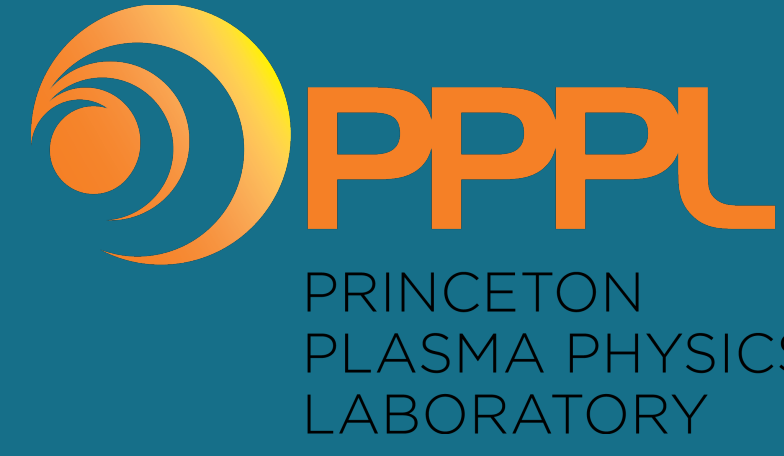


Geometric integration of the Vlasov-Maxwell system with a variational particle-in-cell scheme

