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Discretization of Maxwell-Vlasov Equations based on Discrete Exterior Calculus

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Abstract

We discuss the discretization of Maxwell-Vlasov equations based on a discrete exterior calculus framework, which provides a natural factorization of the discrete field equations into topological (metric-free) and metric-dependent parts. This enables a gain in geometrical flexibility when dealing with general grids and also the *ab initio*, exact preservation of conservation laws through discrete analogues. In particular, we describe a particle-in-cell (PIC) implementation of time-dependent discrete Maxwell-Vlasov equations, whereby the electromagnetic field are discretized using Whitney forms and coupled to particle dynamics by means of a gather-scatter scheme that yields exact charge-conservation on general grids. Numerical examples of PIC simulations such as vacuum diode and backward-wave oscillator are used to illustrate the approach.

1 Introduction

Historically, computational electromagnetics (CEM) has adopted the language of vector calculus when describing initial or boundary value problems involving Maxwell's equations, and for their discretization based on finite-difference, finite-element, or finite-volume techniques [1]. However, when it comes to unveiling the deeper geometric structure of electromagnetism, the exterior calculus of differential forms is a more suitable mathematical language [2, 3, 4]. Among its advantages, exterior calculus provides a natural factorization of the field equations into topological and metric parts [3, 5]. To be specific, the exterior derivative d, which plays the simultaneous role of the gradient, curl, and divergence operators of vector calculus, is the adjoint of the boundary operator ∂. The latter is a purely topological operator which, on a discrete setting, acts on a cell complex based on generalized Stokes theorem [5, 6, 7] so that the associated equations become metric-free. All metric information are incorporated in the constitutive relations generalized as Hodge star operators. The resulting discrete formulation provides a great deal of geometrical flexibility since the metric-free equations depend only on the mesh *connectivity* (topology) and are independent of the geometry of the mesh (i.e. element *shapes*). Consequently, conservation laws such as charge continuity can be verified independently of the mesh geometry [3].

In this summary paper, we discuss the discretization of Maxwell-Vlasov equations based on discrete exterior calculus [3, 5, 6] and some specific algorithmic strategies to improve their accuracy [8, 9]. Maxwell-Vlasov equations consist of time-dependent Maxwell's equations coupled to Lorentz-Newton equations of motion (the latter derived from Vlasov kinetic equation) describing the collective motion of a (typically very large) set of charged particles. Maxwell-Vlasov equations are important in a variety of applications including plasma fusion, vacuum electronic devices, laser ignition, and astrophysics [10]. A common strategy for algorithmic implementation of Maxwell-Vlasov equations is to use a finite-difference or finite-element field solver coupled, via gather-scatter steps, to a particle-in-cell algorithm modeling the particle dynamics, as depicted schematically in Fig. 1. Here, we detail how discrete exterior calculus can unify some of these strategies, as well as provide new design principles for obtaining gather-scatter that yields exact charge-conservation on general grids [8, 9]. Numerical examples involving a vacuum diode and a backward-wave oscillator are provided to illustrate the methodology.

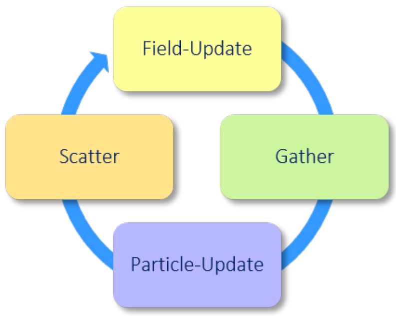

Figure 1. Schematic representation for the four basic steps of a PIC algorithm repeated at each time step.

2 Electromagnetic PIC Algorithm on General Grids

Maxwell-Vlasov equations model the dynamics of collisionless plasmas where the number density of particles per Debye length is very dense. Maxwell-Vlasov equations are typically solved using electromagnetic PIC (EMPIC)

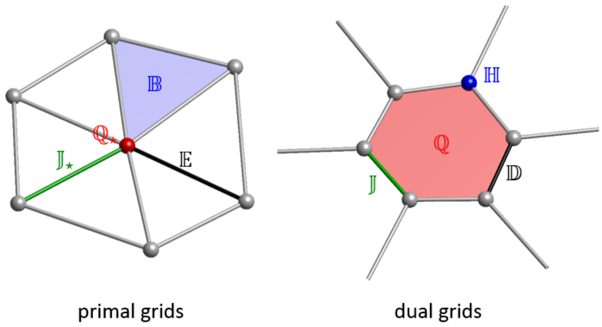

Figure 2. Degrees of freedom for fields and sources at primal and dual grids.

