C. R. Mecanique 342 (2014) 570–582

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Theoretical and numerical approaches for Vlasov–Maxwell equations

Charge-conserving FEM–PIC schemes on general grids ☆

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ARTICLE INFO

Article history:
Received 12 March 2014
Accepted 2 June 2014

Keywords:
Maxwell–Vlasov system
Conservation of charge
Continuity equation
Finite element method
Particle-In-Cell
Unstructured grids

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

☆ This work has been partially supported by Agence Nationale de la Recherche under the grant ANR-06-CIS6-0013.
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http://dx.doi.org/10.1016/j.crme.2014.06.011
1631-0721/

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

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

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 $t \in [0,T]$,

$$\int_\Omega \partial_t E \cdot \varphi^\varepsilon - c^2 \int_\Omega B \cdot \operatorname{curl} \varphi^\varepsilon = -\varepsilon_0^{-1} \int_\Omega J \cdot \varphi^\varepsilon, \quad \varphi^\varepsilon \in V^\varepsilon \tag{7}$$

$$\int_\Omega \partial_t B \cdot \varphi^\mu + \int_\Omega \operatorname{curl} E \cdot \varphi^\mu = 0, \quad \varphi^\mu \in V^\mu \tag{8}$$

where for simplicity we have written $\partial_t E$ instead of $\partial_t E(t,\cdot)$, and so on. In this variational framework, we may formulate the above key equivalence as follows.

Lemma 2.1 *(Variational charge conservation). If V is such that*

$$\operatorname{grad} V \subset V^\varepsilon \tag{9}$$

and if the variational Ampère equation (7) holds for all $t \in [0,T]$, then the following properties are equivalent:

(i) *for all t in $[0,T]$, a variational Gauss law holds,*

$$-\int_\Omega E \cdot \operatorname{grad} \varphi = \varepsilon_0^{-1} \int_\Omega \rho\, \varphi, \quad \varphi \in V \tag{10}$$

(ii) *the above variational Gauss law holds at $t=0$, and for all $t \in [0,T]$, ρ and J satisfy a variational continuity equation,*

$$\int_\Omega \partial_t \rho\, \varphi - \int_\Omega J \cdot \operatorname{grad} \varphi = 0, \quad \varphi \in V \tag{11}$$

Proof. Again, the idea consists in "taking the divergence" of Ampère's law. In this context this is done by writing (7) with $\varphi^\varepsilon := \operatorname{grad} \varphi$, where φ is arbitrary in V. By using that $\operatorname{curl}(\operatorname{grad}) \equiv 0$, this yields

$$\int_\Omega \partial_t E \cdot \operatorname{grad} \varphi = -{\varepsilon_0}^{-1} \int_\Omega J \cdot \operatorname{grad} \varphi$$

Now, (10) implies (11), as $\int_\Omega \partial_t \rho\, \varphi = -\varepsilon_0 \int_\Omega \partial_t E \cdot \operatorname{grad} \varphi = \int_\Omega J \cdot \operatorname{grad} \varphi$ holds for all $\varphi \in V$. Conversely, (11) yields $\frac{\mathrm{d}}{\mathrm{d}t}(\int_\Omega \rho\, \varphi + \varepsilon_0 \int_\Omega E \cdot \operatorname{grad} \varphi) = 0$ for all $\varphi \in V$, which ends the proof. □

Remark 2.1 *(On the embedding $V \subset H_0^1(\Omega)$).* If V satisfies condition (9), then we can assume without restriction that $V \subset H_0^1(\Omega)$. Indeed, by using classical arguments from, e.g., [14], we see that any such V consists of functions φ in $H^1(\Omega)$ which have a constant trace c on $\partial\Omega$. Now if $\int_\Omega \rho \neq 0$, then c must vanish for (10) to hold, and in the opposite case (10) holds equivalently for φ and $\varphi - c$ thus we can always consider that $c = 0$.

Remark 2.2 *(On the weak divergence).* Since $E = E(t,\cdot)$ is in $L^2(\Omega)$, $\operatorname{div} E$ is a distribution in the dual space of $H_0^1(\Omega)$. In particular we have $\langle \operatorname{div} E, \varphi \rangle = -\int_\Omega E \cdot \operatorname{grad} \varphi$ for all $\varphi \in H_0^1(\Omega)$, where $\langle \operatorname{div} E, \varphi \rangle$ can be seen as the continuous extension of the usual duality pairing between a distribution and an infinitely smooth functions of $C_0^\infty(\Omega)$ to any $\varphi \in H_0^1(\Omega)$. We thus infer from Remark 2.1 that (10) involves the weak divergence of E, which justifies calling it a "variational Gauss law". The same argument also justifies the denomination "variational continuity equation" for (11).

2.2. Finite-elements and matrix formulations

When applied to the maximal spaces $V^\varepsilon = H_0(\operatorname{curl};\Omega)$ and $V^\mu = H(\operatorname{div};\Omega)$ Lemma 2.1 gives an abstract condition for the exact (weak formulation of the) Maxwell system to be well posed. Note that in such a case the relevant Gauss and continuity equations involve test functions in $V = H_0^1(\Omega)$, according to Remark 2.1. In order to derive a practical condition for designing charge-conserving schemes, we need instead to apply Lemma 2.1 to discrete finite-element spaces, i.e., piecewise polynomial spaces built on a polygonal or polyhedral mesh Ω_h of Ω. Here condition (6) leads to considering curl-conforming spaces for E, which essentially means that the tangential components of the vector fields in V^ε are continuous across the faces of Ω_h, see, e.g., [15]. To keep track of the polynomial degrees, we let $\underline{p}$ and $\overline{p}$ be the maximum and minimum integers such that

$$\big(\mathcal{P}_{\underline{p}}(\Omega_h)\big)^d \cap H_0(\operatorname{curl};\Omega) \subset V^\varepsilon \subset \big(\mathcal{P}_{\overline{p}}(\Omega_h)\big)^d \cap H_0(\operatorname{curl};\Omega) \tag{12}$$

with $\mathcal{P}_p(\Omega_h)$ denoting the space of (discontinuous) piecewise polynomials on Ω_h with total degree less or equal to p. Examples of such spaces are the first Nédélec family [15] for which $\overline{p} = \underline{p} + 1$, or the second one [16] for which $\overline{p} = \underline{p}$.