J Squire, H Qin, W M Tang jsquire@princeton.edu

Princeton Plasma Physics Laboratory

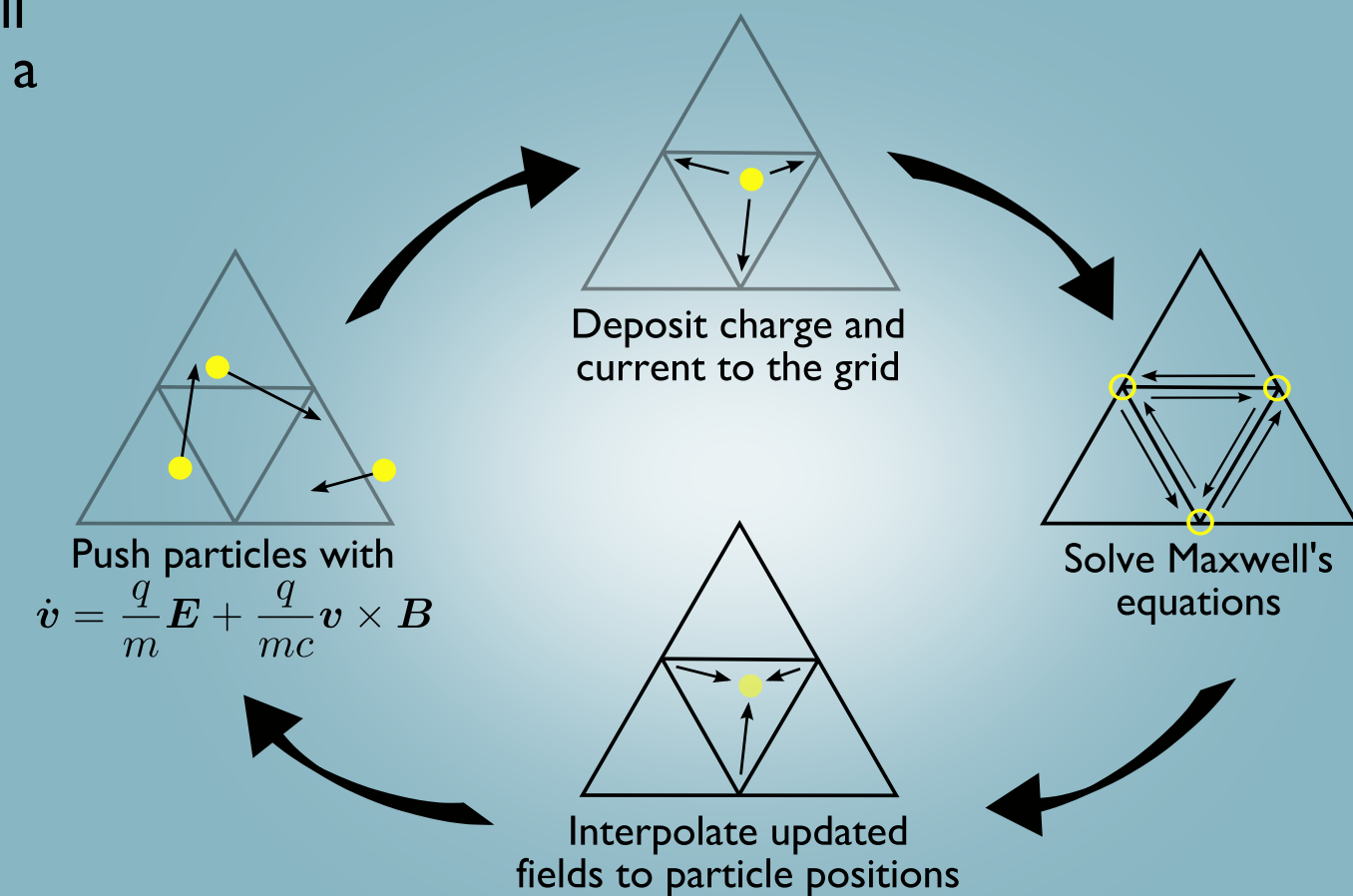


A fully variational, unstructured, electromagnetic particle-in-cell integrator is developed for integration of the Vlasov-Maxwell equations. Using the formalism of Discrete Exterior Calculus [2], the field solver, interpolation scheme and particle advance algorithm are derived through minimization of 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.

Particle-in-Cell

- Through direct solution of the Vlasov-Maxwell system, particle-in-cell (PIC) codes have been a crucial tool in understanding complex plasma dynamics in many application domains.
- A hybrid computational approach is used. Electromagnetic fields are stored on a grid, while discrete plasma quasi-particles are tracked in continuous space.
- Simulations can be very computationally intensive, running with billions of quasi-particles on some of the world's largest supercomputing facilities [3].



Geometric Integration

- Geometric integrators are numerical algorithms designed to respect the underlying geometry of the physical system.
- By ensuring the integrator has various long-time conservation properties, one can better rely upon the fidelity of simulations. This is particularly important as larger and more complex systems are studied.
- A very fruitful approach to designing a geometric integrator is to start by discretizing the variational principle rather than the equations of motion. Using the least action principle in *discrete* space, one obtains a *variational integrator*.
- Some examples of successful variational integrators for finite and infinite dimensional systems include: plasma guiding center equations [4] (see Fig. 1), electrodynamics [5], and magnetohydrodynamics [6].

Figure 1: Comparison of tokamak banana orbits in the guiding center approximation integrated using (a) a Runge-Kutta algorithm (b) the variational symplectic algorithm in [4].