algorithms which track an evolution of a very large number of physical particles coarse-grained in phase space via an ensemble of computational super-particles. The resulting EMPIC algorithms can be built to solve time-dependent Maxwell's equation coupled to Newton-Lorentz equations of motion, while marching in time. By treating forces acting on individual particles and the associated EM field in a collective fashion, EMPIC algorithms lower the $O(N^2)$ computational complexity of the interaction of a system on N charged particles down to $O(N)$. An EMPIC algorithm has four basic steps which are repeated at each time step, viz. field-solver, gather, particle-push, and scatter, as shown in Fig. 1. As the field solver, the present PIC algorithm employs a finite-element method based on discrete exterior calculus [3, 6] whereby, starting from Maxwell's equations written in the language of differential forms [11, 12], fields and sources (node-based charges and edge-based currents) are expanded by a weighted sum of Whitney forms [13, 14]. For example, the electric field 1-form $\mathbb{E}$ and the magnetic flux 2-form $\mathbb{B}$ are expanded via Whitney 1- and 2-forms on primal grid. As illustrated in Fig. 2, the degrees of freedom associated with $\mathbb{E}$ and $\mathbb{B}$ are associated to the edges and faces of the grid, respectively. Dual-grid quantities such as the magnetic field $\mathbb{H}$ and the electric flux $\mathbb{D}$ are linked to primal grid quantities via discrete Hodge star operators $[\star_{\mu^{-1}}]$ and $[\star_\varepsilon]$ which are constructed by Galerkin method with the use of Whitney forms [15, 16]. After applying the generalized Stokes theorem [5] and a leap-frog time discretization, the fully discrete Maxwell's equations can be obtained [6, 14].

The gather step interpolates the discrete fields at the position of each particle via Whitney forms, as shown in Fig. 3a. The interpolated electric field at a particle position (black circle marker) is calculated by a linear combination of the degrees of freedom associated to the three neighbor edges ($\mathbb{E}_1$, $\mathbb{E}_2$, and $\mathbb{E}_3$) and their corresponding Whitney forms. Next, particles are accelerated by solving Newton-Lorentz equations of motion using Boris algorithm with correction [17, 18]. The present PIC algorithm achieves exact charge-conservation on irregular grids through a consistent use of Whitney forms once more for the scatter step [8, 9]. Fig. 3b shows schematically how grid-based sources (node-based changes and edge-based currents) can be associated geometrically to the movement of charged particle in ambient space and how charge conservation is obtained exactly. More details can be found in [8].

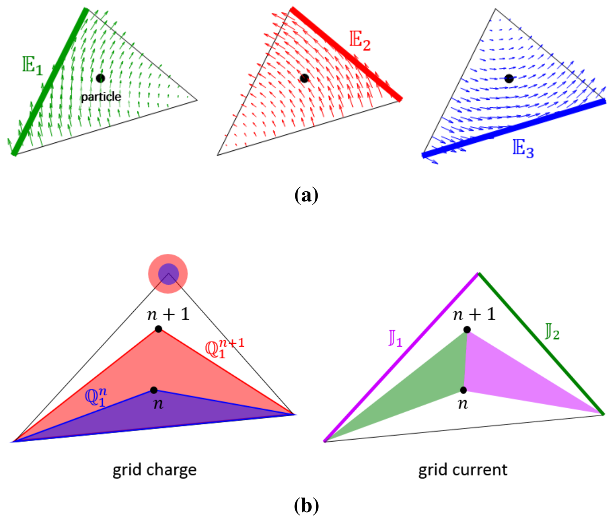

Figure 3. Charge-conservative gather-scatter scheme. (a) field interpolation and (b) assignment of grid sources.

3 Numerical examples

In this section, we provide two numerical examples involving a vacuum diode and a backward-wave oscillator with a slow-wave corrugated waveguide section.

In order to examine late-time charge conservation on general grids, we first simulate a vacuum diode accelerating an electron beam [9]. The domain $\Omega = \{(x,y) \in [0,1]^2\}$ includes anode (right) and cathode (left) surfaces with a potential difference of 1.5×10^5 V. The top and bottom boundaries of the domain are truncated by a perfectly matched layer [14, 19] to model open boundaries. The unstructured mesh adopted has 2301 faces, 3524 edges, and 1224 nodes. The time step interval is set to $\Delta t = 270$ ps, and the simulation ends at 16.2 μs. Each superparticle represents 5×10^7 electrons. For the electron emission from the cathode, an initial velocity of 10^4 [m/s] is assumed. Fig. 4 provides snapshots of the particle distribution and the self-field profile. Fig. 4a and Fig. 4b correspond to the proposed charge-conserving algorithm. Fig. 4c and Fig. 4d are obtained by using a conventional scatter scheme that is non-charge-conserving on irregular grids. In the latter case, violation of the discrete continuity equation produces spurious bunching of the electrons into strips of higher density. In addition, the self field is highly asymmetric near the beam center. These non-physical effects are not present in the charge-conserving simulation.