Hierarchical spaces (suited for varying polynomial orders) were also described by Ainsworth and Coyle in [17,18], for general meshes in two and three dimensions.

In this discrete setting, it is useful to write a matrix version of the above developments. For this purpose, we let $\Phi^\varepsilon = \{\varphi_i^\varepsilon : i = 1, \dots, N_\varepsilon\}$ and $\Phi^\mu = \{\varphi_i^\mu : i = 1, \dots, N_\mu\}$ denote bases of V^ε and V^μ, respectively, and let σ_i^ε, σ_i^μ be the associated degrees of freedom characterized by the relations $\sigma_j^{\varepsilon,\mu}(\varphi_i^{\varepsilon,\mu}) = \delta_{i,j}$ for $i, j = 1, \dots, N_{\varepsilon,\mu}$. Accordingly, we denote

$$\underline{E} := \big(\sigma_i^\varepsilon(E)\big)_{1\le i\le N_\varepsilon}, \qquad \underline{B} := \big(\sigma_i^\mu(B)\big)_{1\le i\le N_\mu} \quad \text{and} \quad \underline{J} := \left(\int_\Omega J\cdot\varphi_i^\varepsilon\right)_{1\le i\le N_\varepsilon}$$

the column vectors containing the (time-dependent) coefficients of $E(t,\cdot)$ and $B(t,\cdot)$ in the appropriate bases, and the moments of $J(t,\cdot)$ with respect to Φ^ε, respectively. The matrix formulation of (7)–(8) reads then

$$\frac{\mathrm{d}}{\mathrm{d}t} M_\varepsilon \underline{E} - c^2 K \underline{B} = -\varepsilon_0^{-1}\underline{J} \tag{13}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} M_\mu \underline{B} + K^{\mathrm{T}}\underline{E} = 0 \tag{14}$$

where

$$M_{\varepsilon,\mu} := \left(\int_\Omega \varphi_i^{\varepsilon,\mu}\cdot\varphi_j^{\varepsilon,\mu}\right)_{1\le i,j\le N_{\varepsilon,\mu}} \quad \text{and} \quad K := \left(\int_\Omega \operatorname{curl}\varphi_i^\varepsilon\cdot\varphi_j^\mu\right)_{\substack{1\le i\le N_\varepsilon\\ 1\le j\le N_\mu}}$$

denote the mass matrices of Φ^ε, Φ^μ, and the matrix representing the curl operator in this variational setting. In order to write Gauss's law in matrix terms, we further denote by $\Phi := \{\varphi_i : i = 1, \dots, N\}$ one basis for the space V, and let

$$\underline{\rho} := \left(\int_\Omega \rho\,\varphi_i\right)_{1\le i\le N} \quad \text{and} \quad D := \left(-\int_\Omega \varphi_j^\varepsilon\cdot\operatorname{grad}\varphi_i\right)_{\substack{1\le i\le N\\ 1\le j\le N_\varepsilon}}$$

be the column vector containing the appropriate moments of ρ and the matrix representing the divergence in this variational setting (see Remark 2.2), respectively. The matrix translation of Lemma 2.1 reads then as follows.

Lemma 2.2 *(Matrix charge conservation). Given the matrix Ampère law (13), the following are equivalent:*

(i) *the matrix Gauss law*

$$D\underline{E} = \varepsilon_0^{-1}\underline{\rho} \tag{15}$$

holds for all $t \in [0, T]$,

(ii) *the matrix Gauss law (15) holds at $t = 0$, and for all $t \in [0, T]$, the source vectors $\underline{\rho}$ and $\underline{J}$ satisfy the matrix continuity equation*

$$\frac{\mathrm{d}\underline{\rho}}{\mathrm{d}t} - G^{\mathrm{T}}\underline{J} = 0 \tag{16}$$

where G is the matrix describing the action of the gradient operator in the bases Φ and Φ^ε, i.e., $G := (\sigma_i^\varepsilon(\operatorname{grad}\varphi_j))_{1\le i\le N_\varepsilon, 1\le j\le N}$.

Proof. Since this is a matrix reformulation of Lemma 2.1, we do not need a proof for it. However, a direct argument is of interest, because it involves key matrix properties that will be useful in the sequel. Indeed, one easily infers from the embedding $\operatorname{grad} V \subset V^\varepsilon$ that

$$D = \left(-\int_\Omega \varphi_j^\varepsilon\cdot\operatorname{grad}\varphi_i\right)_{i,j} = \left(\sum_{k=1}^{N_\varepsilon} -\sigma_k^\varepsilon(\operatorname{grad}\varphi_i)\int_\Omega \varphi_j^\varepsilon\cdot\varphi_k^\varepsilon\right)_{i,j} = -G^{\mathrm{T}}M_\varepsilon \tag{17}$$

and

$$G^{\mathrm{T}}K = \left(\sum_{k=1}^{N_\varepsilon}\sigma_k^\varepsilon(\operatorname{grad}\varphi_i)\int_\Omega \varphi_j^\mu\cdot\operatorname{curl}\varphi_k^\varepsilon\right)_{i,j} = \left(\int_\Omega \varphi_j^\mu\cdot\underbrace{\operatorname{curl}(\operatorname{grad}\varphi_i)}_{=0}\right)_{i,j} = 0 \tag{18}$$

Left-multiplying the matrix Ampère equation (13) by $-G^{\mathrm{T}}$ yields then

$$\frac{\mathrm{d}}{\mathrm{d}t} D\underline{E} = \varepsilon_0^{-1} G^{\mathrm{T}}\underline{J} \tag{19}$$

and the desired result follows easily. □

Remark 2.3 *(On the discrete Gauss law).* According to (12), any continuous piecewise polynomial of total degree less or equal to $\underline{p}+1$ vanishing on $\partial\Omega$ has its gradient in V^ε. Thus, for V we can take a space containing $\mathcal{P}_{\underline{p}+1}(\Omega_h)\cap H_0^1(\Omega)$. It follows that the discrete Gauss law (15) involves continuous finite elements of degree greater than $\underline{p}$.

