymbol{X}_f - \boldsymbol{X}_i)$, which is constant over a single time step of the particle. Upon comparison with the definition for ρ in (3.25*a*), it is clear that (3.31) holds off-shell, as desired. The N2T formalism of Hydon & Mansfield (2011) has succeeded in deriving the off-shell, discrete conservation law.

Before we depart from the Lagrangian formalism, we note that an alternative approach to deriving the conservation laws of the continuous space–time and DEC Vlasov–Maxwell actions – equations (3.2) and (3.21) – entails gauge fixing these actions by setting $\phi(x) = 0$ and $\phi^i_{n+1/2} = 0$, respectively. Such a gauge fixing removes these systems' degeneracy and uniquely determines solutions to their equations of motion. In such an approach, N1T is applied to the time-independent symmetry transformation $\boldsymbol{A}(t, \boldsymbol{x}) \to \boldsymbol{A}(t, \boldsymbol{x}) - \nabla \psi(\boldsymbol{x})$, thereby deriving a non-trivial conservation law in the form of a time evolution of Gauss's law. In the ensuing sections, we pursue an analogous gauge-fixing approach for the Hamiltonian Vlasov–Maxwell system, employing the Hamiltonian formalism's counterpart to N1T – the momentum map.

4. The momentum map and reduction of the Vlasov–Maxwell system

Having derived the N2T charge conservation laws of continuous and discrete Vlasov–Maxwell Lagrangian systems, we now explore the conservation laws of these gauge-symmetric systems in the Hamiltonian formalism. We first develop the

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necessary technical background for §§ 5–6, which study gauge-compatible splitting methods and their application to PIC algorithms. In this section, we review the Poisson structure of the Vlasov–Maxwell system, derived in Morrison (1980) and independently in Iwinski & Turski (1976), and later presented in its complete, correct form in Marsden & Weinstein (1982). Closely following this last reference, we review the Poisson reduction (Marsden & Weinstein 1974; Marsden & Ratiu 1986) of the Vlasov–Maxwell system, which 'spends' the system's gauge symmetries in order to eliminate their associated redundant (gauge) degrees of freedom. As we will discuss at length, this Poisson reduction is achieved via the momentum map, which in turn determines the local charge conservation law of the Vlasov–Maxwell system. The following section serves as a concise pedagogical summary of Marsden & Weinstein (1982), with additional discussion relevant to the more recent plasma physics literature.

4.1. *The Poisson structure of the Vlasov–Maxwell system*

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

$$\{\{F, G\}\}[f, \boldsymbol{A}, \boldsymbol{Y}] = \int \mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{p} f \left\{\frac{\delta F}{\delta f}, \frac{\delta G}{\delta f}\right\}_{\boldsymbol{xp}} + \int \mathrm{d}\boldsymbol{x}\left(\frac{\delta F}{\delta \boldsymbol{A}}\cdot\frac{\delta G}{\delta \boldsymbol{Y}} - \frac{\delta G}{\delta \boldsymbol{A}}\cdot\frac{\delta F}{\delta \boldsymbol{Y}}\right), \tag{4.1}$$

with time evolution defined by the Hamiltonian

$$H[f, \boldsymbol{A}, \boldsymbol{Y}] = \frac{1}{2}\int f\cdot|\boldsymbol{p}-\boldsymbol{A}|^2\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{p} + \frac{1}{2}\int[|\boldsymbol{Y}|^2 + |\nabla\times\boldsymbol{A}|^2]\,\mathrm{d}\boldsymbol{x}. \tag{4.2}$$

Here, F and G represent arbitrary functionals of the distribution function $f(\boldsymbol{x}, \boldsymbol{p})$, the 3-component vector potential $\boldsymbol{A}(\boldsymbol{x})$ and its conjugate momentum $\boldsymbol{Y}(\boldsymbol{x})$. As we shall see momentarily, $\boldsymbol{Y}$ can be readily identified as negative the electric field strength – (i.e. $\boldsymbol{Y} = -\boldsymbol{E}$). We note that our system is rendered in the temporal gauge, wherein the electric potential satisfies $\phi(\boldsymbol{x}) = 0$. As in Marsden & Weinstein (1982), we denote the Poisson bracket in (4.1) by $\{\{\cdot,\cdot\}\}$ merely to distinguish it from other Poisson structures.

The $\int \mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{p} f\{\delta_f\cdot, \delta_f\cdot\}_{\boldsymbol{xp}}$ operator in the first line of (4.1) is a Lie–Poisson bracket (Marsden & Ratiu 1999), which defines a Poisson structure for functions on a dual Lie algebra $\mathfrak{g}^*$. In general, the Lie–Poisson bracket on an arbitrary dual Lie algebra $\mathfrak{g}^*$ is defined to inherit the bracket $[\cdot,\cdot]$ of its underlying Lie algebra $\mathfrak{g}$ as follows:

$$\{F, G\}(\alpha) := -\left\langle \alpha, \left[\frac{\delta F}{\delta \alpha}, \frac{\delta G}{\delta \alpha}\right]\right\rangle. \tag{4.3}$$

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

$$\left\langle \beta, \frac{\delta F}{\delta \alpha}\right\rangle = D_\alpha F\cdot\beta = \left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} F(\alpha + \epsilon\beta). \tag{4.4}$$

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Since $\mathfrak{g}^{**} \cong \mathfrak{g}$, the functional derivative may be interpreted as an element of the Lie algebra.

In the present context, the Lie algebra $\mathfrak{g}$ corresponds to infinitesimal transformations of $(\boldsymbol{x}, \boldsymbol{p}) \cong \mathbb{R}^6$, 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.

$$[\boldsymbol{X}_h, \boldsymbol{X}_k] = -\{h, k\}_{\boldsymbol{xp}}. \tag{4.5}$$

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

$$\{h, k\}_{\boldsymbol{xp}} := (\partial_{\boldsymbol{x}} h \cdot \partial_{\boldsymbol{p}} k - \partial_{\boldsymbol{x}} k \cdot \partial_{\boldsymbol{p}} h). \tag{4.6}$$

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

$$\langle f, h \rangle := \int fh \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}\boldsymbol{p} \tag{4.7}$$

for $f \in \mathfrak{g}^*$, $h \in \mathfrak{g}$.

In this way, the operator $\int \mathrm{d}\boldsymbol{x} \, \mathrm{d}\boldsymbol{p} \, f\{\delta_f \cdot, \delta_f \cdot\}_{\boldsymbol{xp}}$ comprising the first term of (4.1) is seen to be a Lie–Poisson bracket of the form in (4.3). We note that the negative sign of (4.3) cancels with the negative sign of the anti-homomorphism of (4.5) to produce this operator.

The second term of (4.1) represents the electromagnetic 'sector' of our Poisson structure, and derives from the canonical symplectic structure on the cotangent space – $T^*Q = \{(\boldsymbol{A}, \boldsymbol{Y})\}$ – of the configuration space $Q = \{\boldsymbol{A}\}$. Therefore, the complete setting of the Vlasov–Maxwell system is a Poisson manifold, given by

$$M = \mathfrak{g}^* \times T^*Q, \tag{4.8}$$

with its bracket defined in (4.1).