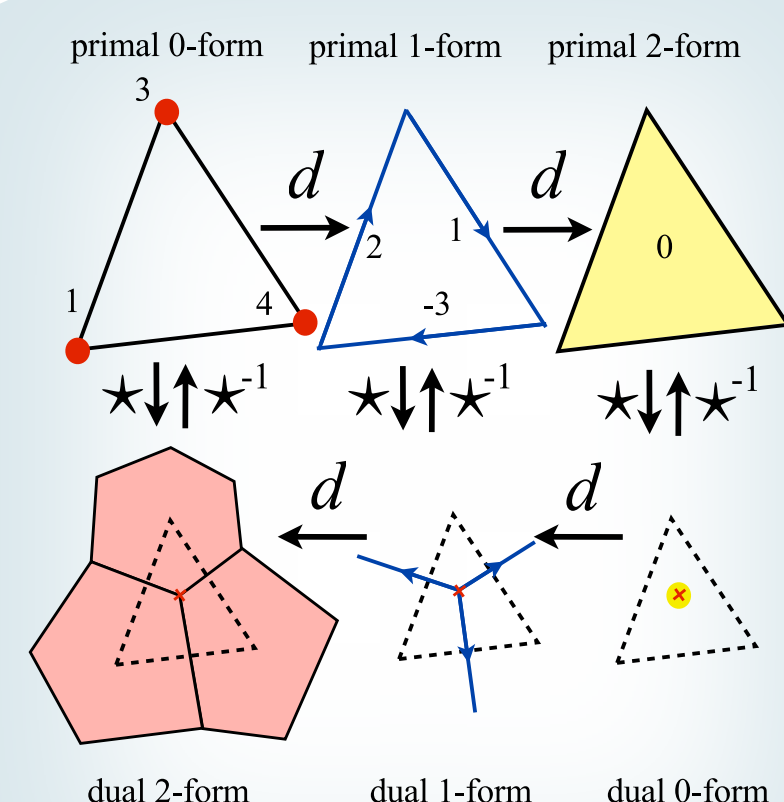
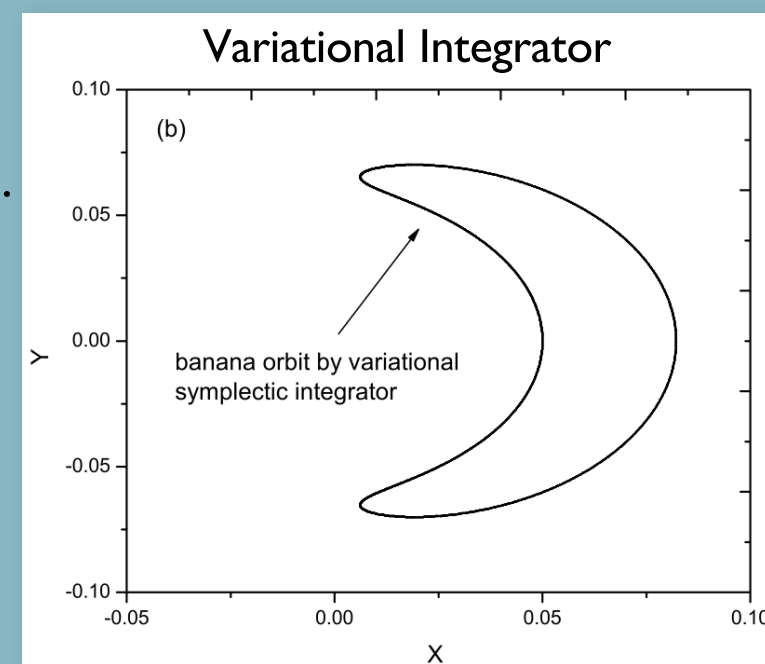
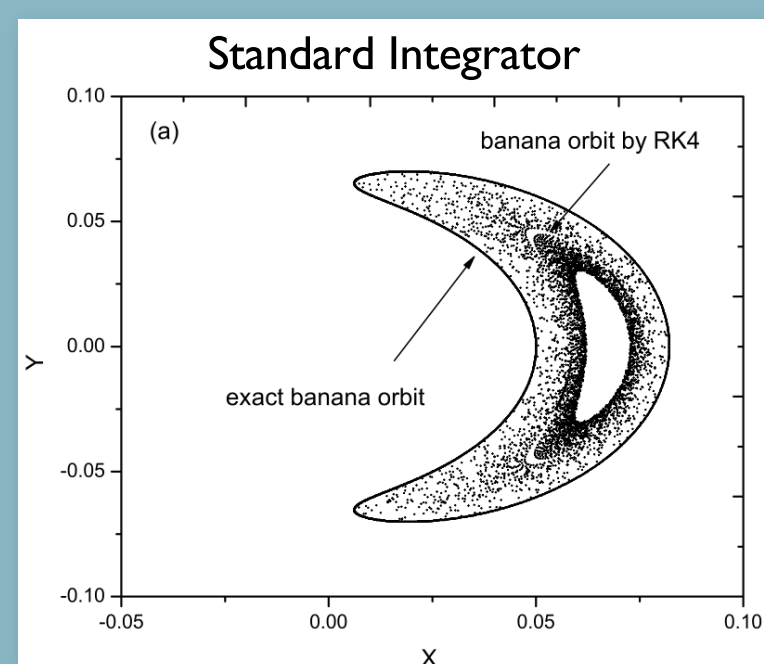


Figure 2: Structure of DEC and operators for a single 2-D simplex.