Remark 2.4 *(On the smoothness of the sources).* Up to now we have implicitely assumed that the sources J,ρ are smooth enough for writing integrals such as $\int_\Omega J\cdot\varphi^\varepsilon$ and $\int_\Omega \rho\,\varphi$. However in Section 3 we will consider discrete sources defined from Dirac particles, for which this is not true. We will thus need to specify how the source vectors are defined in this case. Moreover we shall use a slightly different version of Lemma 2.2 that is better suited to fully discrete settings. To this end we already note that the above proof does not involve properties of either $\underline{J}$ or $\underline{\rho}$, but only the embedding $\operatorname{grad} V\subset V^\varepsilon$.

Remark 2.5 *(On the use of numerical integration).* If the space integral involving the electric field E in the Ampère equation (13) is replaced by a numerical integration (which is often done in practice, e.g., for mass lumping purposes [19]), i.e, if the matrix M_ε is replaced by a new spd matrix $M_{\varepsilon,*}$, then a modified version of Lemma 2.2 still holds true. It suffices to replace the "exact" Gauss law (15) by an approximated one where the integral involved in the left-hand side is again replaced by the same numerical integration. Namely, $D=-G^{\mathrm{T}}M_\varepsilon$ should be replaced by $D_*=-G^{\mathrm{T}}M_{\varepsilon,*}$. Note that this does not change the matrix continuity equation (16).

Remark 2.6 *(On Gauss's law for magnetism).* It is well-known that curl-conforming FEM solvers preserve the Gauss law for magnetism (4), regardless of the sources. Specifically, under the classical assumption that $\operatorname{curl} V^\varepsilon\subset V^\mu$, (8) actually holds in a strong sense, i.e., we have $\partial_t B+\operatorname{curl} E=0$ in V^μ. In particular, $\operatorname{div} B(t)=0$ holds for all t iff it holds at $t=0$.

2.3. Consistency criteria for time-domain FEM schemes

Equipped with the above matrix equations $D=-G^{\mathrm{T}}M_\varepsilon$ and $G^{\mathrm{T}}K=0$ that follow from the embedding $\operatorname{grad} V\subset V^\varepsilon$, we now state consistency criteria for different classes of time-domain Maxwell solvers to be charge-conserving. Here we assume that charge density functions ρ^n are given at discrete time steps $n=0,1,\dots$, such that the moments $\underline{\rho}_i^n:=\langle\rho^n,\varphi_i\rangle$ involving the basis functions of V are well defined, see Remark 2.4. A given Maxwell solver will then be said *charge-conserving* if it computes numerical solutions $\underline{E}^n$ that satisfy the finite-element Gauss laws

$$D\underline{E}^n=\varepsilon_0^{-1}\underline{\rho}^n \tag{20}$$

at each positive time step n, as long as (20) holds for $n=0$. In this article we consider three classes of explicit time discretization schemes: the popular low-order leap-frog scheme, symplectic Runge–Kutta schemes of higher order and Cauchy–Kowalewskaya schemes of arbitrary order. For simplicity the time steps will be assumed uniform (although this could be easily relaxed) and we denote $t_n=n\Delta t$.

We begin with the leap-frog time discretization of the Ampère–Faraday system (13)–(14), which reads

$$\underline{E}^{n+1}:=\underline{E}^n+c^2\Delta t(M_\varepsilon)^{-1}K\,\underline{B}^{n+\frac12}-\Delta t\,(\varepsilon_0M_\varepsilon)^{-1}\underline{J}^{n+\frac12} \tag{21}$$

$$\underline{B}^{n+\frac12}:=\underline{B}^{n-\frac12}-\Delta t(M_\mu)^{-1}K^{\mathrm{T}}\underline{E}^n \tag{22}$$

with a source term $\underline{J}^{n+\frac12}$ that is usually seen as an approximation to $\underline{J}(t_{n+\frac12})$, or better to $\frac{1}{\Delta t}\int_{t_n}^{t_{n+1}}\underline{J}(t)\,\mathrm{d}t$. Left-multiplying (21) by D, and using (17), (18), it is straightforward to derive the following criterion.

Lemma 2.3 *(Consistency criterion for the leap-frog scheme). The leap-frog scheme (21)–(22) is charge-conserving if and only if the discrete sources satisfy the matrix continuity equation*

$$\underline{\rho}^{n+1}-\underline{\rho}^n-\Delta tG^{\mathrm{T}}\underline{J}^{n+\frac12}=0,\quad \text{for all } n \tag{23}$$

We next consider symplectic Runge–Kutta schemes of order $p=1,\dots,4$, that generalize the leap-frog method and are known to be stable and nondissipative [20–22]. Applied to the time-dependent system (13)–(14), they compute auxiliary solutions by first letting $\underline{E}^{n,0}:=\underline{E}^n$, $\underline{B}^{n,0}:=\underline{B}^n$, then for $j=0,\dots,p-1$,

$$\underline{E}^{n,j+1}:=\underline{E}^{n,j}+b_{j+1}\Delta t\big[c^2(M_\varepsilon)^{-1}K\,\underline{B}^{n,j}-(\varepsilon_0M_\varepsilon)^{-1}\underline{J}^{n,j}\big] \tag{24}$$

$$\underline{B}^{n,j+1}:=\underline{B}^{n,j}-a_{j+1}\Delta t(M_\mu)^{-1}K^{\mathrm{T}}\underline{E}^{n,j} \tag{25}$$

and finally $\underline{E}^{n+1}:=\underline{E}^{n,p}$, $\underline{B}^{n+1}:=\underline{B}^{n,p}$. Here the coefficients a_j,b_j, $j=1,\dots,p$ should be taken from available tables, e.g., in [23,20]. Note that for $p=2$, we have $a_1=a_2=1/2$ and $b_1=0,b_2=1$, which corresponds to the leap-frog scheme. By using again (17) and (18), we obtain the following criterion.