We now consider dynamics on this Poisson manifold M. To derive our Hamiltonian EOM, it is convenient to define functionals

$$F(\boldsymbol{u}) := \int \mathrm{d}\boldsymbol{u}' \, F(\boldsymbol{u}') \delta(\boldsymbol{u} - \boldsymbol{u}') \tag{4.9}$$

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

$$\left.\begin{aligned} \dot{f}(\boldsymbol{x}, \boldsymbol{p}) = \{\{f, H\}\} &= -[\partial_{\boldsymbol{x}} f + \partial_{\boldsymbol{p}} f \cdot (\nabla \boldsymbol{A})] \cdot (\boldsymbol{p} - \boldsymbol{A}), \\ \dot{\boldsymbol{A}}(\boldsymbol{x}) = \{\{\boldsymbol{A}, H\}\} &= \boldsymbol{Y}, \\ \dot{\boldsymbol{Y}}(\boldsymbol{x}) = \{\{\boldsymbol{Y}, H\}\} &= \int f \cdot (\boldsymbol{p} - \boldsymbol{A}) \, \mathrm{d}\boldsymbol{p} - \nabla \times \nabla \times \boldsymbol{A}. \end{aligned}\right\} \tag{4.10}$$

We observe that $\boldsymbol{Y}$ plays the role of $-\boldsymbol{E}$, as expected. For convenience, we note that the familiar form of the Vlasov equation may be recovered from the first line of (4.10) by defining a distribution density $\bar{f}$ on $(\boldsymbol{x}, \boldsymbol{v})$ space where $\boldsymbol{v} = \boldsymbol{p} - \boldsymbol{A}$, i.e.

$$f(\boldsymbol{x}, \boldsymbol{p}) = \bar{f}(\boldsymbol{x}, \boldsymbol{p} - \boldsymbol{A}) = \bar{f}(\boldsymbol{x}, \boldsymbol{v}), \tag{4.11}$$

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

$$\boldsymbol{v} \cdot \boldsymbol{A}\boldsymbol{B} \cdot \boldsymbol{w} = v_i A_i B_j w_j \tag{4.12}$$

in Einstein notation.

4.2. *Gauge symmetry and the momentum map*

With our Poisson and Hamiltonian structure 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 Poisson manifold $M = \mathfrak{g}^* \times T^*Q$ of the form

$$\Phi_\psi : (f, \boldsymbol{A}, \boldsymbol{Y}) \mapsto (f \circ \tau_\psi, \boldsymbol{A} - \nabla \psi, \boldsymbol{Y}), \tag{4.13}$$

where

$$\tau_\psi(\boldsymbol{x}, \boldsymbol{p}) := (\boldsymbol{x}, \boldsymbol{p} + \nabla \psi). \tag{4.14}$$

We emphasize that Φ_ψ transforms f, and not $\boldsymbol{p}$ itself. It is straightforward to check that Φ_ψ is a canonical group action, i.e. that the Poisson bracket is preserved by the pullback of Φ_ψ, namely $\Phi_\psi^*\{\{F, G\}\} = \{\{\Phi_\psi^* F, \Phi_\psi^* G\}\}$.

We define such an arbitrary function $\psi \in \mathcal{F}$ as belonging to the abelian group $\mathcal{F} := C^\infty(\mathbb{R}^3)$ of smooth functions on $\mathbb{R}^3$, with the 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 (4.7).

Now let $\phi \in \mathfrak{f}$ denote an arbitrary Lie algebra element, such that $\exp(\epsilon\phi) \in \mathcal{F}$ $\forall$ $\epsilon \in \mathbb{R}$. By differentiating the group action $\Phi_{\exp(\epsilon\phi)}$ on M, we may associate to any such $\phi \in \mathfrak{f}$ the corresponding vector field ϕ_M on M, namely

$$\phi_M := \left. \frac{\mathrm{d}}{\mathrm{d}\epsilon} \right|_{\epsilon=0} \Phi_{\exp(\epsilon\phi)}. \tag{4.15}$$

The vector field ϕ_M is therefore the infinitesimal generator of the group action on M corresponding to $\phi \in \mathfrak{f}$.

For any canonical group action on Poisson manifold M, we may seek a corresponding momentum map. The momentum map $\mu : M \to \mathfrak{f}^*$ of a group action is defined such that, $\forall$ $\phi \in \mathfrak{f}$ and $m \in M$, the induced function

$$\left.\begin{array}{c} \mu^\phi : M \to \mathbb{R} \\ m \mapsto \langle \mu(m), \phi \rangle \end{array}\right\} \tag{4.16}$$

satisfies

$$\{\{F, \mu^\phi\}\} = \phi_M(F) \tag{4.17}$$

for arbitrary $F \in C^\infty(M)$. Here, $\phi_M(F)$ is the Lie derivative of F along the vector field ϕ_M. In particular, the momentum map μ assigns a dual element of $\mathfrak{f}^*$ to each point of M such that, when μ is everywhere paired with an element $\phi \in \mathfrak{f}$ of the Lie algebra, the resulting function μ^ϕ on M is a generating function of the associated vector field ϕ_M.

The preceding definition of μ is general to arbitrary Poisson systems with canonical group actions, and we now apply it to find μ for the Vlasov–Maxwell system of interest. We first note that a single point $m \in M = \mathfrak{g}^* \times T^*Q$ specifies $(f, \boldsymbol{A}, \boldsymbol{Y})$ over

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the entire $(\boldsymbol{x}, \boldsymbol{p})$ phase space. Given the group action defined in (4.13)–(4.14), it is immediately seen that ϕ_M can be expressed as the following infinitesimal operator on M corresponding to $\phi(\boldsymbol{x}) \in \mathfrak{f}$:

$$\{\{\cdot, \mu^\phi\}\} = \int \mathrm{d}\boldsymbol{x}\, \mathrm{d}\boldsymbol{p}\, \nabla\phi \cdot \frac{\partial f}{\partial \boldsymbol{p}} \frac{\delta}{\delta f} - \int \mathrm{d}\boldsymbol{x}\, \nabla\phi \cdot \frac{\delta}{\delta \boldsymbol{A}}. \tag{4.18}$$

Upon inspection, it is evident that to generate the operator of (4.18), the Poisson bracket of (4.1) requires that μ^ϕ be given by

$$\begin{aligned} \mu^\phi(m) &:= \langle \mu(m), \phi \rangle \\ &= \int \mathrm{d}\boldsymbol{x} \left[\int \mathrm{d}\boldsymbol{p} f(\boldsymbol{x}, \boldsymbol{p}) + \nabla \cdot \boldsymbol{Y} \right] \phi(\boldsymbol{x}), \end{aligned} \tag{4.19}$$

where $\langle \cdot, \cdot \rangle = \int \mathrm{d}\boldsymbol{x}$. Therefore, the momentum map must be

$$\begin{aligned} \mu(m) &= \int \mathrm{d}\boldsymbol{p} f(\boldsymbol{x}, \boldsymbol{p}) + \nabla \cdot \boldsymbol{Y} \\ &:= \rho + \nabla \cdot \boldsymbol{Y}, \end{aligned} \tag{4.20}$$

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

For later use, we further observe that μ is group equivariant

$$\mu \circ \Phi_\psi = \mathrm{Ad}^*_{\psi^{-1}} \circ \mu, \tag{4.21}$$

where $\mathrm{Ad}^*_{\psi^{-1}}$ 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 (4.20) that μ is invariant under $\mathcal{F}$ transformations, and since $\mathcal{F}$ is abelian, its coadjoint action on $\mathfrak{f}^*$ is simply the identity map.

4.3. *Deriving the conservation law*

The momentum map μ is defined as above – equations (4.15)–(4.17) – for any Poisson manifold M with a canonical group action Φ. If it should happen that a Hamiltonian H is furthermore defined on M such that H is invariant under Φ, then the momentum map μ so-constructed further guarantees a conservation law for the system.

