Space-Time Finite-Element Exterior Calculus and Variational Discretizations of Gauge Field Theories

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Abstract—Many gauge field theories can be described using a multisymplectic Lagrangian formulation, where the Lagrangian density involves space-time differential forms. While there has been much work on finite-element exterior calculus for spatial and tensor product space-time domains, there has been less done from the perspective of space-time simplicial complexes. One critical aspect is that the Hodge star is now taken with respect to a pseudo-Riemannian metric, and this is most naturally expressed in space-time adapted coordinates, as opposed to the barycentric coordinates that the Whitney forms (and their higher-degree generalizations) are typically expressed in terms of.

We introduce a novel characterization of Whitney forms and their Hodge dual with respect to a pseudo-Riemannian metric that is independent of the choice of coordinates, and then apply it to a variational discretization of the covariant formulation of Maxwell's equations. Since the Lagrangian density for this is expressed in terms of the exterior derivative of the fourpotential, the use of finite-dimensional function spaces that respects the de Rham cohomology results in a discretization that inherits the gauge symmetries of the continuous problem. This then yields a variational discretization that exhibits a discrete Noether's theorem, which implies that an associated multimomentum is automatically conserved by the discretization.

I. INTRODUCTION

A gauge symmetry is a continuous local transformation on the field variables that leaves the system physically indistinguishable. A consequence of this is that the Euler-Lagrange equations are underdetermined, i.e., the evolution equations are insufficient to propagate all the fields. The fields can be classified into kinetic fields that have no physical significance, and the dynamic fields and their conjugate momenta that have physical significance. The Euler-Lagrange equations are underdetermined as the gauge symmetry implies that there is a functional dependence between the equations, but this also results in a constraint (typically elliptic) on the initial data on a Cauchy surface. That is to say the Euler-Lagrange equations derived from the action are underdetermined due to gauge invariance since there are more fields than evolution equations to propagate the field components. However, they are simultaneously overdetermined due to the constraints imposed on the Cauchy data. A comprehensive review of gauge field theories from

the space-time covariant (or multi-Dirac) perspective can be found in [1].

An example of a gauge symmetry arises in Maxwell's equations of electromagnetism, which can be expressed in terms of the scalar potential ϕ , the vector potential **A**, the electric field E, and the magnetic field B.

$$\mathbf{E} = -\nabla \phi - \frac{\partial \mathbf{A}}{\partial t}, \qquad \nabla^2 \phi + \frac{\partial}{\partial t} (\nabla \cdot \mathbf{A}) = 0,$$

$$\mathbf{B} = \nabla \times \mathbf{A}, \qquad \Box \mathbf{A} + \nabla \left(\nabla \cdot \mathbf{A} + \frac{\partial \phi}{\partial t} \right) = 0,$$

where \square is the d'Alembert (or wave) operator. The following gauge transformation leaves the equations invariant,

$$\phi \to \phi - \frac{\partial f}{\partial t},$$
 $\mathbf{A} \to \mathbf{A} + \nabla f,$

where f is an arbitrary scalar-valued function of space-time. Associated with this gauge symmetry is the Cauchy initial data constraint,

$$\nabla \cdot \mathbf{B}^{(0)} = 0. \qquad \nabla \cdot \mathbf{E}^{(0)} = 0.$$

Typically, the indeterminacy in the equations of motion associated with the gauge freedom in the field theory is addressed by imposing a gauge condition. In electromagnetism, two commonly imposed gauge conditions are the Lorenz gauge $\nabla \cdot \mathbf{A} = -\frac{\partial \phi}{\partial t}$, which yields,

$$\Box \phi = 0, \qquad \Box \mathbf{A} = 0,$$

and the Coulomb gauge $\nabla \cdot \mathbf{A} = 0$, which yields,

$$\nabla^2 \phi = 0,$$
 $\Box \mathbf{A} + \nabla \frac{\partial \phi}{\partial t} = 0.$

Given different initial and boundary conditions, some problems may be easier to solve in certain gauges than others. Unfortunately, there is no systematic way of deciding which gauge to use for a given problem. Additionally, as we will see in section II-D, the gauge group is larger on manifolds with more complicated topology.