- The starting point is a discrete manifold, usually just a simplicial complex (collection of lines, triangles and tetrahedra). 0-forms (functions) live on points, 1-forms (co-vectors) live on edges, 2-forms on triangles and 3-forms on tetrahedra, see Fig. 2.
- The exterior derivative operation, d is designed to satisfy Stoke's theorem $\int_{\partial \alpha} d\alpha = \int_{\alpha} \alpha$ (see Fig. 2).
- In 3-D d is equivalent to gradient, curl or divergence (depending on the form it operates on) and the definition above ensures $\nabla \times \nabla f = 0$ and $\nabla \cdot \nabla \times \mathbf{A} = 0$ are automatically satisfied.
- The Hodge star, $\star$ takes a k -form to an $(n-k)$ -form on the dual mesh, which is formed by connecting the circumcenters of the top level simplices (see Fig. 2).
- Electromagnetism is an ideal application for DEC since the equations are written very naturally using exterior calculus [5]. With F the Maxwell field tensor and $\mathcal{J}$ the 4-current (including charge),

$$\left\{ \begin{array}{l} \nabla \times \mathbf{B} = \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} + \frac{4\pi}{c} \mathbf{J} \\ \nabla \cdot \mathbf{E} = 4\pi \rho \end{array} \right\} \iff d \star F = \mathcal{J} \quad \left\{ \begin{array}{l} \nabla \times \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} \\ \nabla \cdot \mathbf{B} = 0 \end{array} \right\} \iff dF = 0$$
- Simply replacing continuous exterior operators with their discrete counterparts leads to a variational integrator [5] with very nice conservation properties. On a cubic mesh this is the FDTD Yee mesh [7].

The Discrete Variational Principle

- Start with the action for a collection of particles interacting with the electromagnetic field. This is just the continuous Vlasov-Maxwell action principle of Low [8] with a discrete distribution function.

$$S = -\frac{1}{2} \int_x dA \wedge \star dA + \int dt \sum_p \left[\frac{1}{2} m_p \dot{x}_p^2 - q_p \phi(x_p) + q_p \dot{x}_p \cdot \mathbf{A}(x_p) \right]$$

DISCRETIZE

$$S_d = \sum_{n=0}^N \left\{ \sum_s -\frac{1}{2} dA \wedge \star dA + h \sum_p \left[\frac{1}{2} m_p \left| \frac{x_{n+\frac{1}{2}}^p - x_{n-\frac{1}{2}}^p}{h} \right|^2 - \frac{q_p}{h} \sum_{i \in \sigma_0} A_{n-\frac{1}{2}}^i \varphi_i(x_{n-\frac{1}{2}}^p) + q_p \left(\frac{x_{n+\frac{1}{2}}^p - x_{n-\frac{1}{2}}^p}{h} \right) \cdot \int_{t_{n-\frac{1}{2}}}^{t_{n+\frac{1}{2}}} \frac{dt}{h} \left(\sum_{ij \in \sigma_1} A_n^{ij} \varphi_{\sigma_{ij}}(x^p(t)) \right) \right] \right\}$$

- Stationarity of the discrete action with respect to variation in A leads to the discrete Maxwell's equations

$$d \star dA = \mathcal{J} \quad \iff \quad \begin{aligned} d_s E_{n+\frac{1}{2}} + \frac{B_{n+1} - B_n}{h} &= 0 & d_s D_{n-\frac{1}{2}} &= \sum_p q_p \varphi_i |x_{n-\frac{1}{2}}^p \\ d_s H_n - \frac{D_{n+\frac{1}{2}} - D_{n-\frac{1}{2}}}{h} &= \sum_p q_p v_n^p \cdot \int_{t_{n-\frac{1}{2}}}^{t_{n+\frac{1}{2}}} \frac{dt}{h} \varphi_{\sigma_{ij}} |x^p(t), & d_s B &= 0 \end{aligned}$$

$E_{n+\frac{1}{2}} = -\frac{1}{h} (A_{n+1} - A_n) - d_s A_{n+\frac{1}{2}}$, $B_n = d_s A_n$

- The ability to split Maxwell's equations in this way comes from the primal structure of the mesh (see Fig. 3). d_s denotes the exterior derivative on the spatial mesh.