Let us show this for our Vlasov–Maxwell system. We first note that Φ_ψ leaves the Hamiltonian invariant, $\Phi^*_\psi H = H$. By differentiating this expression with respect to ψ as in (4.15), it is seen that, infinitesimally

$$0 = \phi_M(H) = \{\{H, \mu^\phi\}\} = -\{\{\mu^\phi, H\}\} = -\dot{\mu}^\phi. \tag{4.22}$$

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

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

$$\dot{\mu} = \{\{\mu, H\}\} = 0. \tag{4.23}$$

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

$$0 = \dot{\mu} = \dot{\rho} + \nabla \cdot \dot{\boldsymbol{Y}}. \tag{4.24}$$

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This completes the canonical derivation of the Vlasov–Maxwell local conservation law – $\dot{\mu} = 0$ – in the continuous Hamiltonian formalism. We note that, setting $\boldsymbol{Y} = -\boldsymbol{E}$, equation (4.24) is the time evolution of Gauss's law.

With an additional substitution to (4.24) from the EOM for $\dot{\boldsymbol{Y}}$ in (4.10), we may re-express this canonical conservation law in the form

$$0 = \dot{\rho} + \boldsymbol{\nabla} \cdot \boldsymbol{J}, \tag{4.25}$$

where $\boldsymbol{J} := \int f \cdot (\boldsymbol{p} - \boldsymbol{A})\, \mathrm{d}\boldsymbol{p}$. Here ρ and $\boldsymbol{J}$ are (scalar and vector) densities over $\mathbb{R}^3$ and functionals in the sense of (4.9). This charge conservation law may be immediately checked by substituting the expression for $\dot{f}$ from (4.10). In the present Hamiltonian context, it is evident that (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. *Reduction of the Vlasov–Maxwell system*

Finally, we undertake the Poisson reduction (Marsden & Weinstein 1974; Marsden & Ratiu 1986) of the Vlasov–Maxwell system. Given a Poisson manifold $(M, \{\cdot,\cdot\}_M)$ on which a Lie group G acts by Poisson diffeomorphisms, the Poisson reduction of M is the unique quotient map $\pi : (M, \{\cdot,\cdot\}_M) \to (M/G, \{\cdot,\cdot\}_{M/G})$ satisfying $\pi^*\{f, g\}_{M/G} = \{\pi^* f, \pi^* g\}_M$. For a Poisson system equipped with a group-equivariant momentum map μ satisfying (4.21) – as in the Vlasov–Maxwell system of interest – such a quotient map may be defined on level sets of μ, as we now describe.

Consider the preimage of an arbitrary $\alpha \in \mathfrak{f}^*$ under $\mu : M \to \mathfrak{f}^*$, that is, the level set $\mu^{-1}(\alpha) \subset M$. We may take equivalence classes of this preimage under the full action of $\Phi_\psi \ \forall \ \psi \in \mathcal{F}$. That is, we reduce $\mu^{-1}(\alpha)$ to the quotient manifold $\mu^{-1}(\alpha)/\mathcal{F}$, and thereby take a 'slice' of the orbit of $\mu^{-1}(\alpha)$ under the action of $\mathcal{F}$. Because μ is equivariant in the sense of (4.21), this quotient is well defined. The reduced manifold $\mu^{-1}(\alpha)/\mathcal{F}$ will again be a Poisson manifold, as we now show.

Let us consider the particular case $\alpha = 0$, and define $M_0 := \mu^{-1}(0)$. By (4.20), M_0 corresponds to the submanifold of M on which $\rho = -\boldsymbol{\nabla} \cdot \boldsymbol{Y}$. 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 (4.13), namely

$$\left.\begin{aligned} \bar{f}(\boldsymbol{x}, \boldsymbol{v}) &= f(\boldsymbol{x}, \boldsymbol{p} = \boldsymbol{v} + \boldsymbol{A}), \\ \boldsymbol{B} &= \boldsymbol{\nabla} \times \boldsymbol{A}, \\ \boldsymbol{E} &= -\boldsymbol{Y}. \end{aligned}\right\} \tag{4.26}$$

We therefore identify the manifold of equivalence classes $\tilde{M}_0 := M_0/\mathcal{F}$ with the manifold $(\bar{f}, \boldsymbol{B}, \boldsymbol{E})$ of densities $\bar{f}$ defined on $(\boldsymbol{x}, \boldsymbol{v})$ space, vector fields $\boldsymbol{B}$ that satisfy $\boldsymbol{\nabla} \cdot \boldsymbol{B} = 0$, and vector fields $\boldsymbol{E}$ that satisfy $\bar{\rho} = \boldsymbol{\nabla} \cdot \boldsymbol{E}$, where now $\bar{\rho} := \int \bar{f}\, \mathrm{d}\boldsymbol{v}$. (We note that the choice to constrain M to $\{m \in M \mid \mu(m) = 0\}$ evidently corresponds to the physical case $\boldsymbol{\nabla} \cdot \boldsymbol{E} - \bar{\rho} = 0$, in which no 'external' charges are present in the system. Such a choice must be made when determining the Vlasov–Maxwell system's initial conditions, as we shall see.) Our reduction map is therefore summarized by

$$\begin{array}{rccc} \pi_{\mathrm{red}} : & \mu^{-1}(0) \subset M & \longrightarrow & \tilde{M}_0 := \mu^{-1}(0)/\mathcal{F} \\ & (f(\boldsymbol{x}, \boldsymbol{p}), \boldsymbol{A}, \boldsymbol{Y}) & \longmapsto & (\bar{f}(\boldsymbol{x}, \boldsymbol{v}), \boldsymbol{B}, \boldsymbol{E}). \end{array} \tag{4.27}$$

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As calculated in Marsden & Weinstein (1982) § 7, the substitution of (4.26) into the bracket of (4.1) yields the following reduced Poisson bracket on $\tilde{M}_0$:

$$\begin{aligned}\{\{F,G\}\}^{\mathrm{red}}[\bar{f},\boldsymbol{B},\boldsymbol{E}] = &\int \mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{v}\left[\bar{f}\left\{\frac{\delta F}{\delta \bar{f}},\frac{\delta G}{\delta \bar{f}}\right\}_{\boldsymbol{x}\boldsymbol{v}}\right.\\ &\left.+\bar{f}\boldsymbol{B}\cdot\left(\frac{\partial}{\partial \boldsymbol{v}}\frac{\delta F}{\delta \bar{f}}\times\frac{\partial}{\partial \boldsymbol{v}}\frac{\delta G}{\delta \bar{f}}\right)+\left(\frac{\delta F}{\delta \boldsymbol{E}}\cdot\frac{\partial \bar{f}}{\partial \boldsymbol{v}}\frac{\delta G}{\delta \bar{f}}-\frac{\delta G}{\delta \boldsymbol{E}}\cdot\frac{\partial \bar{f}}{\partial \boldsymbol{v}}\frac{\delta F}{\delta \bar{f}}\right)\right]\\ &+\int \mathrm{d}\boldsymbol{x}\left(\frac{\delta F}{\delta \boldsymbol{E}}\cdot\nabla\times\frac{\delta G}{\delta \boldsymbol{B}}-\frac{\delta G}{\delta \boldsymbol{E}}\cdot\nabla\times\frac{\delta F}{\delta \boldsymbol{B}}\right).\end{aligned} \tag{4.28}$$

We note that this process of Poisson reduction preserves the $\dot{\mu}=0$ conservation law associated with the unreduced Poisson manifold M. After all, the image of π_{red} restricts M to (quotients of) a submanifold $M_0\subset M$ on which μ is constant – in particular, level sets of a single value of μ. The conservation law of (4.24) is clearly respected by this reduction, and may simply be re-expressed in the phase space variables of the reduced manifold $\tilde{M}_0$, along with its form in (4.25), i.e.

$$\begin{aligned}0=\dot{\bar{\mu}} &= \dot{\bar{\rho}}-\nabla\cdot\dot{\boldsymbol{E}}\\ &= \dot{\bar{\rho}}+\nabla\cdot\bar{\boldsymbol{J}},\end{aligned} \tag{4.29}$$

where

$$\begin{aligned}\bar{\mu} &= \int \mathrm{d}\boldsymbol{v}\bar{f}(\boldsymbol{x},\boldsymbol{v})-\nabla\cdot\boldsymbol{E}\\ &= \bar{\rho}-\nabla\cdot\boldsymbol{E},\end{aligned} \tag{4.30}$$

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

We note that the reduced bracket of (4.28) is a well-defined Poisson bracket specifically on the quotient submanifold $\tilde{M}_0$. Some of the plasma physics literature (e.g. Morrison 1982, 2013; Kraus *et al.* 2017) notes that (4.28) generally fails to satisfy a Jacobi identity, however, so we pause to elucidate the source of this contrasting point of view.