Lemma 2.4 *(Consistency criterion for symplectic RK schemes). The symplectic Runge–Kutta scheme of order p (24)–(25) is charge-conserving if and only if the auxiliary current vectors satisfy (23) for all n, with* $\underline{J}^{n+1/2}$ *now denoting* $\sum_{j=0}^{p-1} b_{j+1}\underline{J}^{n,j}$.

Note that the foregoing criterion can also be applied to the higher-order symplectic schemes of Yoshida [24], obtained by composing RK schemes of intermediate orders.

We finally turn to Cauchy–Kowalewskaya schemes of arbitrary order p, see, e.g., [25–27]. They can be derived from the time-dependent Ampère and Faraday equations (13)–(14) by first reformulating them into a single matrix ODE

$$\frac{\mathrm{d}}{\mathrm{d}t}\underline{U}(t) = A\underline{U}(t) + \underline{b}(t) \tag{26}$$

with $\underline{U} := \begin{pmatrix}\underline{E}\\ \underline{B}\end{pmatrix}$, $A := \begin{pmatrix}0 & c^2(M_\varepsilon)^{-1}K\\ -(M_\mu)^{-1}K^{\mathrm{T}} & 0\end{pmatrix}$ and $\underline{b} := -\begin{pmatrix}(\varepsilon_0 M_\varepsilon)^{-1}\underline{J}\\ 0\end{pmatrix}$. We next write the p-th order Taylor expansion of $\underline{U}$,

$$\underline{U}(t_{n+1}) \approx \sum_{m=0}^{p} \frac{\Delta t^m}{m!}\frac{\mathrm{d}^m}{\mathrm{d}t^m}\underline{U}(t_n)$$

and replace there every time derivative of $\underline{U}$ by a power of the evolution operator A. By a straightforward induction argument, we indeed infer from (26) that

$$\frac{\mathrm{d}^m}{\mathrm{d}t^m}\underline{U}(t) = A^m\underline{U}(t) + \sum_{\nu=0}^{m-1} A^{m-1-\nu}\frac{\mathrm{d}^\nu}{\mathrm{d}t^\nu}\underline{b}(t) \quad \text{for } m \in \mathbb{N} \tag{27}$$

which yields an explicit scheme of the form

$$\underline{U}^{n+1} := \left(I + \sum_{m=1}^{p}\frac{\Delta t^m}{m!}A^m\right)\underline{U}^n + \underline{L}^n \quad \text{with } \underline{U}^n = \begin{pmatrix}\underline{E}^n\\ \underline{B}^n\end{pmatrix} \tag{28}$$

and where the load vector $\underline{L}^n$ can be seen as an approximation to the sum of all terms involving the current density, $\sum_{m=1}^{p}\sum_{\nu=0}^{m-1}\frac{\Delta t^m}{m!}A^{m-1-\nu}\frac{\mathrm{d}^\nu}{\mathrm{d}t^\nu}\underline{b}(t_n)$. Now, even though we can provide a consistency criterion for arbitrary load vectors, it is of interest to specify the structure of $\underline{L}^n$ that should appear in such a scheme. Indeed, we can decompose the above sum into two parts, namely one part that can be factorized by the matrix A, and a remainder. Thus, $\underline{L}^n \approx A\tilde{\underline{L}}^n + \sum_{m=1}^{p}\frac{\Delta t^m}{m!}\frac{\mathrm{d}^{m-1}}{\mathrm{d}t^{m-1}}\underline{b}(t_n)$, and writing $\underline{c}(t) := \int_{t_n}^{t}\underline{b}(t')\,\mathrm{d}t'$ we further obtain

$$\underline{L}^n \approx A\tilde{\underline{L}}^n + \sum_{m=1}^{p}\frac{\Delta t^m}{m!}\frac{\mathrm{d}^m}{\mathrm{d}t^m}\underline{c}(t_n) \approx A\tilde{\underline{L}}^n + \underline{c}(t_{n+1}) = A\tilde{\underline{L}}^n + \int_{t_n}^{t_{n+1}}\underline{b}(t)\,\mathrm{d}t$$

where the second approximation is again a Taylor expansion and uses the fact that $\underline{c}(t_n) = 0$. According to the definition of $\underline{b}$, we thus find that the load vector in the CK scheme (28) may be written as

$$\underline{L}^n = A\tilde{\underline{L}}^n - \Delta t\begin{pmatrix}(\varepsilon_0 M_\varepsilon)^{-1}\underline{J}^{n+\frac{1}{2}}\\ 0\end{pmatrix} \tag{29}$$

where $\underline{J}^{n+\frac{1}{2}}$ now clearly appears to be an approximation to $\frac{1}{\Delta t}\int_{t_n}^{t_{n+1}}\underline{J}(t)\,\mathrm{d}t$. For such schemes, the consistency criterion reads as follows.