The second example consists of a backward-wave oscillator. The kinetic energy carried on an electron beam is transferred to the RF field via Cerenkov radiation. This occurs

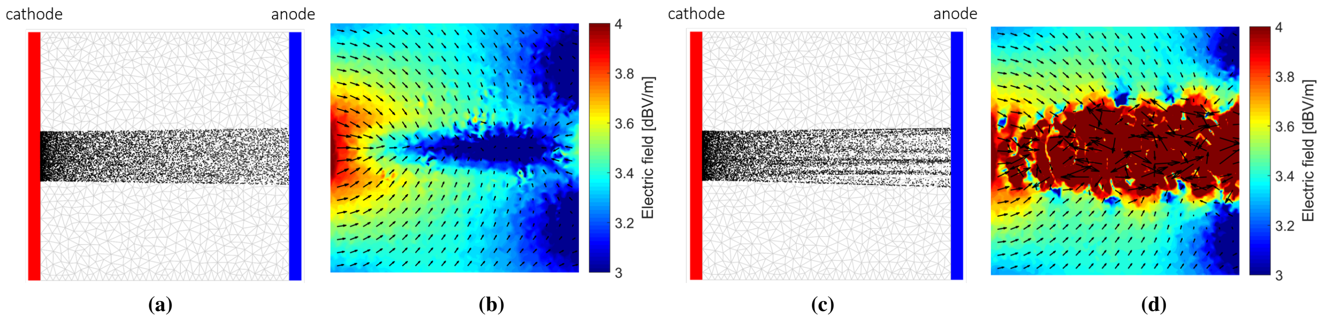

Figure 4. 2D vacuum diode example. (a) and (b) are snapshots of particle and self-field distributions based on the charge-conserving scatter scheme. (c) and (d) are those by using conventional scatter scheme that is non-charge-conserving.

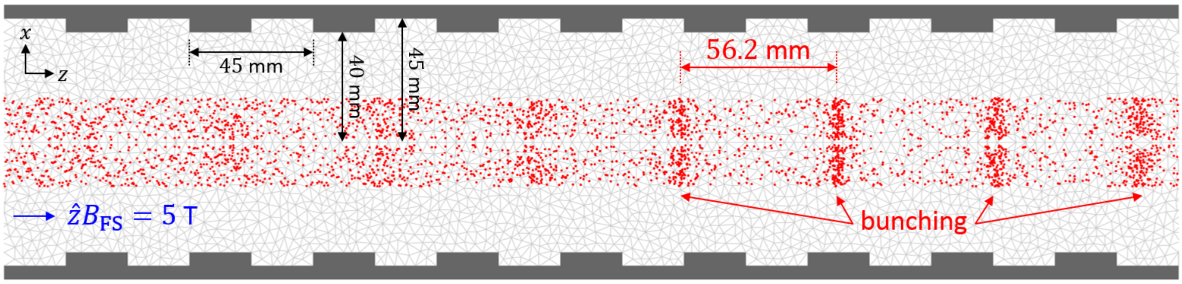

Figure 5. Snapshot of a bunched electron beam in a slow-wave structure at 200 ns.

when charged particles moves faster than the phase speed of the modal field in the device. In order to decrease the phase velocity, a corrugated waveguide is utilized as a slow-wave structure. As a result, Cerenkov interactions between the electron beam and the modal fields produce high power RF coherent signals. Here, we consider a cylindrical waveguide with rectangular corrugation. The corrugation period and depth are 45 mm and 5 mm respectively, and the average radius of the waveguide is 42.5 mm, as shown in Fig. 5. An axially symmetric relativistic electron beam with velocity 2.5×10^8 m/s and radius 20 mm is injected from the cathode. Fig. 5 illustrates a snapshot of the electron beam distribution at $t = 200$ ns along the device. The desired bunching effect due to the beam-structure interaction is clearly visible. Also, it is seen that the beam focusing system (realized by an axial magnetic field) is able to confine the beam within the center of the waveguide.

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