In particular, the aforementioned literature defines the Vlasov–Maxwell system on an augmented manifold that includes all unconstrained vector fields $\boldsymbol{E},\boldsymbol{B}\in\mathbb{R}^3$:

$$\tilde{M}_0^+ := \tilde{M}_0\sqcup\{\boldsymbol{E},\boldsymbol{B}\mid \nabla\cdot\boldsymbol{E}\neq\bar{\rho},\,\nabla\cdot\boldsymbol{B}\neq 0\}. \tag{4.31}$$

When the bracket of (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 $\nabla\cdot\boldsymbol{B}=0$. Indeed, the constraint $\nabla\cdot\boldsymbol{B}=0$ appears as an exogenous defect that must be satisfied for $(\tilde{M}_0^+,\{\{\cdot,\cdot\}\}^{\mathrm{red}})$ to be considered a Poisson manifold. On $\tilde{M}_0^+$, the bracket of (4.28) also acquires additional Casimirs,

$$\left.\begin{aligned}\{\{\cdot,\bar{\rho}-\nabla\cdot\boldsymbol{E}\}\}=0\\ \{\{\cdot,\nabla\cdot\boldsymbol{B}\}\}=0,\end{aligned}\right\} \tag{4.32}$$

in much the same way that a Poisson structure on $\mathbb{R}^2=\{(x,y)\}$ acquires a z Casimir when the system is embedded in $\mathbb{R}^3$.

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We adopt the point of view that it is more natural to regard the bracket of (4.28) as a Poisson bracket defined on the submanifold of physical interest – $\tilde{M}_0 = \mu^{-1}(0)/\mathcal{F}$ – rather than a defected bracket defined on the larger manifold including arbitrary vector fields $\boldsymbol{E}$ and $\boldsymbol{B}$. In a sense, it is merely a lack of economical notation that leads us to coordinatize $\tilde{M}_0$ with vector symbols $\boldsymbol{E}$ and $\boldsymbol{B}$ that are more commonly defined over all of $\mathbb{R}^3$.

It is clear from this discussion, however, that care must be taken in any numerical implementation of the reduced Vlasov–Maxwell bracket to constrain one's fields to the phase space of $\tilde{M}_0$; generic, unconstrained vector fields $\boldsymbol{E}, \boldsymbol{B} \in \mathbb{R}^3$ are to 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 (for example, see 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

$$H = \sum_{i=1}^{N} H_i. \tag{5.1}$$

The system's dynamical variables $\boldsymbol{u}$ are then evolved by each subsystem individually, arranged in a sequence chosen to minimize discretization error, e.g.

$$\begin{aligned} \boldsymbol{u}(t+\Delta t) &= \exp(\Delta t H)\boldsymbol{u}(t) \\ &\approx \exp\left(\frac{\Delta t}{2} H_1\right) \exp(\Delta t H_2) \exp\left(\frac{\Delta t}{2} H_1\right) \boldsymbol{u}(t), \end{aligned} \tag{5.2}$$

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

The advantage afforded by this subdivision of the Hamiltonian is that its subsystems $\{H_i\}$ are often more easily integrated individually than the full system H. In fact, each sub-Hamiltonian H_i can at times 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 § 6.

Our interest concerns the status of the momentum map μ in such algorithms. A sufficient condition for the exact preservation of μ 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

$$\Phi_g^* H_i = H_i \quad \forall i \text{ and } g \in G. \tag{5.3}$$

Then, differentiating with respect to g – as in (4.15) – we find by the same argument of (4.22)–(4.23) that $\dot{\mu} = 0$ in each Hamiltonian subsystem, where μ is the total system's momentum map associated with the group action Φ_g.

This claim follows simply from the observation that μ is an object defined by its Poisson manifold $(M, \{\cdot,\cdot\})$, separate and apart from the Hamiltonian defined on that manifold. (One might say that μ is defined kinematically (Morrison 1993) on M, independently of dynamics.) μ is therefore preserved along the flow generated by any gauge-invariant function. Consequently, if each sub-Hamiltonian is gauge invariant and its flow is exactly integrated, then the momentum map is exactly preserved by its evolution during each discrete time step. We summarize this result as a theorem.

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THEOREM. *Let Φ be a canonical group action of a Lie group G on Poisson manifold M with momentum map μ, and let $H : M \to \mathbb{R}$ satisfy $\Phi_g^* H = H$, $\forall\ g \in G$. Suppose a splitting method $H = \sum_{i=1}^{N} H_i$ satisfies:*

(i) *$\Phi_g^* H_i = H_i$, $\forall\ i$ and $g \in G$;*
(ii) *subsystem H_i is solved exactly $\forall\ i$.*

Then μ 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. *An 'unreduced' Hamiltonian PIC method*

With the formalism we have developed, we proceed to explore PIC methods in the Hamiltonian setting, by defining 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 unreduced Poisson bracket of (4.1), while the former implements a splitting method for the reduced bracket of (4.28). We shall synthesize the two, defining a gauge-compatible splitting method for the unreduced bracket of (4.1) and, in so doing, demonstrate the merit of this new class of splitting methods. The result is an explicit-time-advance, canonical, locally charge-conserving PIC method, whose momentum map and conservation law we shall systematically derive.

In Qin *et al.* (2016), a Klimontovich–Maxwell PIC method is derived from the unreduced bracket of (4.1) by specifying the following form for the distribution function $f(\boldsymbol{x}, \boldsymbol{p})$ of L particles, analogous to (3.1)

$$f(\boldsymbol{x}, \boldsymbol{p}) = \sum_{i=1}^{L} \delta^{(3)}(\boldsymbol{x} - \boldsymbol{X}_i)\delta^{(3)}(\boldsymbol{p} - \boldsymbol{P}_i). \tag{6.1}$$

Here, $(\boldsymbol{X}_i, \boldsymbol{P}_i)$ denotes the dynamical coordinates of particle i in phase space. The fields $\boldsymbol{A}$ and $\boldsymbol{Y}$ are also discretized on a (three-dimensional) spatial lattice and are denoted $(\boldsymbol{A}_n, \boldsymbol{Y}_n)$ at lattice site n. We shall further require the interpolation of $\boldsymbol{A}$

$$\boldsymbol{A}(\boldsymbol{x}) = \sum_{n=1}^{N} \boldsymbol{A}_n W_{\sigma_1}(\boldsymbol{x} - \boldsymbol{x}_n), \tag{6.2}$$

where n is an index over all N lattice sites and W_{σ_1} is an (as yet unspecified) interpolation function for $\boldsymbol{A}$.

A Poisson bracket for this discrete system simply follows from the canonical symplectic structure of its variables. In particular, we define the symplectic manifold

$$M_d = T^*X \times T^*Q, \tag{6.3}$$

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 lattice, such that $T^*X = \{(\boldsymbol{X}_i, \boldsymbol{P}_i)\}$ and $T^*Q = \{(\boldsymbol{A}_n, \boldsymbol{Y}_n)\}$.