Lemma 2.5 *(Consistency criterion for the CK schemes). The p-th order CK scheme (28) is charge-conserving if and only if the load vector* $\underline{L}^n$ *satisfies*

$$\underline{\rho}^{n+1} - \underline{\rho}^n - \varepsilon_0\hat{D}\underline{L}^n = 0 \tag{30}$$

for all n, with $\hat{D} := (D\ 0)$ *being the* $N \times (N_\varepsilon + N_\mu)$ *matrix obtained by completing D with a zero block. If* $\underline{L}^n$ *has the form (29), this criterion coincides with (23).*

Proof. From the matrix equations (17), (18), we easily infer that

$$\hat{D}A = (D\quad 0)\begin{pmatrix}0 & c^2(M_\varepsilon)^{-1}K\\ -(M_\mu)^{-1}K^{\mathrm{T}} & 0\end{pmatrix} = (0\quad -c^2G^{\mathrm{T}}K) = 0$$

Left-multiplying the CK scheme (28) by $\hat{D}$, we thus obtain

$$D\underline{E}^{n+1} - D\underline{E}^n = \hat{D}\underline{U}^{n+1} - \hat{D}\underline{U}^n = \hat{D}\underline{L}^n$$

which easily yields (30). □

3. Consistent coupling with particles

In this section we propose a generic algorithm to compute charge-conserving currents that generalizes the early virtual particle method of Eastwood [6]. In the case of a leap-frog time discretization, for instance, our algorithm computes a load vector $\underline{J}^{n+\frac{1}{2}}$ that satisfies the consistency criterion (23). Despite its simplicity, our algorithm covers a large class of particle schemes. In particular, it is valid for arbitrary shape factors, piecewise polynomial trajectories of arbitrary degree, and for any curl-conforming FEM in two and three dimensions.

3.1. Particle approximations

We now consider the situation where the Maxwell system is coupled with the Vlasov equation

$$\partial_t f + v \cdot \nabla_x f + \frac{q}{m} F \cdot \nabla_v f = 0 \tag{31}$$

involving the phase space distribution function $f = f(t, x, v)$ of the charged particles, and the Lorentz force $F := E + v \times B$. For simplicity, we consider a single species (say, electrons) thus q, m denote the charge and mass of an electron. With such a model the charge and current densities are given by the first moments of f,

$$\rho(t,x) := q \int f(t,x,v)\,\mathrm{d}v \qquad J(t,x) := q \int v f(t,x,v)\,\mathrm{d}v \tag{32}$$

In the context of approximating the Vlasov equation by a particle method, the distribution function f is approached at every time step $t_n = n\Delta t$ by a sum of (macro) particles with shape factor S,

$$f(t_n,x,v) \approx f_h^n(x,v) := \sum_{k=1}^{N_{\mathrm{part}}} \omega_k S\big(x - x_k^n\big) S\big(v - v_k^n\big) \tag{33}$$

In practice S is either a Dirac distribution, or a compactly supported, nonnegative continuous function of mass one, such as a B-spline [1]. As for the particles positions x_k^n and velocities v_k^n, they are updated by the following approximated characteristic curves, which consists in a numerical integration of the differential system $\dot{x}(t) = v(t)$, $\dot{v}(t) = \frac{q}{m} F(t, x(t), v(t))$ on $[t_n, t_{n+1}]$, with initial condition $x(t_n) = x_k^n$, $v(t_n) = v_k^n$. In a standard leap-frog scheme, one could for instance use piecewise affine trajectories $x_k(t) = x_k^n + v_k^{n+1/2}(t - t_n)$ with constant speeds on $[t_n, t_{n+1}]$ updated either by $v_k^{n+1/2} - v_k^{n-1/2} = \frac{q\Delta t}{m}(E_k^n + (v_k^{n-1/2} + v_k^{n+1/2})/2 \times B_k^n)$ with $E_k^n := E(t_n, x_k^n)$, $B_k^n := B(t_n, x_k^n)$, or by the Boris scheme that avoids accelerations by the magnetic field [1], $v^- = v_k^{n-1/2} + \frac{q}{2m} E_k^n$, $v^+ - v^- = \frac{q\Delta t}{2m}(v^+ + v^-) \times B_k^n$, $v_k^{n+1/2} = v^+ + \frac{q}{2m} E_k^n$. Now, as we aim for a greater generality, we will simply assume in the sequel that the numerical trajectories $x_k(t)$ are globally continuous, polynomial (or piecewise polynomial) on every $[t_n, t_{n+1}]$ and such that $\dot{x}_k(t) = v_k(t)$. For later purposes, we denote by p_T the maximum degree of these polynomials. It is then possible to define time-dependent particle, charge and current densities,

$$\begin{aligned}
f_h(t,x,v) &:= \sum_{k=1}^{N_{\mathrm{part}}} \omega_k S\big(x - x_k(t)\big) S\big(v - v_k(t)\big) \\
\rho_h(t,x) &:= \sum_{k=1}^{N_{\mathrm{part}}} q\omega_k S\big(x - x_k(t)\big) \\
J_h(t,x) &:= \sum_{k=1}^{N_{\mathrm{part}}} q\omega_k v_k(t) S\big(x - x_k(t)\big)
\end{aligned} \tag{34}$$

Note that we have $\rho_h = q\int f_h\,\mathrm{d}v$ and $J_h = q\int v f_h\,\mathrm{d}v$ as long as S is symmetric, see (32). Since the early works of Eastwood [6], it is known that charge-conserving currents can be obtained in particle schemes by averaging the time-dependent current density over the time step, and evaluating the charge density at t_n. With our notations, this corresponds to setting

$$\begin{aligned}
J_h^{n+\frac{1}{2}}(x) &:= \int_{t_n}^{t_{n+1}} J_h(t,x)\frac{\mathrm{d}t}{\Delta t} = q\sum_{k=1}^{N_{\mathrm{part}}} \omega_k \int_{t_n}^{t_{n+1}} v_k(t) S\big(x - x_k(t)\big)\frac{\mathrm{d}t}{\Delta t} \\
\rho_h^n(x) &:= \rho_h(t_n,x) = q\sum_{k=1}^{N_{\mathrm{part}}} \omega_k S\big(x - x_k^n\big)
\end{aligned} \tag{35}$$

and to defining the FEM vectors sources by the moments

$$\underline{J}^{n+\frac{1}{2}} := \big(\langle J_h^{n+\frac{1}{2}}, \varphi_i^\varepsilon\rangle\big)_{1\le i\le N_\varepsilon} \quad \text{and} \quad \underline{\rho}^n := \big(\langle \rho_h^n, \varphi_i\rangle\big)_{1\le i\le N}$$

see Remark 2.4. Here we need to verify that the former products are well defined in the case of Dirac shape factors, since the curl-conforming basis functions φ_i^ε of V^ε are not continuous.