An important consequence of gauge symmetries is the presence of associated conserved quantities. Noether's first theorem states that for every differentiable, local symmetry of an action, there exists a Noether current obeying a continuity equation. Integrating this current over a spacelike surface yields a conserved quantity called a Noether charge. In electromagnetism, the Noether currents are given by

$$j_0 = \mathbf{E} \cdot \nabla f,$$
 $\mathbf{j} = -\mathbf{E} \frac{\partial f}{\partial t} + (\mathbf{B} \times \nabla) f.$

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Our long-term goal is to develop geometric structurepreserving numerical discretizations that systematically addresses the issue of gauge symmetries. Eventually, we wish to study discretizations of general relativity that address the issue of general covariance. Towards this end, we will consider multi-Dirac mechanics based on a Hamilton-Pontryagin variational principle for field theories [2] that is well adapted to degenerate field theories. The issue of general covariance also leads us to avoid using a tensor product discretization that presupposes a slicing of space-time, rather we will consider 4-simplicial complexes in space-time. More generally, we will need to study discretizations that are invariant with respect to some discrete analogue of the gauge symmetry group.

II. MULTI-DIRAC FORMULATION OF FIELD THEORIES

The Dirac [3], [4] and multi-Dirac formulation [2] of mechanics and field theories can be viewed as a generalization of the Lagrangian and multi-symplectic formulation to the case whether the Lagrangian is degenerate, i.e., the Legendre transformation is not onto. This approach is critical to gauge field theories, as the gauge symmetries naturally lead to degenerate Lagrangians.

A. Hamilton-Pontryagin Principle for Mechanics

Consider a configuration manifold Q with associated tangent bundle TQ and phase space T^*Q . Dirac mechanics is described on the Pontryagin bundle $TQ \oplus T^*Q$, which has position, velocity and momentum (q,v,p) as local coordinates. The dynamics on the Pontryagin bundle is described by the Hamilton–Pontryagin variational principle, where the Lagrange multiplier (and momentum) p imposes the second-order condition $v = \dot{q}$,

$$\delta \int_{t_{*}}^{t_{2}} L(q, v) - p(\dot{q} - v)dt = 0.$$
 (1)

It provides a variational description of both Lagrangian and Hamiltonian mechanics, and yields the implicit Euler–Lagrange equations,

$$\dot{q} = v, \qquad \dot{p} = \frac{\partial L}{\partial q}, \qquad p = \frac{\partial L}{\partial v}.$$
 (2)

The last equation is the Legendre transform $\mathbb{F}L:(q,\dot{q})\mapsto (q,\frac{\partial L}{\partial \dot{q}})$. This is important for degenerate systems as it enforces the primary constraints that arise when the Legendre transform is not onto.

B. Multisymplectic Geometry

The geometric setting for Lagrangian PDEs is multisymplectic geometry [5], [6]. The base space X consists of independent variables, denoted by $(x^0,\ldots,x^n)\equiv(t,x)$, where $x^0\equiv t$ is time, and $(x^1,\ldots,x^n)\equiv x$ are space variables. The dependent field variables, $(y^1,\ldots,y^m)\equiv y$, form a fiber over each space-time basepoint. The independent and field variables form the configuration bundle, $\rho:Y\to X$. The configuration of the system is specified by a section of Y over X, which is a continuous map $\phi:X\to Y$, such that $\rho\circ\phi=1_X$, i.e., for every $(t,x)\in X$, $\phi((t,x))$ is in the

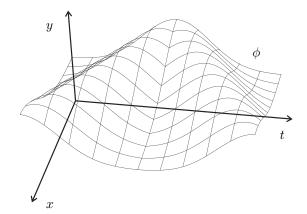


Fig. 1. A section of the configuration bundle: the horizontal axes represent spacetime, and the vertical axis represent dependent field variables. The section ϕ gives the value of the field variables at every point of spacetime.

fiber over (t, x), which is $\rho^{-1}((t, x))$. This is illustrated in Figure 1.