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A point $m \in M_d$ correspondingly specifies $(\boldsymbol{X}_i, \boldsymbol{P}_i, \boldsymbol{A}_n, \boldsymbol{Y}_n)\ \forall\ i, n$ (where the subscript d denotes discretization).

The Poisson bracket for this symplectic manifold therefore takes its usual Darboux-coordinate form

$$\{\{F, G\}\}_d[\boldsymbol{X}_i, \boldsymbol{P}_i, \boldsymbol{A}_n, \boldsymbol{Y}_n] = \sum_{i=1}^{L}\left(\frac{\partial F}{\partial \boldsymbol{X}_i}\cdot\frac{\partial G}{\partial \boldsymbol{P}_i} - \frac{\partial G}{\partial \boldsymbol{X}_i}\cdot\frac{\partial F}{\partial \boldsymbol{P}_i}\right) + \sum_{n=1}^{N}\left(\frac{\partial F}{\partial \boldsymbol{A}_n}\cdot\frac{\partial G}{\partial \boldsymbol{Y}_n} - \frac{\partial G}{\partial \boldsymbol{A}_n}\cdot\frac{\partial F}{\partial \boldsymbol{Y}_n}\right). \tag{6.4}$$

We observe that, unlike its continuous counterpart in (4.1), the bracket of (6.4) is non-degenerate; it defines M_d not only as a Poisson manifold, but as a symplectic manifold.

The discrete Hamiltonian of Qin *et al.* (2016) is derived from (4.2) by substituting the Klimontovich distribution of (6.1) and expanding terms of the form $|\boldsymbol{P}_i - \boldsymbol{A}(\boldsymbol{X}_i)|^2$ using (6.2)

$$H_d[\boldsymbol{X}_i, \boldsymbol{P}_i, \boldsymbol{A}_n, \boldsymbol{Y}_n] = \frac{1}{2}\sum_{i=1}^{L}\left[\boldsymbol{P}_i^2 - 2\boldsymbol{P}_i\cdot\sum_{n=1}^{N}\boldsymbol{A}_n W_{\sigma_1}(\boldsymbol{X}_i - \boldsymbol{x}_n) + \sum_{m,n=1}^{N}\boldsymbol{A}_m\cdot\boldsymbol{A}_n W_{\sigma_1}(\boldsymbol{X}_i - \boldsymbol{x}_m)W_{\sigma_1}(\boldsymbol{X}_i - \boldsymbol{x}_n)\right] + \frac{1}{2}\sum_{n=1}^{N}[\boldsymbol{Y}_n^2 + |\nabla_d^+ \times \boldsymbol{A}|_n^2]. \tag{6.5}$$

Here, the operator $(\nabla_d^{\pm}\times)_n$ represents a discrete curl, defined by

$$(\nabla_d^{\pm}\times\boldsymbol{A})_n := \pm\begin{pmatrix} \dfrac{A^3_{i,j\pm1,k} - A^3_{i,j,k}}{\Delta y} - \dfrac{A^2_{i,j,k\pm1} - A^2_{i,j,k}}{\Delta z} \\ \dfrac{A^1_{i,j,k\pm1} - A^1_{i,j,k}}{\Delta z} - \dfrac{A^3_{i\pm1,j,k} - A^3_{i,j,k}}{\Delta x} \\ \dfrac{A^2_{i\pm1,j,k} - A^2_{i,j,k}}{\Delta x} - \dfrac{A^1_{i,j\pm1,k} - A^1_{i,j,k}}{\Delta y} \end{pmatrix} \tag{6.6}$$

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

We now describe the gauge symmetry of this discrete Hamiltonian system. We define the group action Φ_f on M_d by analogy with (4.13)

$$\Phi_f(\boldsymbol{X}_i, \boldsymbol{P}_i, \boldsymbol{A}_n, \boldsymbol{Y}_n) = (\boldsymbol{X}_i, [\boldsymbol{P}_i - \nabla_d^+ f(\boldsymbol{X}_i)], [\boldsymbol{A}_n - (\nabla_d^+ f)_n], \boldsymbol{Y}_n), \tag{6.7}$$

where

$$\nabla_d^+ f(\boldsymbol{x}) = \sum_{n=1}^{N}(\nabla_d^+ f)_n W_{\sigma_1}(\boldsymbol{x} - \boldsymbol{x}_n) \tag{6.8}$$

and where $(\nabla_d^{\pm})_n$ is a discrete gradient defined by

$$(\nabla_d^{\pm} f)_n := \pm\begin{pmatrix} \dfrac{f_{i\pm1,j,k} - f_{i,j,k}}{\Delta x} \\ \dfrac{f_{i,j\pm1,k} - f_{i,j,k}}{\Delta y} \\ \dfrac{f_{i,j,k\pm1} - f_{i,j,k}}{\Delta z} \end{pmatrix}. \tag{6.9}$$

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We note that $\nabla_d^{\pm} \times \nabla_d^{\pm} = 0$ as an operator. (If the $\pm$ signs agree, this relation holds identically; if they disagree, it holds only after a summation over lattice points, $\sum_n$.) We also note that – in contrast with (4.13)–(4.14) – $\boldsymbol{P}_i$ and $\boldsymbol{A}_n$ are shifted in the same direction in (6.7), reflecting the fact that $\boldsymbol{p}$ and $\boldsymbol{P}_i$ have opposite signs in (6.1) when we reinterpret the transformation of (4.14) as a transformation of $\boldsymbol{P}_i$.

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

$$\langle \alpha, \phi \rangle := \sum_{n=1}^{N} \alpha_n \phi_n \quad \forall\ \alpha \in \mathfrak{f}_d^*, \phi \in \mathfrak{f}_d. \tag{6.10}$$

We must verify that the group action is canonical, a task most easily approached infinitesimally. In particular, we ask whether the following infinitesimal form of $\{\{\Phi_f^* F, \Phi_f^* G\}\}_d = \Phi_f^* \{\{F, G\}\}_d$ holds:

$$\begin{aligned} &\left\{ \left\{ -\nabla_d^+ \phi(\boldsymbol{X}_i) \cdot \frac{\partial F}{\partial \boldsymbol{P}_i} - \nabla_d^+ \phi_n \cdot \frac{\partial F}{\partial \boldsymbol{A}_n}, G \right\} \right\}_d - (F \leftrightarrow G) \\ &\quad = -\nabla_d^+ \phi(\boldsymbol{X}_i) \cdot \frac{\partial \{\{F, G\}\}_d}{\partial \boldsymbol{P}_i} - \nabla_d^+ \phi_n \cdot \frac{\partial \{\{F, G\}\}_d}{\partial \boldsymbol{A}_n}, \end{aligned} \tag{6.11}$$

where summation over repeated indices is implicit. After applying (6.4) to evaluate each bracket, equation (6.11) is seen to be true only when $\nabla \times \nabla_d^+ \phi(\boldsymbol{X}_i) = 0$. This requires the operator relation

$$\nabla \times \nabla_d^+ = 0. \tag{6.12}$$

Here, $\nabla \equiv \partial_{\boldsymbol{X}_i}$ is a continuous spatial gradient.

Equation (6.12) therefore necessitates the following condition on the interpolation function W_{σ_1}:

$$\sum_{n=1}^{N} (\nabla_d^+ \phi)_n W_{\sigma_1}(\boldsymbol{x} - \boldsymbol{x}_n) = \nabla \sum_{n=1}^{N} \phi_n W_{\sigma_0}(\boldsymbol{x} - \boldsymbol{x}_n) \tag{6.13}$$

for some interpolation function W_{σ_0}. This condition was already discovered in Xiao *et al.* (2015), and is analogous to a property of the simplicial Whitney forms described earlier (Bossavit 1988). Our discussion of this condition merely contributes that, in a Hamiltonian context, the motivation for the constraint in (6.13) is the canonicality of the group action.

