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Geometric integration of the Vlasov-Maxwell system with a variational particle-in-cell scheme

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Abstract

A fully variational, unstructured, electromagnetic particle-in-cell integrator is developed for integration of the Vlasov-Maxwell equations. Using the formalism of Discrete Exterior Calculus [1], the field solver, interpolation scheme and particle advance algorithm are derived through minimization of a single discrete field theory action. As a consequence of ensuring that the action is invariant under discrete electromagnetic gauge transformations, the integrator exactly conserves Gauss's law.

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Particle in cell (PIC) codes have been a crucial tool in understanding complex plasma dynamics through solution of the Vlasov-Maxwell equations. The underlying idea of PIC is to advance electromagnetic fields on a fixed grid, while individual quasiparticles are tracked in continuous space. This is realized by interpolating fields to particle positions, advancing positions and velocities in time, then interpolating charge densities and currents from new particle positions back to the fixed grid. As modern supercomputers move into the exaflop (10^{18} floating point operations per second) regime and beyond, PIC codes are increasingly being used for simulations of larger and more complex systems [2]. To be able to rely upon the fidelity of simulation results and thus fully utilize computational resources, it is critical that algorithms have good long time conservation properties. This is the underlying idea behind geometric integrators: integrators designed to respect geometric principles of the underlying physical system being studied, thereby reducing spurious numerical effects damaging to the fidelity of simulations. In the past decade there has been rapid development of these techniques, both for time discretization, with variational integrators [3–5], and for spatial discretization, with Discrete Exterior Calculus (DEC) and mimetic finite elements [1, 6, 7].

In this letter we use the ideas of discrete exterior calculus (DEC) and variational integrators to formulate a geometric PIC scheme that conserves a space-time multi-symplectic structure [4]. While symplectic particle pushing algorithms and multi-symplectic electromagnetic field solvers exist, coupling two such schemes does not guarantee multi-symplecticity of the PIC algorithm as a whole. Our method is to devise a single *space-time* discrete Lagrangian, then use the principle of least action to derive the entire PIC scheme. This approach is motivated by the success of numerous integrators of this type for other field theories. These include integrators for continuum mechanics [8], electromagnetism [9], incompressible fluids [10], and more complex fluids, such as ideal magnetohydrodynamics [11]. In all cases, the algorithms have very good long time energy conservation as well as other desirable properties.

In addition to multi-symplecticity, discrete current conservation $\partial_t \rho + \nabla \cdot \mathbf{J} = 0$, is a natural property of the variational formulation: it is a direct consequence of discrete electromagnetic gauge invariance of the discrete action. Current conservation ensures Gauss’s law, $\nabla \cdot \mathbf{E} = \rho/\epsilon_0$, remains satisfied at all times. This is important both from a physics and computational standpoint, since Gauss’s law is non-local and can be difficult to solve efficiently on modern, massively parallel computing systems. Understanding current conservation in terms of discrete gauge invariance could be crucial in the future design of geometrical PIC schemes for more complicated field theories, for instance gyrokinetics [12].

The classical action for a collection of particles interacting with a self-generated electromagnetic field is,

$$\mathcal{S} = -\frac{1}{2} \int_x dA \wedge \star dA + \int \sum_p (q_p A + p) |_{\mathbf{x}_p(t)}. \quad (1)$$

Here A and p are 1-forms on 4-D space-time, respectively the 4-vector potential of the field and the particle momentum 1-form, and q_p is the particle charge. \int_x denotes integration over space-time and \sum_p denotes the sum over all particles with A and p evaluated at particle positions, $\mathbf{x}_p(t)$. The exterior derivative, hodge star and wedge product are all operating in 4-D space-time. In terms of fields $-\frac{1}{2}dA \wedge \star dA$ is simply $E^2 - B^2$, where we have chosen the geometric notation for the sake of clarity in the discretization of the action principle. Throughout this letter natural units are used with $c = \varepsilon_0 = 1$.