The multisymplectic analogue of the tangent bundle is the first jet bundle J^1Y , which is a fiber bundle over X that consists of the configuration bundle Y and the first partial derivatives $v_\mu^a = \partial y^a/\partial x^\mu$ of the field variables with respect to the independent variables. Given a section $\phi: X \to Y, \ \phi(x^0,\ldots,x^n) = (x^0,\ldots x^n,y^1,\ldots y^m)$, its first jet extension $j^1\phi: X \to J^1Y$ is a section of J^1Y over X given by

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

The dual jet bundle J^1Y^* is affine, with fiber coordinates (p, p_a^μ) , corresponding to the affine map $v_\mu^a \mapsto (p + p_a^\mu v_\mu^a)d^{n+1}x$, where $d^{n+1}x = dx^1 \wedge \cdots \wedge dx^n \wedge dx^0$.

C. Hamilton-Pontryagin Principle for Classical Fields

The (first-order) Lagrangian density is a map $\mathcal{L}: J^1Y \to \bigwedge^{n+1}(X)$, and let $\mathcal{L}(j^1\phi) = L(j^1\phi)\,dV = L(x^\mu,y^a,v^a_\mu)\,dV$, where $\bigwedge^{n+1}(X)$ is the space of alternating (n+1)-forms over X and $L(j^1\phi)$ is a scalar function on J^1Y . For field theories, the analogue of the Pontryagin bundle is $J^1Y\times_YJ^1Y^\star$, and the first-jet condition $\frac{\partial y^a}{\partial x^\mu}=v^a_\mu$ replaces $v=\dot{q}$, so the Hamilton-Pontryagin principle is

$$0 = \delta S(y^a, y^a_\mu, p^\mu_a)$$

$$= \delta \int_U \left[p^\mu_a \left(\frac{\partial y^a}{\partial x^\mu} - v^a_\mu \right) + L(x^\mu, y^a, v^a_\mu) \right] d^{n+1} x. \quad (3)$$

Taking variations with respect to y^a , v^a_μ and p^μ_a (where δy^a vanishes on the boundary ∂U) yields the implicit Euler–Lagrange equations,

$$\frac{\partial p_a^{\mu}}{\partial x^{\mu}} = \frac{\partial L}{\partial y^a}, \quad p_a^{\mu} = \frac{\partial L}{\partial v_u^a}, \quad \text{and} \quad \frac{\partial y^a}{\partial x^{\mu}} = v_{\mu}^a, \quad (4)$$

which generalizes (2) to the case of field theories; see [7] for more details. As the jet bundle is an affine bundle, the duality pairing used implicitly in (3) is more complicated.

The second equation of (4) yields the covariant Legendre transform, $\mathbb{F}\mathcal{L}: J^1Y \to J^1Y^*$,

$$p_a^{\mu} = \frac{\partial L}{\partial v_{\mu}^a}, \qquad p = L - \frac{\partial L}{\partial v_{\mu}^a} v_{\mu}^a.$$
 (5)

This unifies the two aspects of the Legendre transform by combining the definitions of the momenta and the Hamiltonian into a single covariant entity.

D. Multi-Dirac formulation of Maxwell's equations

The electromagnetic Lagrangian density is given by

$$\mathcal{L}(A, j^1 A) = -\frac{1}{4} \mathbf{d}A \wedge \star \mathbf{d}A = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu}, \qquad (6)$$

where $F_{\mu\nu} = A_{\mu,\nu} - A_{\nu,\mu}$, **d** is the exterior derivative, and \star is the Minkowski Hodge star $\star : \bigwedge^k(M) \to \bigwedge^{n-k}(M)$ defined uniquely by the identity,

$$\langle \langle \alpha^k, \beta^k \rangle \rangle \mathbf{v} = \alpha^k \wedge \star \beta^k,$$

where $\langle\langle \, , \, \rangle\rangle$ is the Minkowski metric on differential forms, and ${\bf v}$ is the volume form. For example, for standard Minkowski spacetime with metric signature (+---), the Hodge star acts on 2-forms as follows:

$$\star dt \wedge dx = dz \wedge dy, \qquad \star dy \wedge dz = dt \wedge dx,$$

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For a more in-depth discussion, see, for example, page 411 of [8].