Lemma 3.1. *If the current density is defined by (35) with $S = \delta$, then the product $\langle J_h^{n+\frac{1}{2}}, \varphi^\varepsilon\rangle$ is well defined for $\varphi^\varepsilon \in H(\mathrm{curl};\Omega)$.*

Proof. Since every trajectory x_k is continuous and piecewise polynomial, we can subdivide $[t_n, t_{n+1}]$ into a finite set of subintervals $[\tau_k^{n,m}, \tau_k^{n,m+1}]$, $m = 1,\dots,M$, on which $x_k(t)$ stays within a closed cell K_m of Ω_h. We can thus set

$$\begin{aligned}\big\langle J_h^{n+\frac{1}{2}}, \varphi_i^\varepsilon\big\rangle &:= \sum_{k=1}^{N_{\mathrm{part}}} q\omega_k \sum_{m=1}^{M} \int_{\tau_k^{n,m}}^{\tau_k^{n,m+1}} \big\langle v_k(t)\delta_{x_k(t)}, \varphi_{i\,|K_m}^\varepsilon\big\rangle \frac{\mathrm{d}t}{\Delta t}\\ &= \sum_{k=1}^{N_{\mathrm{part}}} q\omega_k \sum_{m=1}^{M} \int_{\tau_k^{n,m}}^{\tau_k^{n,m+1}} v_k(t)\cdot\varphi_{i\,|K_m}^\varepsilon\big(x_k(t)\big) \frac{\mathrm{d}t}{\Delta t}\end{aligned} \tag{36}$$

by using the fact that φ_i^ε is continuous inside every K_m. Now, if the trajectory x_k runs simultaneously within two closed cells K_m, K'_m on $[\tau_k^{n,m}, \tau_k^{n,m+1}]$, it does not matter which one is considered in the above computation. Indeed in such a case $v_k(t)$ is directed along the face $K_m \cap K'_m$, so that $v_k(t)\cdot\varphi_{i\,|K_m}^\varepsilon(x_k(t)) = v_k(t)\cdot\varphi_{i\,|K'_m}^\varepsilon(x_k(t))$ follows from the curl-conformity of φ_i^ε. □

We can next prove that these sources satisfy a proper continuity equation, either in a distributional sense or in the more practical finite element framework.

Lemma 3.2. *For any distribution S, the sources given by (35) satisfy a continuity equation in distribution's sense, i.e.,*

$$\big\langle \rho_h^{n+1} - \rho_h^n + \Delta t\,\mathrm{div}\, J_h^{n+\frac{1}{2}}, \varphi\big\rangle = 0 \tag{37}$$

holds for all φ in $\mathcal{C}_0^\infty(\Omega)$.

Proof. For $\varphi \in \mathcal{C}_0^\infty(\Omega)$ we have $\langle S(\cdot - x_k(t)), \varphi\rangle = \langle S, \varphi(\cdot + x_k(t))\rangle$, hence we may compute

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\big\langle S\big(\cdot - x_k(t)\big), \varphi\big\rangle &= \Big\langle S, \frac{\mathrm{d}}{\mathrm{d}t}\big[\varphi\big(\cdot + x_k(t)\big)\big]\Big\rangle\\ &= \big\langle S, v_k(t)\cdot\mathrm{grad}\,\varphi\big(\cdot + x_k(t)\big)\big\rangle\\ &= \big\langle v_k(t)S, \mathrm{grad}\,\varphi\big(\cdot + x_k(t)\big)\big\rangle\\ &= -\big\langle \mathrm{div}\big(v_k(t)S\big), \varphi\big(\cdot + x_k(t)\big)\big\rangle\\ &= -\big\langle \mathrm{div}\big[v_k(t)S\big(\cdot - x_k(t)\big)\big], \varphi\big\rangle\end{aligned} \tag{38}$$

Now, as v_k is bounded we see that $\langle v_k(t)S, \mathrm{grad}\,\varphi(\cdot + x_k(t))\rangle$ is also bounded (by a constant depending on φ). Thus $\langle S(\cdot - x_k(t)), \varphi\rangle$ is a Lipschitz function of t, and summing on k we can write

$$\begin{aligned}\big\langle \rho_h^{n+1} - \rho_h^n, \varphi\big\rangle &= \int_{t_n}^{t_{n+1}} \frac{\mathrm{d}}{\mathrm{d}t}\big\langle \rho_h(t), \varphi\big\rangle\,\mathrm{d}t\\ &= \int_{t_n}^{t_{n+1}} \sum_{k=1}^{N_{\mathrm{part}}} q\omega_k \frac{\mathrm{d}}{\mathrm{d}t}\big\langle S\big(\cdot - x_k(t)\big), \varphi\big\rangle\,\mathrm{d}t\\ &= -\left\langle \int_{t_n}^{t_{n+1}} \mathrm{div}\left[\sum_{k=1}^{N_{\mathrm{part}}} q\omega_k v_k(t) S\big(\cdot - x_k(t)\big)\right]\mathrm{d}t, \varphi\right\rangle\\ &= -\big\langle \Delta t\,\mathrm{div}\, J_h^{n+\frac{1}{2}}, \varphi\big\rangle \qquad \square\end{aligned}$$

For practical use, we need to check that Lemma 3.2 extends to the finite element framework, where the test functions φ are globally continuous but only piecewise $\mathcal{C}^1$ on an unstructured mesh. This is done in the following lemma where we denote by $\mathcal{C}^1(\Omega_h)$ the space of all functions φ that are continuous on Ω and such that $\varphi_{|K} \in \mathcal{C}^1(K)$ for all $K \in \Omega_h$.