We now solve for μ_d, the momentum map on M_d associated with the group action of (6.7), using the symplectic structure of (6.4). First, we must find the infinitesimal generator ϕ_{M_d} of our group action on M_d, defined analogously to (4.15). Given the group action of (6.7) we expect ϕ_{M_d} to take the form (already implicitly used in (6.11))

$$\{\{\cdot, \mu_d^{\phi}\}\}_d = -\sum_{i=1}^{L} \nabla_d^+ \phi(\boldsymbol{X}_i) \cdot \frac{\partial}{\partial \boldsymbol{P}_i} - \sum_{n=1}^{N} (\nabla_d^+ \phi)_n \cdot \frac{\partial}{\partial \boldsymbol{A}_n}, \tag{6.14}$$

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where we denote the pairing of the momentum map with ϕ by $\langle \mu_d, \phi \rangle = \mu_d^\phi$. The Poisson bracket of (6.4) therefore requires that μ_d^ϕ be given by

$$\begin{aligned}\mu_d^\phi(m) &= \sum_{n=1}^{N} (\nabla_d^+ \phi)_n \cdot \left[\sum_{i=1}^{L} \int_{-\infty}^{\boldsymbol{X}_i} \mathrm{d}\boldsymbol{X}_i' \, W_{\sigma_1}(\boldsymbol{X}_i' - \boldsymbol{x}_n) - \boldsymbol{Y}_n \right] \\ &= \sum_{n=1}^{N} \phi_n \nabla_d^- \cdot \left[-\sum_{i=1}^{L} \int_{-\infty}^{\boldsymbol{X}_i} \mathrm{d}\boldsymbol{X}_i' \, W_{\sigma_1}(\boldsymbol{X}_i' - \boldsymbol{x}_n) + \boldsymbol{Y}_n \right], \end{aligned} \tag{6.15}$$

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

$$\nabla_d^\pm \cdot \boldsymbol{v}_n := \pm \sum_{\alpha=1}^{3} \frac{v_{n\pm\hat{\alpha}}^\alpha - v_n^\alpha}{\Delta x^\alpha}. \tag{6.16}$$

Note that $\mathrm{d}\boldsymbol{X}_i'$ is treated in (6.15) and hereafter as a vector, with each component integrated individually. We observe that $\nabla_d^\pm \cdot \nabla_d^\pm \times = 0$ as an operator (when $\pm$ signs agree).

Given the pairing defined in (6.10), the momentum map μ_d must therefore be

$$(\mu_d(m))_n = -\nabla_d^- \cdot \sum_{i=1}^{L} \int_{-\infty}^{\boldsymbol{X}_i} \mathrm{d}\boldsymbol{X}_i' \, W_{\sigma_1}(\boldsymbol{X}_i' - \boldsymbol{x}_n) + \nabla_d^- \cdot \boldsymbol{Y}_n \tag{6.17}$$

defined at each lattice site $n \in [1, N]$. Due to the gauge invariance of H_d in (6.5) – 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 Vlasov–Maxwell system of § 4. Equations (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 (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:

$$\left.\begin{aligned} \dot{\boldsymbol{X}}_i &= \{\{\boldsymbol{X}_i, H_d\}\}_d = \boldsymbol{P}_i - \sum_{m=1}^{N} \boldsymbol{A}_m W_{\sigma_1}(\boldsymbol{X}_i - \boldsymbol{x}_m), \\ \dot{\boldsymbol{P}}_i &= \{\{\boldsymbol{P}_i, H_d\}\}_d = \sum_{m=1}^{N} (\dot{\boldsymbol{X}}_i \cdot \boldsymbol{A}_m) \nabla W_{\sigma_1}(\boldsymbol{X}_i - \boldsymbol{x}_m), \\ \dot{\boldsymbol{A}}_n &= \{\{\boldsymbol{A}_n, H_d\}\}_d = \boldsymbol{Y}_n, \\ \dot{\boldsymbol{Y}}_n &= \{\{\boldsymbol{Y}_n, H_d\}\}_d = \sum_{i=1}^{L} \dot{\boldsymbol{X}}_i W_{\sigma_1}(\boldsymbol{X}_i - \boldsymbol{x}_n) - (\nabla_d^- \times \nabla_d^+ \times \boldsymbol{A})_n. \end{aligned}\right\} \tag{6.19}$$

Now substituting $\dot{\boldsymbol{Y}}_n$ into the charge conservation law equations (6.17)–(6.18), we note that

$$0 = \dot{\rho}_n + \nabla_d^- \cdot \boldsymbol{J}_n, \tag{6.20}$$

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where

$$\left.\begin{aligned}\rho_n &:= -\nabla_d^- \cdot \sum_{i=1}^{L} \int_{-\infty}^{X_i} \mathrm{d}\boldsymbol{X}_i' \, W_{\sigma_1}(\boldsymbol{X}_i' - \boldsymbol{x}_n), \\ \boldsymbol{J}_n &:= \sum_{i=1}^{L} \dot{\boldsymbol{X}}_i W_{\sigma_1}(\boldsymbol{X}_i - \boldsymbol{x}_n).\end{aligned}\right\} \tag{6.21}$$

This is an alternative form of the charge conservation law equation (6.18) for the continuous-time evolution of the Hamiltonian system of Qin *et al.* (2016). (We observe that, unlike its counterpart in (4.25), it is an off-shell identity.)

The form of ρ_n in (6.21) can be justified by a schematic one-dimensional example in which $W_{\sigma_1}(x) = 1$ on $0 \leqslant x < \Delta x$ and 0 otherwise. For a single particle at $X_i = 0.2$, we have

$$\rho_n = -\nabla_d^- \cdot \int_{-\infty}^{0.2} \mathrm{d}X_i' \, W_{\sigma_1}(X_i' - x_n) = \begin{cases} 0.8/\Delta x & n = 0, \\ 0.2/\Delta x & n = 1, \\ 0 & n \neq 0, 1. \end{cases} \tag{6.22}$$

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 μ_d. To algorithmically evolve this system in discrete time, we define a gauge-compatible splitting method adapted from He *et al.* (2015, 2016). We define Hamiltonian subsystems

$$H_d = \sum_{\alpha=1}^{3} H_{\mathrm{Klim}}^{\alpha} + H_{\boldsymbol{A}} + H_{\boldsymbol{Y}}, \tag{6.23}$$

where

$$\left.\begin{aligned} H_{\mathrm{Klim}}^{\alpha} &:= \frac{1}{2} \sum_{i=1}^{L} (P_i^{\alpha} - A^{\alpha}(\boldsymbol{X}_i))^2, \\ H_{\boldsymbol{A}} &:= \frac{1}{2} \sum_{n=1}^{N} |\nabla_d^+ \times \boldsymbol{A}|_n^2, \\ H_{\boldsymbol{Y}} &:= \frac{1}{2} \sum_{n=1}^{N} \boldsymbol{Y}_n^2. \end{aligned}\right\} \tag{6.24}$$

We immediately note that these subsystems are all gauge invariant for the group action of (6.7) – $\Phi_f^* H_i = H_i \ \forall f \in \mathcal{F}_d$ and i – and will therefore comprise a gauge-compatible splitting – and preserve μ_d – if they can be exactly solved.