- Stationary of the discrete action with respect to variation of $x_{n-\frac{1}{2}}^p$ leads to particle update equations

$$\frac{1}{h^2} \left(x_{n+\frac{1}{2}}^p - 2x_{n-\frac{1}{2}}^p + x_{n-\frac{3}{2}}^p \right) = \frac{q_p}{m_p} \left(\tilde{E}_{n-\frac{1}{2}}^p + \frac{1}{2} v_n^p \times \tilde{B}_n^p + \frac{1}{2} v_{n-1}^p \times \tilde{B}_{n-1}^p \right) \quad \text{with} \quad \begin{aligned} \tilde{E}_{n-\frac{1}{2}}^p &= (E_{n-\frac{1}{2}})_{interp} |x_{n-\frac{1}{2}}^p \\ \tilde{B}_n^p &= \int_{t_{n-\frac{1}{2}}}^{t_{n+\frac{1}{2}}} \frac{dt}{h} \left(\frac{t_{n+\frac{1}{2}} - t}{h} \right) (B_n^p)_{interp} |x^p(t) \\ \tilde{B}_{n-1}^p &= \int_{t_{n-\frac{1}{2}}}^{t_{n-\frac{1}{2}}} \frac{dt}{h} \left(\frac{t - t_{n-\frac{1}{2}}}{h} \right) (B_{n-1}^p)_{interp} |x^p(t) \end{aligned}$$

$()_{interp}$ is used to denote interpolation (using Whitney forms) of a discrete form to continuous space.

- The time integrals in the action and equations of motion are required for discrete gauge invariance, see "Gauge Invariance" section.

- While variational formulations have been used for PIC methods in the past, 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.

- The algorithm is relatively similar to that presented in [9]. The crucial difference is that our particle mover is set to a particular form by the discrete action.

Whitney Forms

- To interpolate fields to particles in the action principle we use Whitney forms [10], a generalization of the "hat function" (finite element) to differential forms.
- The Whitney 1-form for the edge (ij) is defined as $\varphi_{ij}(x) = \varphi_i d\varphi_j - \varphi_j d\varphi_i$ where $\varphi_i(x)$ is the hat function associated with node i .
- There is a straightforward generalization to higher order forms.