The Hamilton-Pontryagin action principle is given in coordinates by

$$S = \int_{U} \left[p^{\mu,\nu} \left(\frac{\partial A_{\mu}}{\partial x^{\nu}} - A_{\mu,\nu} \right) - \frac{1}{4} F_{\mu\nu} F^{\mu\nu} \right] d^{4}x,$$

where U is an open subset of X. The implicit Euler–Lagrange equations are given by

$$p^{\mu,\nu} = F^{\mu\nu}, \quad A_{\mu,\nu} = \frac{\partial A_{\mu}}{\partial x^{\nu}}, \quad \frac{\partial p^{\mu,\nu}}{\partial x^{\nu}} = 0,$$

and by eliminating $p^{\mu,\nu}$ lead to Maxwell's equations: $\partial_{\nu}F^{\mu\nu}=0.$

Note that the gauge symmetry of the action given in (6) is more general than what is typically considered in the standard formulation of electromagnetism. Since the action only depends on ${\bf d}A$, then the Lagrangian density is invariant under shifts of A by any closed 1-form, in other words, 1-forms ω such that ${\bf d}\omega=0$. Contrast this with the standard formulation shown in section I, which implies that only exact 1-forms $\omega={\bf d}f$ leave the dynamics invariant.

E. Discrete Multi-Dirac Variational Integrators

The theory of variational integrators provide a way of discretizing Lagrangian mechanical systems so as to obtain numerical integration schemes that are automatically symplectic. They are based on the concept of a discrete Lagrangian $L_d: Q \times Q \to \mathbb{R}$, which can be viewed as a

Type I generating function of a symplectic map, which is intended to approximate the exact discrete Lagrangian,

$$L_d^{\text{exact}}(q_0, q_1) \equiv \int_0^h L(q_{0,1}(t), \dot{q}_{0,1}(t)) dt,$$

where $q_{0,1}(t)$ satisfies the Euler-Lagrange boundary-value problem. There are systematic methods of constructing computable approximations of the discrete Lagrangian [9], [10], and it can be shown that if the computable discrete Lagrangian approximates the exact discrete Lagrangian to a given order of accuracy, then the resulting variational integrator exhibits the same order of accuracy [11], [12].

In the case of field theories, the boundary Lagrangian [13], which is a scalar-valued function on the space of boundary data, plays a similar role, and the exact boundary Lagrangian has the form

$$L_{\partial U}^{\mathrm{exact}}(\varphi|_{\partial U}) \equiv \int_{U} L(j^{1}\tilde{\varphi})$$

where $\tilde{\varphi}$ satisfies the boundary conditions $\tilde{\varphi}|_{\partial U} = \varphi|_{\partial U}$, and $\tilde{\varphi}$ satisfies the Euler–Lagrange equation in the interior of U. As with the case for Lagrangian ODEs, a computable approximation of the boundary Lagrangian can be obtained by replacing the space-time integral with a quadrature rule, and considering a finite-element approximation of the configuration bundle. As we will see, in the case of Maxwell's equations, this involves the use of Whitney forms as the finite-dimensional configuration bundle.

III. SPACE-TIME WHITNEY FORMS

The Whitney k-forms are a finite-dimensional subspace of k-differential forms, and they are dual to k-simplices via integration pairing. They were introduced by Whitney in [14], and they are typically expressed in terms of barycentric coordinates. The barycentric coordinates λ_i are defined on a k-simplex with vertex vectors $v_0, v_1, \ldots v_k$ as functions of the position vector x such that

$$\sum_{i=0}^{k} \lambda_i v_i = x \qquad \sum_{i=0}^{k} \lambda_i = 1.$$

Then, on a k-simplex $\rho := [v_0, v_1, \dots v_k]$, the Whitney k-form ${}^k w_{\rho}$ is

$$^{k}w_{\rho}=k!\sum_{i=0}^{k}(-1)^{i}\lambda_{i}d\lambda_{0}\wedge d\lambda_{1}\wedge\ldots\widehat{d\lambda_{i}}\wedge\cdots\wedge d\lambda_{k},$$

where the hat indicates an omitted term and the superscript k is usually dropped when the order of the form is clear. Whitney forms are a crucial ingredient in Finite Element Exterior Calculus (FEEC), a finite element framework that encompasses all standard and mixed finite element formulations through the use of the de Rham complex formed by the exterior derivative \mathbf{d} and the Koszul operator κ . The framework is described in terms of the $\mathcal{P}_r\Lambda^k$ spaces, which are the spaces of order r polynomials on differential k-forms. Indeed, Whitney forms characterize $\mathcal{P}_r^-\Lambda^k\subseteq\mathcal{P}_r\Lambda^k$. For more details, see [15], [16].