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Let us examine the EOM for each subsystem H_i in turn

$$H^{\alpha}_{\text{Klim}} \begin{cases} \dot{X}^{\beta}_i = \delta^{\beta}_{\alpha}\left[P^{\alpha}_i - \sum_{m=1}^{N} A^{\alpha}_m W_{\sigma_1}(\boldsymbol{X}_i - \boldsymbol{x}_m)\right], \\ \dot{P}^{\beta}_i = \dot{X}^{\alpha}_i \sum_{m=1}^{N} A^{\alpha}_m \partial_{\beta} W_{\sigma_1}(\boldsymbol{X}_i - \boldsymbol{x}_m), \\ \dot{A}^{\beta}_n = 0, \\ \dot{Y}^{\beta}_n = \delta^{\beta}_{\alpha} \sum_{i=1}^{L} \dot{X}^{\alpha}_i W_{\sigma_1}(\boldsymbol{X}_i - \boldsymbol{x}_n), \end{cases} \tag{6.25}$$

$$H_{\boldsymbol{A}} \begin{cases} \dot{\boldsymbol{X}}_i = 0, \\ \dot{\boldsymbol{P}}_i = 0, \\ \dot{\boldsymbol{A}}_n = 0, \\ \dot{\boldsymbol{Y}}_n = -(\boldsymbol{\nabla}^{-}_d \times \boldsymbol{\nabla}^{+}_d \times \boldsymbol{A})_n, \end{cases} \tag{6.26}$$

$$H_{\boldsymbol{Y}} \begin{cases} \dot{\boldsymbol{X}}_i = 0, \\ \dot{\boldsymbol{P}}_i = 0, \\ \dot{\boldsymbol{A}}_n = \boldsymbol{Y}_n, \\ \dot{\boldsymbol{Y}}_n = 0, \end{cases} \tag{6.27}$$

where $\partial_{\beta} \equiv \partial/\partial X^{\beta}_i$. (We emphasize that α is fixed, and is not summed over in the expressions for H^{α}_{Klim}.) $H_{\boldsymbol{A}}$ and $H_{\boldsymbol{Y}}$ are exactly solvable at a glance. Furthermore, H^{α}_{Klim} is seen to be exactly solvable by noting that $\ddot{X}^{\beta}_i = 0$; $\dot{X}^{\beta}_i$ is therefore a constant determined by a time step's initial conditions. The evolutions of $\dot{\boldsymbol{P}}_i$ and $\dot{\boldsymbol{Y}}_n$ in H^{α}_{Klim} follow immediately from this analysis.

The exact time evolutions of $H_{\boldsymbol{A}}$, $H_{\boldsymbol{Y}}$ and H^{α}_{Klim} are therefore explicitly solved, defining by construction an explicit-time-advance gauge-compatible splitting method that exactly preserves the momentum map, $\dot{\mu}_d = 0$, as desired. The alternative form of the charge conservation law given in (6.20) – that is, $\dot{\rho}_n + \boldsymbol{\nabla}^{-}_d \cdot \boldsymbol{J}_n = 0$ – is also exactly preserved in this algorithm, because the substitution that led from (6.18) to (6.20) – that is, $\boldsymbol{\nabla}^{-}_d \cdot \dot{\boldsymbol{Y}}_n = \boldsymbol{\nabla}^{-}_d \cdot \boldsymbol{J}_n$ – holds for each Hamiltonian subsystem above.

Finally, we note that the momentum map μ_d has significant ramifications for the appropriate initial conditions of the preceding algorithm. We refer the reader to a brief but important discussion of these initial conditions in the text following (6.30) below.

6.2. *A '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 (4.28).

We will mirror Xiao *et al.* (2015) and derive this PIC scheme by undertaking the symplectic reduction (Marsden & Weinstein 1974) of the discrete canonical bracket defined in (6.4). As in § 4.4, we define a mapping to the reduced symplectic manifold $\tilde{M}_{d_0} = \mu_d^{-1}(0)/\mathcal{F}_d$, with coordinates given by

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$$\pi_{d,\mathrm{red}}: \begin{array}{ccc} \mu_d^{-1}(0) \subset M_d & \longrightarrow & \tilde{M}_{d_0} = \mu_d^{-1}(0)/\mathcal{F}_d \\ (\boldsymbol{X}_i, \boldsymbol{P}_i, \boldsymbol{A}_n, \boldsymbol{Y}_n) & \longmapsto & (\boldsymbol{X}_i, \boldsymbol{V}_i, \boldsymbol{B}_n, \boldsymbol{E}_n), \end{array} \tag{6.28}$$

where

$$\left.\begin{array}{c} \boldsymbol{X}_i = \boldsymbol{X}_i, \\ \boldsymbol{V}_i = \boldsymbol{P}_i - \boldsymbol{A}(\boldsymbol{X}_i), \\ \boldsymbol{B}_n = (\nabla_d^+ \times \boldsymbol{A})_n, \\ \boldsymbol{E}_n = -\boldsymbol{Y}_n. \end{array}\right\} \tag{6.29}$$

As discussed earlier, care must be taken to ensure that the discrete fields $\boldsymbol{B}_n$ and $\boldsymbol{E}_n$ of $\tilde{M}_{d_0}$ obey the reduced manifold constraints

$$\left.\begin{array}{c} (\nabla_d^+ \cdot \boldsymbol{B})_n = 0, \\ -\nabla_d^- \cdot \sum_{i=1}^{L} \int_{-\infty}^{\boldsymbol{X}_i} \mathrm{d}\boldsymbol{X}_i' W_{\sigma_1}(\boldsymbol{X}_i' - \boldsymbol{x}_n) - (\nabla_d^- \cdot \boldsymbol{E})_n = 0. \end{array}\right\} \tag{6.30}$$

We note that these constraints must also be satisfied by any initial condition of the algorithm. The former condition is necessary to enforce a physically valid magnetic field. If the latter condition (Gauss's law) is not satisfied initially, it will have the effect of adding fixed 'external' charges at the corresponding vertex n. In particular, a non-zero initial Gauss's law condition will evolve the system along some other reduced manifold $\tilde{M}_{d_\alpha} = \mu_d^{-1}(\alpha)/\mathcal{F}_d$ with fixed external charge density α.

A similar initial condition must be determined for the unreduced algorithm of § 6.1 as well. The unreduced algorithm enforces the constraint $(\nabla_d^+ \cdot \nabla_d^+ \times \boldsymbol{A})_n = 0$ automatically. However, for simulations without external charges, care should be taken so that the value of $(\mu_d(m))_n$ in (6.17) is everywhere initialized to zero. (Alternatively, equation (6.17) can be used to properly initialize a simulation with external charges that remain fixed for all time.) We note that our derivation of the momentum map is essential to this correct specification of initial conditions.

We therefore proceed with the reduction of our discrete system and substitute equation (6.29) into the bracket of (6.4) to find

$$\begin{aligned} &\{\{F, G\}\}_d^{\mathrm{red}}[\boldsymbol{X}_i, \boldsymbol{V}_i, \boldsymbol{B}_n, \boldsymbol{E}_n] \\ &= \sum_{i=1}^{L} \left(\frac{\partial F}{\partial \boldsymbol{X}_i} \cdot \frac{\partial G}{\partial \boldsymbol{V}_i} - \frac{\partial G}{\partial \boldsymbol{X}_i} \cdot \frac{\partial F}{\partial \boldsymbol{V}_i} + \left[\frac{\partial F}{\partial \boldsymbol{V}_i} \times \frac{\partial G}{\partial \boldsymbol{V}_i} \right] \cdot \sum_{n=1}^{N} \boldsymbol{B}_n W_{\sigma_2}(\boldsymbol{X}_i - \boldsymbol{x}_n) \right) \\ &\quad + \sum_{n=1}^{N} \left(\left[\sum_{i=1}^{L} \frac{\partial F}{\partial \boldsymbol{V}_i} W_{\sigma_1}(\boldsymbol{X}_i - \boldsymbol{x}_n) - \left(\nabla_d^- \times \frac{\partial F}{\partial \boldsymbol{B}} \right)_n \right] \cdot \frac{\partial G}{\partial \boldsymbol{E}_n} \right. \\ &\quad \left. - \left[\sum_{i=1}^{L} \frac{\partial G}{\partial \boldsymbol{V}_i} W_{\sigma_1}(\boldsymbol{X}_i - \boldsymbol{x}_n) - \left(\nabla_d^- \times \frac{\partial G}{\partial \boldsymbol{B}} \right)_n \right] \cdot \frac{\partial F}{\partial \boldsymbol{E}_n} \right). \end{aligned} \tag{6.31}$$

