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Theoretical and numerical approaches for Vlasov–Maxwell equations

Charge-conserving FEM–PIC schemes on general grids ☆

Martin Campos Pinto [a], Sébastien Jund [b], Stéphanie Salmon [c], Éric Sonnendrücker [d,e,*]

[a] UPMC Université Paris 06, UMR 7598, Laboratoire Jacques-Louis Lions, 4, place Jussieu, 75005, Paris, France
[b] IRMA – Université de Strasbourg and CNRS, CALVI – INRIA Nancy-Grand Est, France
[c] Laboratoire de mathématiques, EA 4535, Fédération ARC CNRS FR 3399, Université de Reims–Champagne-Ardenne, UFR Sciences Exactes et Naturelles, Moulin de la Housse, BP 1039, 51687 Reims cedex 2, France
[d] Max-Planck Institute for Plasma Physics, Boltzmannstr. 2, 85748 Garching, Germany
[e] Mathematics Center, TU Munich, Boltzmannstr. 3, 85748 Garching, Germany

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ABSTRACT

In this article, we aim at proposing a general mathematical formulation for charge-conserving finite-element Maxwell solvers coupled with particle schemes. In particular, we identify the finite-element continuity equations that must be satisfied by the discrete current sources for several classes of time-domain Vlasov–Maxwell simulations to preserve the Gauss law at each time step, and propose a generic algorithm for computing such consistent sources. Since our results cover a wide range of schemes (namely curl-conforming finite element methods of arbitrary degree, general meshes in two or three dimensions, several classes of time discretization schemes, particles with arbitrary shape factors and piecewise polynomial trajectories of arbitrary degree), we believe that they provide a useful roadmap in the design of high-order charge-conserving FEM–PIC numerical schemes.

1. Introduction

Particle-In-Cell (PIC) solvers are a major tool for the understanding of the complex behavior of a plasma or a particle beam in many situations. An important issue for electromagnetic PIC solvers, where the fields are computed using Maxwell's equations, is the problem of discrete charge conservation. In a nutshell, the problem consists in updating the electromagnetic field via Ampère and Faraday's equations in such a way that it satisfies a discrete Gauss law at each time step. Indeed the charge and current densities ρ and J computed numerically from the particles do not necessarily verify a proper continuity equation, so that Maxwell's equations with these sources might be ill-posed.

Existing answers to this issue can be decomposed into two classes, namely field correction methods, which consist in modifying the inconsistent electric field resulting from an ill-posed Maxwell solver, see, e.g., [1–5], and charge-conserving methods, which compute the current density in a specific way so as to enforce a discrete continuity equation, see, e.g., [6–9]. The zigzag method of Umeda et al. [9] has been extended to higher orders by Yu et al. [10]. Note also the recent extension of the Esirkepov method [8] to high-order time schemes, given in [11]. Compared to those of the former class, methods enforcing a discrete continuity equation have the advantage to be local and not to modify the electromagnetic field away from the source, which may generate causality errors for some applications. However, their application to arbitrary

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* Corresponding author at: Max-Planck Institute for Plasma Physics, Boltzmannstr. 2, 85748 Garching, Germany.

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finite-element methods (FEM) built on unstructured simplicial meshes is not straightforward. For example, the early virtual particle method of Eastwood [6,12] has been essentially described in the context of structured grids such as straight or curvilinear Cartesian meshes, and for particles with simple shape factors.

In this work, we aim at bridging this gap and propose a unified formulation for curl-conforming finite elements (the so-called edge elements) coupled with particle schemes. This allows us to derive a general roadmap for the design of charge-conserving FEM–PIC schemes of arbitrary order both in time and space, that are built on general polygonal or polyhedral meshes. In particular, we extend the virtual particle method of Eastwood into a compact algorithm that also covers the case of arbitrary shape factors and piecewise polynomial trajectories of arbitrary degree.

The article is organized as follows. In Section 2, we provide a rigorous finite-element formulation of the continuity equation that should be satisfied by the sources for the discrete Maxwell system to be well posed. We next derive consistency criteria for several classes of time integration schemes such as the leap-frog scheme, higher-order symplectic Runge–Kutta and Cauchy–Kowalewskaya schemes of arbitrary order. In Section 3, we then establish that the time-averaged current densities based on particle representations with arbitrary shape factors satisfy the appropriate finite-element continuity equation. We also propose a generic algorithm for computing the resulting charge-conserving currents, that is valid for arbitrary particle shapes, high-order trajectories and any choice of finite-element basis functions. Finally, in Section 4 we illustrate the validity of the algorithm with a 2D diode test case and the Landau damping problem, and in Section 5 we summarize our findings.

2. Charge conserving FEM Maxwell solvers

In this section we recall the curl-conforming variational formulation of Maxwell's equations

$$\partial_t E - c^2 \operatorname{curl} B = -{\varepsilon_0}^{-1} J \tag{1}$$

$$\partial_t B + \operatorname{curl} E = 0 \tag{2}$$

$$\operatorname{div} E = {\varepsilon_0}^{-1} \rho \tag{3}$$

$$\operatorname{div} B = 0 \tag{4}$$

and derive proper consistency criteria for associated FEM discretizations.

Throughout the article, we assume that Ω is a bounded, Lipschitz-continuous polyhedral domain in $\mathbb{R}^d$, $d = 2, 3$, and we consider the above system complemented with both smooth initial data E_0, B_0, and boundary conditions of either metallic or absorbing type, i.e.,

$$E \times n = \begin{cases} 0 & \text{on } \Gamma_M \\ c\mu_0 (H \times n) \times n & \text{on } \Gamma_A \end{cases} \quad \text{with } \partial\Omega = \Gamma_M \cup \Gamma_A$$

As the absorbing boundary conditions are only used in regions of space where there are no particles, they play no role in our discussion.

What will guide us throughout this exercise is the following well-known formal observation: if Ampère's law (1) is satisfied at all times, then Gauss's law (3) is satisfied at all times if and only if it is satisfied at the initial time and the sources satisfy a continuity equation

$$\partial_t \rho + \operatorname{div} J = 0 \tag{5}$$

which simply states that the current density J is the flow of the electric charge density ρ. Aside from an elementary proof—take the divergence of Ampère's law and invoke the fact that a curl is always divergence free—this equivalence has indeed an essential corollary. Namely, since ρ and J *must* satisfy (5) for the Maxwell system to be well-posed, it suffices to satisfy Gauss's law at initial time for it to hold at any time. We shall now see how this basic property translates into a variational framework.

2.1. Variational charge conservation

Throughout the article, we will denote by V^ε and V^μ the function spaces used to represent the fields E and B, respectively. In particular, the variational forms of Ampère's and Faraday's law will involve test functions from these respective spaces. The space of test functions involved by the variational Gauss law will be denoted by V. It can be seen as the natural space for representing the electrostatic potential ϕ. Since we consider curl-conforming formulations, and because for simplicity we restrict ourselves to homogeneous conditions corresponding to perfectly conducting boundaries, we shall assume that

$$V^\varepsilon \subset H_0(\mathrm{curl}; \Omega) \quad \text{and} \quad V^\mu \subset H(\mathrm{div}; \Omega) \tag{6}$$

The variational form of Ampère and Faraday's laws is then usually obtained by integration by parts [13]. It consists in looking for E and B in the respective spaces $\mathcal{C}^1([0,T]; V^\varepsilon)$ and $\mathcal{C}^1([0,T]; V^\mu)$, such that for all $t \in [0,T]$,