The problem with the representation of Whitney forms in terms of barycentric coordinates is that the Hodge star

of a differential form is significantly easier to compute in space-time adapted coordinates, and the Hodge star shows up in the Lagrangian density for electromagnetism. Even though this does not present much of an obstacle for vacuum electromagnetism, an explicit characterization of the Hodge star simplifies the calculations when matter sources and material properties are added into the dynamics. This is perhaps best seen through the permittivity ϵ and permeability μ tensors; any variation in their values mimic the effects of a varying metric tensor. In particular, the electric field $\bf E$ and electric displacement field $\bf D$ are related by the Hodge star with respect to a metric induced by the permittivity, and the magnetic induction $\bf B$ and the magnetic intensity $\bf H$ are related by the the Hodge star with respect to a metric induced by the permeability.

A. Space-time Whitney Forms

To simplify the task of using Whitney forms in space-time multi-Dirac discretizations of Maxwell's equations, we introduce a characterization of Whitney forms that is coordinate independent. The proofs of these results can be found in [17]. In the following, v^{\flat} represents the co-vector associated with the vector v.

Theorem 1: Let $\sigma:=[v_0,v_1,...v_n]$, an ordered set of vertex vectors, represent an oriented n-simplex on a flat n-dimensional manifold, with position vector x. Let $\rho\subseteq\sigma$ be a k-subsimplex, and $\tau=\sigma\smallsetminus\rho$ be the ordered complement of ρ in σ . The Whitney k-form over ρ can be written as

$${}^{k}w_{\rho}(x) = \frac{sgn(\rho \cup \tau)}{\star vol(\sigma)} \frac{k!}{n!} \left(\star \bigwedge_{v_{j} \in \tau} (v_{j} - x)^{\flat} \right), \quad (7)$$

with $vol(\sigma) = \frac{1}{n!} \bigwedge_{i=1}^{n} (v_i - v_0)^{\flat}$, the volume form of σ .

Note that the term outside the parenthesis is simply a normalization factor, and the expression inside the parenthesis can be understood in terms of the observation that the Whitney form vanishes on the complementary subsimplex, and the $(v_i - x)^b$ terms ensure that the proposed differential form vanishes on each of the generators of the complementary subsimplex, and by linearity, it vanishes on the entire complementary subsimplex. Since there are n-k vertices in the complementary subsimplex τ , one then uses the Hodge star \star to convert the (n-k)-differential form $\bigwedge_{v_j \in \tau} (v_j - x)^{\mathsf{p}}$ to a k-form. The overall effect of the above formula is a covector field that "rotates" about the complementary simplex. The proof of the correct normalization is more involved, and the most direct proof involves introducing an equivalent characterization of Whitney forms in terms of vector proxies, which is given in the following Proposition.

Proposition 2: Let $\sigma:=[v_0,v_1,...v_n]$, an ordered set of vertex vectors, represent an oriented n-simplex on a flat n-dimensional manifold. Let $\rho\subseteq\sigma$ be a k-subsimplex, and $\tau=\sigma\smallsetminus\rho$ be the ordered complement of ρ in σ . The Whitney k-form over ρ , evaluated on a k-multivector $W_k=\bigwedge_{i=1}^k w_i$

is given by

$${}^{k}w_{\rho}[W_{k}] = sgn(\rho \cup \tau) \frac{k!}{n!} \cdot \frac{\left\langle \bigwedge_{i=1}^{n} (v_{i} - v_{0}), (\bigwedge_{v_{j} \in \tau} (v_{j} - x)) \wedge W_{k} \right\rangle}{\left\langle \bigwedge_{i=1}^{n} (v_{i} - v_{0}), \bigwedge_{i=1}^{n} (v_{i} - v_{0}) \right\rangle}$$

Then, one can show that the characterization of Whitney k-forms presented in Proposition 2 and Theorem 1 are equivalent. Since the Hodge star applied twice is the identity map (up to a sign), the coordinate-independent characterization of Whitney forms given in Theorem 1 provide an explicit characterization of the Hodge dual of the space of Whitney k-forms.