Primal

Dual

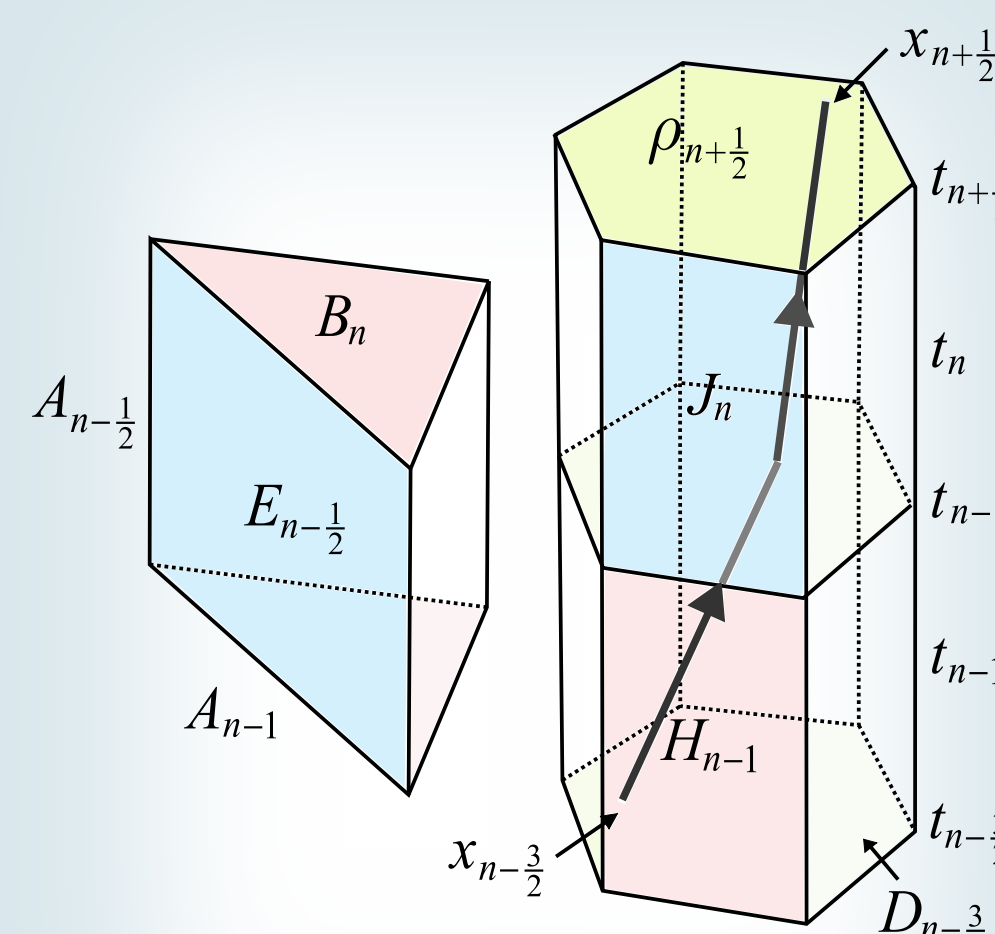


Figure 3: Space-time mesh in 2-D used for DEC based Maxwell solver. Mesh is primal in the time direction. Geometric positions of the various electromagnetic fields are shown along with a sample particle track.