In the non-relativistic limit,

$$(A + p) |_{\mathbf{x}_p(t)} = q_p \mathbf{A}(\mathbf{x}_p) \cdot d\mathbf{x} - q_p \phi(\mathbf{x}_p) dt + m_p \mathbf{v}_p \cdot d\mathbf{x} - \frac{1}{2} m_p v_p^2 dt, \quad (2)$$

with \mathbf{A} and ϕ the usual electromagnetic potentials and m_p particle mass. In this limit, the action, Eq. (1), is simply the mixed Eulerian-Lagrangian action principle of Low expressed in geometric notation [12, 13], with the distribution function $\sum_p \delta(\mathbf{x} - \mathbf{x}_p) \delta(\mathbf{v} - \mathbf{v}_p)$. The equations of motion for the system are

$$\begin{aligned} \dot{\mathbf{x}}_p &= \frac{q_p}{m_p} \left[\left(-\nabla \phi - \frac{\partial \mathbf{A}}{\partial t} \right) |_{\mathbf{x}_p} + \mathbf{v}_p \times (\nabla \times \mathbf{A}) |_{\mathbf{x}_p} \right] \\ \dot{\mathbf{x}}_p &= \mathbf{v}_p \\ d \star dA &= \mathcal{J}. \end{aligned} \quad (3)$$

Here, $\mathcal{J} = \star(\mathbf{J} \cdot d\mathbf{x} - \rho dt)$, with \mathbf{J} the current density $\sum_p q_p \mathbf{v}_p \delta(\mathbf{x} - \mathbf{x}_p)$ and ρ the charge density $\sum_p q_p \delta(\mathbf{x} - \mathbf{x}_p)$.

Eqs. (3) are gauge invariant, meaning an exact 1-form, df , can be added to A without changing the dynamics. This follows directly from symmetry of the action, Eq. (1), under the transformation $A \rightarrow A + df$. The symmetry leads to the conserved quantity $d_s D - \rho$, ($d_s D$ is the divergence of the electric displacement), which is simply Gauss's law [9]. This principle, that gauge invariance of the action will lead to equations that conserve Gauss's law, is critical for our discretization of the problem. Note that this is equivalent to current conservation, $d\mathcal{J} = 0$ ($\partial_t \rho + \nabla \cdot \mathbf{J} = 0$ in standard notation).

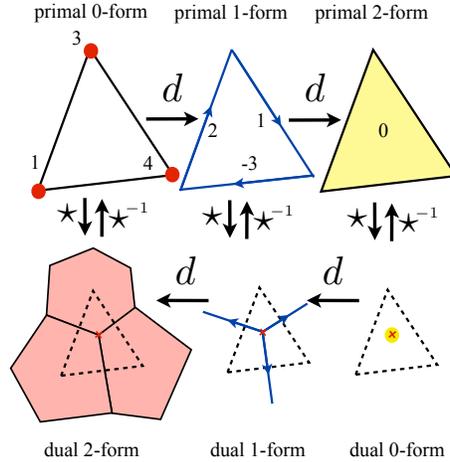


FIG. 1. Structure of DEC and operators for a single 2-D simplex.

The formalism used to develop our discrete variational principle is that of discrete exterior calculus (DEC). A brief overview of the basic elements is given here, with details found in [1, 7, 14, 15]. The starting point for DEC is a discrete manifold. In the simplest case, this is a simplicial complex, essentially a collection of simplices (lines, triangles, tetrahedra in 1-D, 2-D and 3-D respectively) embedded in n -dimensional space. For example, a region in 3-D space discretized using a tetrahedral mesh. The structure of differential forms in DEC is illustrated in Figure 1, with k -forms located on k -simplices (0-forms on vertices, 1-forms on edges etc.). The exterior derivative operator, d , that takes a k -form to a $(k+1)$ -form, is defined so as to exactly satisfy Stoke’s theorem $\int_{\chi} d\alpha = \int_{\partial\chi} \alpha$. Importantly, with this definition, d is purely topological and $d(d\alpha) = 0$.

For operations involving the metric, it is necessary to define a dual mesh, formed in this work by connecting the circumcenters of each n -simplex (circumcentric dual). The discrete Hodge-star operator takes a k -form on the primal mesh to an $(n-k)$ -form on the dual mesh, see Figure 1. The Hodge-star we use is simply a diagonal matrix, more complex operators can give higher order accurate theories. DEC is very well suited to the analysis of electromagnetism, in that replacing continuous operators and forms with their discrete counterparts gives a variational integrator with very nice properties. In fact, the very popular Yee staggered mesh [16] is simply an application of DEC on a cubic mesh [9].