B. Space-time Whitney forms in Electromagnetism

We now apply our space-time FEEC discretization to the vacuum electromagnetic action

$$S = -\frac{1}{4} \int_{M} \mathbf{d}A \wedge \star \mathbf{d}A.$$

Assume the manifold M has a simplicial triangulation into simplices σ_p . Discretizing the vector potential A to linear order yields $A_p = \sum_{i < j} a^p_{ij} w_{ij} + b^p_{ij} \mathbf{d}(\lambda_i \lambda_j)$ on the edges of a given simplex σ_p . This implies $dA_p = \sum_{k,i < j} a^p_{ij} w_{ijk}$ on the faces of the simplex. Applying our discretization to the Maxwell action gives

$$S = -\frac{1}{4} \sum_{p,k,n} \int_{\sigma_p} \sum_{i < j,l < m} a_{ij}^p a_{kl}^p \langle w_{ijk}, w_{lmn} \rangle vol(\sigma_p).$$

Let's now investigate the issue of gauge invariance at this linear order of approximation. We'd like to shift our potential A_p by a closed 1-form ω_p . However, at the simplicial level, all closed forms are exact, so we can take $\omega_p=df_p$, where f_p is a 0-form. Taking f_p to quadratic order, $f_p=\sum_{ij}c_{ij}^p\lambda_i\lambda_j$, which yields the gauge-shifted potential:

$$A'_p = A_p + \mathbf{d}f_p = \sum_{i < j} a_{ij}^p w_{ij} + (b_{ij}^p + c_{ij}^p) \mathbf{d}(\lambda_i \lambda_j).$$

This represents all allowed gauge transformations to linear order. The full gauge group can be better approximated as the order of approximation increases as well. In fact, at linear order, A_p automatically satisfies the Lorenz gauge, $\delta A_p = -\star \mathbf{d} \star A_p = 0$, where δ is the codifferential, defined as $\delta = (-1)^{nk+n+1} s \star d \star$ with s as the signature of the metric. The Lorenz gauge is automatically satisfied since the codifferential of any Whitney form is zero, as can be seen from (7). If we now calculate $\mathbf{d} A_p'$, we find that

$$\mathbf{d}A_p' = \sum_{i < j} \sum_{k} a_{ij}^p w_{ijk} = \mathbf{d}A_p,$$

thus, our space-time FEEC discretization automatically satisfies gauge invariance at linear order, and in particular, dF=0 is automatically satisfied. Therefore, integrating the associated discrete Noether current j_p over an arbitrary 1-chain loop ρ yields

$$\int_{a} j_{p} = \int_{a} \star (F_{p} \wedge \mathbf{d} f_{p}) = 0,$$

implying Noether's first theorem is upheld within this framework.

IV. CONCLUSIONS

In summary, gauge field theories exhibit gauge symmetries that impose Cauchy initial value constraints, and are also underdetermined. These result in degenerate field theories that can be described using multi-Dirac mechanics. There is a systematic framework for constructing and analyzing Galerkin variational integrators for Hamiltonian PDEs based on a suitable choice of numerical quadrature and finiteelement approximation of the configuration bundle. In order to develop a discretization of Maxwell's equations, which involves a space-time variational principle on differential forms that involves the Hodge star with respect to a Minkowski metric, we introduced a coordinate-independent expression for Whitney forms that provided an explicit characterization for the Hodge dual of Whitney forms. Finally, space-time Whitney forms provide a method for preserving the gauge symmetry of electromagnetism at a discrete level.

We are currently exploring extensions of our space-time characterization of Whitney forms to higher-degree approximation spaces by considering the construction introduced by Rapetti and Bossavit in [18] that is related to geometric subdivision and rescalings of the simplices in a simplicial complex. In addition, we are investigating extending this construction to include both material properties and matter sources as to simulate the full theory of electrodynamics.

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