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

$$\nabla \times \sum_{n=1}^{N} \boldsymbol{A}_n W_{\sigma_1}(\boldsymbol{x} - \boldsymbol{x}_n) = \sum_{n=1}^{N} (\nabla_d^+ \times \boldsymbol{A})_n W_{\sigma_2}(\boldsymbol{x} - \boldsymbol{x}_n) \tag{6.32}$$

for some interpolation function W_{σ_2}. As in (6.13), this is a generalized, higher-dimensional analogue of the simplicial Whitney interpolant constraint.

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Lastly, we re-express the Hamiltonian in the reduced coordinates of $\tilde{M}_{d_0}$ as

$$H_d^{\text{red}}[\boldsymbol{X}_i, \boldsymbol{V}_i, \boldsymbol{B}_n, \boldsymbol{E}_n] = \frac{1}{2}\sum_{i=1}^{L} \boldsymbol{V}_i^2 + \frac{1}{2}\sum_{n=1}^{N}(\boldsymbol{E}_n^2 + \boldsymbol{B}_n^2). \tag{6.33}$$

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

As discussed in § 4.4 for spatially continuous systems, this reduced Hamiltonian system is automatically guaranteed to preserve the momentum map of its parent, as long as it 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)

$$H_d^{\text{red}} = \sum_{\alpha=1}^{3} H_{\boldsymbol{V}}^{\alpha} + H_{\boldsymbol{B}} + H_{\boldsymbol{E}}, \tag{6.34}$$

where

$$\left.\begin{aligned} H_{\boldsymbol{V}}^{\alpha} &:= \frac{1}{2}\sum_{i=1}^{L}(V_i^{\alpha})^2, \\ H_{\boldsymbol{B}} &:= \frac{1}{2}\sum_{n=1}^{N}\boldsymbol{B}_n^2, \\ H_{\boldsymbol{E}} &:= \frac{1}{2}\sum_{n=1}^{N}\boldsymbol{E}_n^2. \end{aligned}\right\} \tag{6.35}$$

These subsystems generate the following EOM:

$$H_{\boldsymbol{V}}^{\alpha}\begin{cases} \dot{X}_i^{\beta} = \delta_{\alpha}^{\beta} V_i^{\alpha}, \\ \dot{V}_i^{\beta} = \epsilon_{\beta\alpha\gamma} V_i^{\alpha} \displaystyle\sum_{n=1}^{N} B_n^{\gamma} W_{\sigma_2}(\boldsymbol{X}_i - \boldsymbol{x}_n), \\ \dot{B}_n^{\beta} = 0, \\ \dot{E}_n^{\beta} = -\delta_{\alpha}^{\beta} \displaystyle\sum_{i=1}^{L} V_i^{\alpha} W_{\sigma_1}(\boldsymbol{X}_i - \boldsymbol{x}_n), \end{cases} \tag{6.36}$$

$$H_{\boldsymbol{B}}\begin{cases} \dot{\boldsymbol{X}}_i = 0, \\ \dot{\boldsymbol{V}}_i = 0, \\ \dot{\boldsymbol{B}}_n = 0, \\ \dot{\boldsymbol{E}}_n = (\boldsymbol{\nabla}_d^{-} \times \boldsymbol{B})_n, \end{cases} \tag{6.37}$$

$$H_{\boldsymbol{E}}\begin{cases} \dot{\boldsymbol{X}}_i = 0, \\ \dot{\boldsymbol{V}}_i = \displaystyle\sum_{n=1}^{N} \boldsymbol{E}_n W_{\sigma_1}(\boldsymbol{X}_i - \boldsymbol{x}_n), \\ \dot{\boldsymbol{B}}_n = -(\boldsymbol{\nabla}_d^{+} \times \boldsymbol{E})_n, \\ \dot{\boldsymbol{E}}_n = 0. \end{cases} \tag{6.38}$$

We note again that α is not summed over in the expressions for subsystem $H_{\boldsymbol{V}}^{\alpha}$.

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Upon inspection, it is evident that the $\tilde{M}_{d_0}$ constraints of (6.30) are obeyed in each subsystem when they are exactly solved. (As in the unreduced case, the above subsystems are readily exactly solved. In particular, note that $\dot{V}_i^\alpha = 0$ in H_V^α.) Consequently, the exact conservation law of the reduced system is systematically derived by simply expressing the unreduced momentum map of (6.17) in $\tilde{M}_{d_0}$ coordinates

$$\begin{aligned}(\bar{\mu}_d)_n &= -\boldsymbol{\nabla}_d^- \cdot \sum_{i=1}^{L} \int_{-\infty}^{\boldsymbol{X}_i} \mathrm{d}\boldsymbol{X}_i' \, W_{\sigma_1}(\boldsymbol{X}_i' - \boldsymbol{x}_n) - \boldsymbol{\nabla}_d^- \cdot \boldsymbol{E}_n \\ &:= \rho_n - \boldsymbol{\nabla}_d^- \cdot \boldsymbol{E}_n \\ &= 0, \end{aligned} \tag{6.39}$$

where in the final line we have noted that $\bar{\mu}_d$ vanishes by our previous choice of reduction to the preimage submanifold ${\mu_d}^{-1}(0)$. Equation (6.39) is Gauss's law, for which we are by construction guaranteed

$$\dot{\bar{\mu}}_d = 0, \tag{6.40}$$

as desired. (An analogous observation was made for the reduced bracket in Kraus *et al.* (2017), where the momentum map was treated as a Casimir.) The local charge conservation law of (6.20) – whose expression is unmodified in the reduced submanifold – is furthermore satisfied, since $\boldsymbol{\nabla}_d^- \cdot \dot{\boldsymbol{E}}_n = -\boldsymbol{\nabla}_d^- \cdot \boldsymbol{J}_n$ holds in each subsystem of H_d^{red}.

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, while our approach for Hamiltonian systems 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 (see § 5); when the sub-Hamiltonians of a splitting method are chosen to be gauge invariant and exactly solvable, such methods exactly preserve the momentum map associated with this gauge symmetry, as well as its corresponding conservation laws.

Our study further demonstrated the importance of deriving the momentum map of a discrete Hamiltonian system 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 (see (6.21)) enables the precise assignment (or, more commonly, avoidance) of 'external' fixed charges at each lattice site n as an initial condition.

The techniques we have developed are more widely applicable to the simulation of gauge theories, and in principle provide a template for the derivation of exact conservation laws in any gauge-symmetric variational or gauge-compatible splitting algorithm. Our classification of gauge-compatible splitting methods also provides a general framework for the construction of Hamiltonian splitting algorithms that obey exact conservation laws.

As a final note, these results convey an overall impression of the adaptability of gauge theories to the discrete structures of algorithms. Internal gauge symmetries are characterized by the transformation of fields defined against the background of space–time, and their geometric structure can therefore be maintained even after

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the algorithmic discretization of this background. The present effort demonstrates that much of the formalism that gauge theories employ in continuous space–time – whether in Lagrangian or Hamiltonian systems – is readily ported to discrete settings more suitable for computation.

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