Lemma 3.3. *If the shape factor S is a continuous function, then the sources (35) satisfy the analog of (37), i.e.,*

$$\int_\Omega (\rho_h^{n+1} - \rho_h^n)\varphi = \Delta t \int_\Omega J_h^{n+\frac{1}{2}} \cdot \operatorname{grad} \varphi \tag{39}$$

for all φ in $W^{1,1}(\Omega)$, hence all φ in $\mathcal{C}^1(\Omega_h)$. Finally, if S is the Dirac mass, the sources satisfy

$$\langle \rho_h^{n+1} - \rho_h^n, \varphi \rangle = \Delta t \langle J_h^{n+\frac{1}{2}}, \operatorname{grad} \varphi \rangle \tag{40}$$

for all φ in $\mathcal{C}^1(\Omega_h)$.

Remark 3.1. Because $\operatorname{grad}\varphi$ is not continuous, the right-hand side in (40) must be understood as in (36). From Lemma 3.1 this is valid, indeed the gradient of a $\mathcal{C}^1(\Omega_h)$ function is piecewise continuous and globally curl-conforming.

Proof. The proof presents no difficulty in the case where S is continuous. As for the Dirac case where $S(\cdot - x_k(t)) = \delta_{x_k(t)}$, we again subdivide $[t_n, t_{n+1}]$ into subintervals $[\tau_k^{n,m}, \tau_k^{n,m+1}]$, $m = 1, \dots, M$, on which $x_k(t)$ is in a closed cell K_m of Ω_h. For every such k, m, we thus have

$$\begin{aligned}
\langle \delta_{x_k(\tau_k^{n,m+1})} - \delta_{x_k(\tau_k^{n,m})}, \varphi \rangle &= \varphi_{|K_m}\big(x_k(\tau_k^{n,m+1})\big) - \varphi_{|K_m}\big(x_k(\tau_k^{n,m})\big) \\
&= \int_{\tau_k^{n,m}}^{\tau_k^{n,m+1}} v_k(t) \cdot \operatorname{grad} \varphi_{|K_m}\big(x_k(t)\big)\, \mathrm{d}t \\
&= \int_{\tau_k^{n,m}}^{\tau_k^{n,m+1}} \big\langle v_k(t)\delta_{x_k(t)}, \operatorname{grad} \varphi_{|K_m} \big\rangle \mathrm{d}t
\end{aligned}$$

by using the fact that $\varphi_{|K_m} \in \mathcal{C}^1(K_m)$. As in the proof of Lemma 3.1, we observe that the above product is well defined when x_k runs simultaneously in two adjacent cells K_m, K'_m. The result follows by summing over m and k. □

3.2. Generic algorithm for charge-conserving currents

We now give an algorithm for computing the charge-conserving current vector defined in (35). We shall first consider the simpler case of Dirac shape factors where the computation can be made exact. For arbitrary continuous shape factors S, we then propose an approximation that is consistent with the conservation of charge.

If $S = \delta$, the entries of the current vector read

$$\underline{J}_i^{n+\frac{1}{2}} = \langle J_h^{n+\frac{1}{2}}, \varphi_i^\varepsilon \rangle = q \sum_{k=1}^{N_{\text{part}}} \omega_k \int_{t_n}^{t_{n+1}} v_k(t) \cdot \varphi_i^\varepsilon\big(x_k(t)\big) \frac{\mathrm{d}t}{\Delta t}, \quad i = 1, \dots N_\varepsilon$$

see (36). Now, since every particle trajectory x_k is a polynomial of maximum degree p_T on $[t_n, t_{n+1}]$, the piecewise polynomial structure (12) of the finite-element basis function φ_i^ε can be exploited as follows. As above, we first subdivide the time step $[t_n, t_{n+1}]$ into subintervals $[\tau_k^{n,m}, \tau_k^{n,m+1}]$, where x_k stays within a mesh cell K_m. There the function $t \to v_k(t) \cdot \varphi_i^\varepsilon(x_k(t))$ is a polynomial of degree less or equal to $p_T(\overline{p}+1)-1$. It follows that a univariate Gauss–Legendre quadrature formula with a sufficient number of points, namely $p' \geq p_T(\overline{p}+1)/2$, is exact for the associated integral, as already noticed by Eastwood [6]. More precisely, we have

$$\int_{\tau_k^{n,m}}^{\tau_k^{n,m+1}} v_k(t) \cdot \varphi_i^\varepsilon\big(x_k(t)\big)\, \mathrm{d}t = \frac{\Delta \tau_k^{n,m}}{2} \sum_{j=1}^{p'} \lambda_j\, v_k\big(\tau_{k,j}^{n,m}\big) \cdot \varphi_i^\varepsilon\big(x_k\big(\tau_{k,j}^{n,m}\big)\big)$$

where we have set $\Delta\tau_k^{n,m} := \tau_k^{n,m+1} - \tau_k^{n,m}$ and $\tau_{k,j}^{n,m} := \tau_k^{n,m} + \frac{(1+s_j)\Delta\tau_k^{n,m}}{2}$, and where λ_j, s_j, $j = 1, \dots p'$, denote the Gauss–Legendre weights and nodes for the reference interval $[-1, 1]$. The i-th entry of $\underline{J}^{n+1/2}$ is then obtained by summing these contributions over m and k, see (36).