The interpolation of fields to continuous space is achieved with Whitney forms [7, 14, 17], which associate an interpolation k -form to each discrete k -simplex. Using a first order scheme, Whitney 0-forms are simply familiar “hat-functions,” defined as $\varphi_i(\mathbf{x}) = 1$ at vertex i , $\varphi_i(\mathbf{x}) = 0$ at

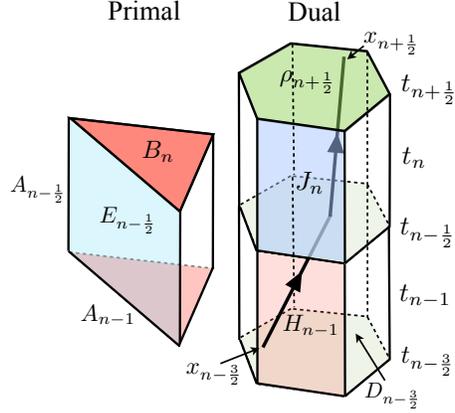


FIG. 2. Primal and dual cells, shown in two spatial dimensions for clarity. A is a primal 1-form, B and E are primal 2-forms, D and H are dual 2-forms, and $\star\mathcal{J}$ (J and ρ) is a dual 2-form. Structure of these forms in 3 spatial dimensions is outlined in the text. Also shown is a sample particle track.

all other vertices, with linear dependence in the neighborhood of vertex i . Higher degree Whitney forms are a generalization of this. For instance, the Whitney 1-form for the edge between node i and node j is simply $\varphi_{ij} = \varphi_i d\varphi_j - \varphi_j d\varphi_i$, which is equal to $\varphi_i \nabla\varphi_j - \varphi_j \nabla\varphi_i$ if working in Euclidian space.

The discrete manifold we use in our discretization is simplex primal in 3+1 or 2+1 dimensions; that is, tetrahedrons or triangles projected through time as illustrated in Figure 2. The simpler case of an integrator on a structured cubic mesh could also easily be derived (not done here). Since the manifold is a direct product of a time discretization with a spatial mesh, we can split operators into time and space components. This allows for a simpler implementation of Maxwells equations in terms of familiar E , B , D and H forms rather than the full Maxwell field tensor, $F = dA$. It is also convenient to split A into a purely spatial 1-form (analogous to vector potential, \mathbf{A}) and a space-time component that can be thought of as a spatial 0-form (analogous to the scalar potential, ϕ). These we denote by A_n^{ij} and $A_{n+1/2}^i$ respectively, due to their location on the space-time manifold. Additionally, we split the current dual 3-form into a space-time component J (spatial primal 1-form or dual 2-form) and a purely spatial component ρ (spatial primal 0-form or dual 3-form), see Figure 2. Field equations of motion as derived from the action principle are given below.

In analogy with the continuous case, symmetry of a discrete action under the transformation $A \rightarrow A + df$ (where A and f are discrete forms) will guarantee exact preservation of the discrete Gauss's law for all time. The method for achieving this gauge symmetry was motivated by Eastwood's current conserving scheme [18] and its recent generalization to an unstructured mesh [19].

This relies on integration of the particle trajectories through time in the calculation of the discrete current. With this idea, our discrete space-time Vlasov-Maxwell action, which is a discrete approximation of Eq. (1), is

$$\begin{aligned} \mathcal{S}_d = \sum_{n=0}^N \left\{ \sum_{\varepsilon_s} -\frac{1}{2} dA \wedge \star dA + h \sum_p \left[\frac{1}{2} m_p \left| \frac{\mathbf{x}_{n+1/2}^p - \mathbf{x}_{n-1/2}^p}{h} \right|^2 \right. \right. \\ \left. \left. + q_p \left(\frac{\mathbf{x}_{n+1/2}^p - \mathbf{x}_{n-1/2}^p}{h} \right) \cdot \int_{t_{n-1/2}}^{t_{n+1/2}} \frac{dt}{h} \left(\sum_{ij \in \sigma_1} A_n^{ij} \boldsymbol{\varphi}_{\sigma_{ij}}(\mathbf{x}^p(t)) \right) \right. \right. \\ \left. \left. - \frac{q_p}{h} \sum_{i \in \sigma_0} A_{n-1/2}^i \varphi_i(\mathbf{x}_{n-1/2}^p) \right] \right\}. \end{aligned} \quad (4)$$

Here, h is the time-step, n is the time index and p the particle index. \sum_{ε_s} denotes the spatial sum of the volume form $-\frac{1}{2}dA \wedge \star dA$, and $\sum_{ij \in \sigma_1}$ and $\sum_{i \in \sigma_0}$ denote the sum over edges and vertices respectively. $\boldsymbol{\varphi}_{\sigma_{ij}}$ is the Whitney 1-form associated to edge ij . The particle path $\mathbf{x}^p(t)$ is taken to be linear with constant velocity between $\mathbf{x}_{n-1/2}^p$ and $\mathbf{x}_{n+1/2}^p$. As is standard in variational integrators, the particle Lagrangian is designed to approximate $\int_{t_{n-1/2}}^{t_{n+1/2}} dt L_c^p$ where L_c^p is the continuous Lagrangian. The present case is that of a single particle in the discrete electromagnetic field.