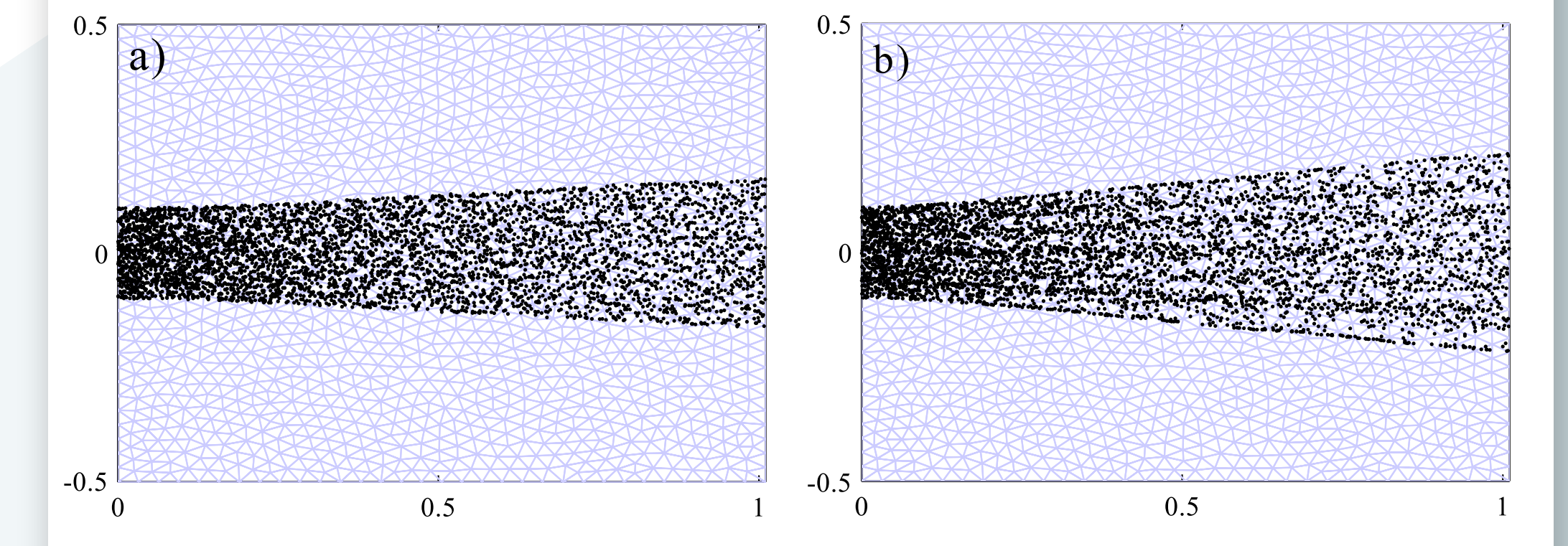
Gauge Invariance

- The electromagnetic action is symmetric under gauge transformations, $A \rightarrow A + df$ ($A \rightarrow A + \nabla f$, $\phi \rightarrow \phi - \partial_t f$ in co-ordinate notation).
- As a direct consequence $\nabla \cdot \mathbf{E} - 4\pi\rho$ is a conserved quantity, i.e., Gauss's law is just an initial condition.
- The same principle holds in the discrete setting; invariance of the discrete action under the transformation $A \rightarrow A + df$ will lead to an algorithm that conserves a discrete Gauss's law.
 - This implies the scheme can be entirely local, a very important property for modern high performance computing on massively parallel systems.
- Gauge invariance of the action is achieved by integrating the particle trajectory through time. This is motivated by Eastwood's current conserving scheme [11] and its recent generalization to an unstructured mesh [9].
 - Discrete gauge invariance is straightforward to prove; the field part is obvious since $d^2 = 0$, while the particle part follows using $d((\alpha)_{interp}) = (d\alpha)_{interp}$ for the discrete 0-form α .
- Note that the update equations depend on A only through $E_{n+1/2}$ and B_n . This property is also a consequence of gauge invariance.

Numerical Example

- The DEC based Maxwell solver is very simple to implement, even on an unstructured grid.
- All DEC operators are simply sparse matrices.
- Since the particle trajectory and the interpolated fields, $(E_{n-1/2})_{interp}$ and $(B_n)_{interp}$, are piecewise polynomial, time integrals are calculated exactly using Gaussian quadrature [9].
 - For example, with piecewise linear interpolation functions, the time integral is the weighted sum of values at the midpoints of each section of the path.
- In the case where a particle remains in the same cell, it can be advanced without requiring an iterative scheme.
- For a particle that changes cells an iterative scheme must be utilized. However, as the current deposition can be calculated in the same step, the extra computational expense is minimal.
- As a test-case we have implemented a 2-D version in MATLAB. Figure 4 is a numerical example to illustrate the importance of satisfying Gauss's law.

Figure 4: A beam of electrons accelerated (from left to right) by an external voltage calculated to satisfy the Child-Langmuir law. The left and right panels show distributions integrated using symplectic PIC and an integrator that does not conserve current respectively, both at $t=40$. Local violations in Gauss's law due to lack of current conservation are manifested through unphysical bunching of charge into lines in (b).



Future Work

- The discretization is relatively arbitrary. To better understand some advantages of a multi-symplectic scheme, one could study integrators from different action principles.
- In this vein, an implicit variational PIC scheme could be developed, which would circumvent some numerical instabilities of explicit PIC.
- A more complex mesh could be used. For instance, a 4-D simplicial complex could be a practical way to design a general relativistic PIC code. The variational formulation could be invaluable in formulating field advancement and current conservation for such a scheme.
- The method could be helpful in the design of geometric integrators for gyrokinetics, which is a more complex field theory. An algorithm would discretely conserve current if one could find a gauge invariant discrete action.

References

- J. Squire, H. Qin, and W. M. Tang, Physics of Plasmas 19, 052501 (2012).
- M. Desbrun, A. N. Hirani, M. Leok, and J. E. Marsden, (2005), arXiv:math/0508341
- R. Rosner (DoE Advanced Scientific Computing Advisory Committee Report), (2010)
- H. Qin and X. Guan, Phys. Rev. Lett. 100, 035006 (2008).
- A. Stern, Y. Tong, M. Desbrun, and J. E. Marsden, (2007), arXiv:0707.4470v3 [math.NA]
- E. Gawlik, P. Mullen, D. Pavlov, J. E. Marsden, and M. Desbrun, Physica D 240, 1724 (2011).
- K. S. Yee, IEEE Trans. Ant. Prop. , 302 (1966).
- F. Low, Proc. R. Soc. A , 282 (1958).
- M. Campos-Pinto, S. Jund, S. Salmon, and E. Sonnendrücker (Projet Calvi (INRIA), ANR Houpic.), (2009).
- H. Whitney, Geometric integration theory (Princeton university press, 1957).
- J. Eastwood, Comp. phys. comm. 64, 252 (1991).

This research was supported by the U.S. Department of Energy under Contract No. AC02-09CH11466.