The field part of Eq. (4) is obviously gauge invariant since $d^2 = 0$. Since the particle part is linear in A , gauge invariance can be seen by substituting $A = df$ and showing that this only gives contributions from the endpoints. This is straightforward using $d_c((\alpha)_{interp}) = (d_d \alpha)_{interp}$ for a 0-form α , where d_c and d_d are the continuous and discrete exterior derivatives and $(\)_{interp}$ signifies Whitney interpolation of the form.

Field equations arise from variation of the discrete action with respect to the potential, A , yielding (see [9])

$$d \star dA = \mathcal{J}. \quad (5)$$

Due to the tensor product nature of the discrete manifold this is equivalent to

$$d_s E_{n+1/2} + \frac{B_{n+1} - B_n}{h} = 0 \quad (6)$$

$$d_s H_n - \frac{D_{n+1/2} - D_{n-1/2}}{h} = q_p \mathbf{v}_n \cdot \int_{t_{n-1/2}}^{t_{n+1/2}} \frac{dt}{h} \sum_{ij \in \sigma_1} \boldsymbol{\varphi}_{\sigma_{ij}}|_{\mathbf{x}^p(t)}, \quad (7)$$

and

$$d_s D_{n+1/2} = q_p \sum_{i \in \sigma_0} \varphi_i(\mathbf{x}_{n-1/2}^p) \quad (8)$$

$$d_s B = 0. \quad (9)$$

Here $E_{n+1/2} = -\frac{1}{h}(A_{n+1} - A_n) - d_s A_{n+1/2}$ is a spatial primal 1-form, $B_n = d_s A_n$ is a spatial primal 2-form, $D = \star_s E$ and $H = \star_s B$, with the subscript s indicating the spatial part of a DEC operator. Note that Eqns. (8) and (9) are constraints and need only be applied as initial conditions. The particle equations of motion are derived from variations of Eq. (4) with respect to $\mathbf{x}_{n-1/2}^p$. This leads to the particle equations of motion,

$$\begin{aligned} & \frac{1}{h^2} (\mathbf{x}_{n+1/2}^p - 2\mathbf{x}_{n-1/2}^p + \mathbf{x}_{n-3/2}^p) \\ &= \frac{q_p}{m_p} \left(\tilde{\mathbf{E}}_{n-1/2}^p + \frac{1}{2} \mathbf{v}_n^p \times \tilde{\mathbf{B}}_n^p + \frac{1}{2} \mathbf{v}_{n-1}^p \times \tilde{\mathbf{B}}_{n-1}^p \right), \end{aligned} \quad (10)$$

where

$$\tilde{\mathbf{E}}_{n-1/2}^p = (E_{n-1/2})_{interp} |_{\mathbf{x}_{n-1/2}^p} \quad (11)$$

$$\tilde{\mathbf{B}}_n^p = \int_{t_{n-1/2}}^{t_{n+1/2}} \frac{dt}{h} \left(\frac{t_{n+1/2} - t}{h} \right) (B_n^p)_{interp} |_{\mathbf{x}^p(t)} \quad (12)$$

$$\tilde{\mathbf{B}}_{n-1}^p = \int_{t_{n-3/2}}^{t_{n-1/2}} \frac{dt}{h} \left(\frac{t - t_{n-3/2}}{h} \right) (B_{n-1}^p)_{interp} |_{\mathbf{x}^p(t)} \quad (13)$$

$$\mathbf{v}_n^p = \frac{1}{h} (\mathbf{x}_{n+1/2}^p - \mathbf{x}_{n-1/2}^p). \quad (14)$$

Since particle trajectories are linear and fields, $(E_{n-1/2})_{interp}$ and $(B_n^p)_{interp}$, are piecewise polynomial, time integrals can be performed exactly using Gaussian quadrature (see [19]). Because of the $\tilde{\mathbf{B}}_n^p$ term, the algorithm is implicit. However, if a quasi-particle stays in the same cell, as is the case for the majority of time-steps, Eq. (10) can be easily solved without resorting to an iterative scheme.

While variational formulations have been used for PIC methods in the past (see [20]), this is, to our knowledge, the first PIC scheme to use a full space-time variational principle. As a consequence, the algorithm as a whole is multi-symplectic (see [9, 21]), an important geometrical property proven to have profound consequences for the integration of systems of ordinary differ-

ential equations [4, 22]. Though presented from a somewhat different standpoint, the algorithm is similar to those in [19]. The crucial difference is that our particle mover is constrained to a particular form by the discrete action, which is necessary for a fully multi-symplectic method.

Using the ideas in [15], the unstructured Maxwell solver is very simple to implement. Field advancement is governed by Eqs. (6) and (7), and simply involves sparse matrix multiplication. As a test case, we have implemented a 2-D version of variational PIC in `MATLAB`, with a magnetic field directed out of the plane. In this case, the equations of motion and definitions of E , B , D , and H are exactly the same as the 3-D case. Particle advancement is implemented by first assuming the particles stay in the same cell. In the case where this is not true and an implicit solver is needed, the current contribution to the grid is calculated at the same time as particle advancement. As a consequence, the extra computational expense over an explicit particle pusher scheme is minimal.

Investigations are ongoing into the numerical properties of variational PIC, with special focus on the importance of the multi-symplectic nature of the algorithm. Here we give a brief numerical example, motivated by Refs. [19, 23], to illustrate the importance of numerical current conservation. On a triangular mesh, a beam of electrons is accelerated by an external voltage (from left to right) calculated to satisfy the Child-Langmuir law. Figure 3(a) shows the particle distribution at $t = 40$ using symplectic PIC, while Figure 3(b) illustrates the distribution for the same initial conditions, advanced using an integrator that does not conserve current. Local violations in Gauss's law caused by lack of current conservation are manifested through unphysical bunching of the charge into lines of higher density, as evident in Figure 3(b). The beam also widens more than in the current conserving case, showing that there is an overestimation of the average self electric field.

Our discretization of the variational principle [Eq. (4)] is relatively arbitrary. As an avenue for future work it could be interesting to explore different discretizations of the same system (for instance, different particle pushers, particle shape factors or field Hodge-star operators) to better understand some advantages of a fully multi-symplectic scheme. Another approach would be to design a fully implicit variational PIC integrator. At the cost of complexity, implicit PIC schemes circumvent many of the numerical instabilities inherent in explicit PIC [20, 24] and allow larger time-steps.

The methods presented above will allow relatively simple generalizations to more complex mesh schemes. One such idea would be an Asynchronous Variational Integrator, in which each grid cell and particle could be advanced with a different time-step set by its own Courant condition

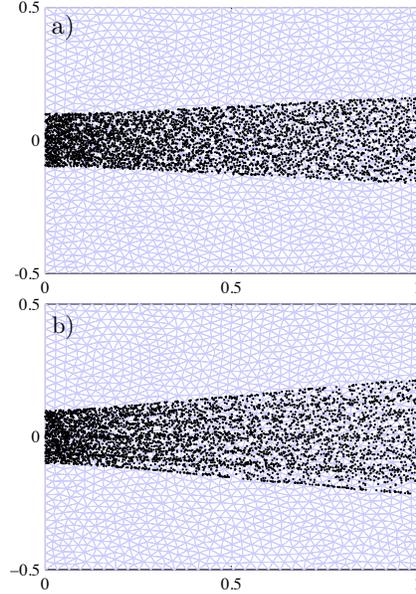


FIG. 3. Electron beam particle distribution accelerated by external potential. Evolved in time using: (a) symplectic PIC (current conserving) (b) non current conserving algorithm producing spurious bunching of the charge into lines due to violations of Gauss’s law.

[8, 9]. Time savings can be substantial on highly irregular meshes. As a further generalization of this type of idea, a 4-D simplicial complex could be used in a completely covariant general relativistic PIC code, which would have many astrophysical applications. The DEC and variational formalisms could be very important in formulating methods for field advancement and current conservation in these complex systems.

Perhaps one of the most exciting areas of future research is in the design of geometric PIC algorithms for more complex field theories, in particular gyrokinetics [12]. Being non-local, gyrokinetics presents a great challenge in algorithm design if one is to respect important geometrical properties of the system. The question of how to ensure current conservation is answered very cleanly by the realization that it is simply the requirement that a discrete variational principle be electromagnetically gauge invariant.

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