We next turn to the case of arbitrary shape factors S where the entries of the current vector read

$$\begin{aligned}\underline{J}_i^{n+\frac{1}{2}} &= \int_\Omega J_h^{n+\frac{1}{2}} \cdot \varphi_i^\varepsilon \\ &= \int_\Omega q \sum_{k=1}^{N_{\text{part}}} \omega_k \left[\int_{t_n}^{t_{n+1}} S\big(x - x_k(t)\big) v_k(t) \cdot \varphi_i^\varepsilon(x) \frac{\mathrm{d}t}{\Delta t} \right] \mathrm{d}x \\ &= \int_{\Omega^S} q \sum_{k=1}^{N_{\text{part}}} \omega_k \left[\int_{t_n}^{t_{n+1}} v_k(t) \cdot \varphi_i^\varepsilon\big(x' + x_k(t)\big) \frac{\mathrm{d}t}{\Delta t} \right] S\big(x'\big)\, \mathrm{d}x'\end{aligned}$$

with $\Omega^S \subset \mathbb{R}^d$ denoting the compact support of S. There we propose to replace the space integral by a quadrature formula using N_S points,

$$\underline{J}_i^{n+\frac{1}{2}} \approx \underline{\tilde{J}}_i^{n+\frac{1}{2}} := q \sum_{k=1}^{N_{\text{part}}} \omega_k \sum_{\ell=1}^{N_S} \lambda_\ell^S \int_{t_n}^{t_{n+1}} v_k(t) \cdot \varphi_i^\varepsilon\big(x_\ell^S + x_k(t)\big) \frac{\mathrm{d}t}{\Delta t} \tag{41}$$

with λ_ℓ^S, x_ℓ^S thus denoting quadrature weights and nodes for the weighted integral $\int S(x')\,\mathrm{d}x'$. In other terms, we propose to replace every smooth particle with weight ω_k and trajectory $x_k(t)$ by a bunch of "auxiliary" Dirac particles with weights $\lambda_\ell^S \omega_k$ and trajectories $x_\ell^S + x_k(t)$, $\ell = 1, \dots, N_S$. Let us emphasize that evaluating a space integral by means of a numerical integration rule is of common practice in finite-element methods. And that even though it represents an approximation of $\underline{J}^{n+1/2}$, it is consistent with the conservation of charge, as long as the discrete charge density vectors $\underline{\rho}^n$ are defined through the same quadrature formula. It is easily seen indeed that Lemma 3.3 extends to this case without difficulty. Moreover, we observe that this approximation preserves the total charge and current carried by the particles, as long as these smoothing weights satisfy $\sum_{\ell=1}^{N_S} \lambda_\ell^S = 1$.

Finally, we note that in this framework the Dirac shape factor case $S = \delta$ is obtained by setting $N_S = 1$. We can thus summarize the foregoing developments in a generic algorithm (see Fig. 1 for a graphical depiction).

Algorithm 3.4 *(Charge-conserving current).*
Input: N_ε and φ_i^ε, the dimension and basis functions of the finite-element space V^ε used for the electric field; N_{part}, the number of (macro) particles; $\omega_k, x_k(t), v_k(t)$, the particles weights, positions and velocities at time t; N_S, the number of quadrature nodes for the shape factors; λ_ℓ^S, x_ℓ^S, the quadrature weights and nodes for representing the shape factor S; p_T and $\bar{p}$, the maximum degree for the trajectories and the finite elements.
Output: $\underline{J}^{n+1/2}$, the charge-conserving current vector.

1. set $p' := \lceil \frac{p_T(\bar{p}+1)}{2} \rceil$, and let λ_j, s_j, $j = 1, \dots, p'$ be the Gauss–Legendre weights and nodes for the reference interval $[-1, 1]$
2. for $i = 1, \dots, N_\varepsilon$, set J_tmp$[i] := 0$
3. for $k = 1, \dots, N_{\text{part}}$, and for $\ell = 1, \dots, N_S$, do {
   (a) define $q_{k,\ell} := q\lambda_\ell^S \omega_k$ and $x_{k,\ell}(t) := x_\ell^S + x_k(t)$
   (b) set $\tau := t_n$, and let K be the cell containing $x_{k,\ell}(\tau + 0^+)$
   (c) while $(\Delta\tau := \min(t_{n+1} - \tau, \inf\{t > 0 : x_{k,\ell}(\tau + t) \notin K\}) > 0)$ do {
      i. for $i = 1, \dots, N_\varepsilon$ such that $K \cap \operatorname{supp}(\varphi_i^\varepsilon) \neq \emptyset$, do

$$\text{J\_tmp}[i] \mathrel{+}= \frac{\Delta\tau}{2\Delta t} q_{k,\ell} \sum_{j=1}^{p'} \lambda_j v_k(\tau_j) \cdot \varphi_i^\varepsilon\big(x_{k,\ell}(\tau_j)\big)$$

      where $\tau_j := \tau + \frac{\Delta\tau}{2}(1 + s_j)$.
      ii. set $\tau := \tau + \Delta\tau$, and let K be the cell containing $x_{k,\ell}(\tau + 0^+)$
   }
   }
4. for $i = 1, \dots, N_\varepsilon$, set $\underline{J}_i^{n+\frac{1}{2}} :=$ J_tmp$[i]$

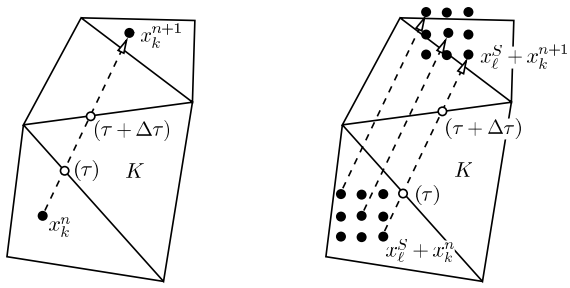

Fig. 1. Graphical depiction of Algorithm 3.4 with a Dirac particle (left), and a smooth particle represented by $N_S = 9$ auxiliary particles (right).

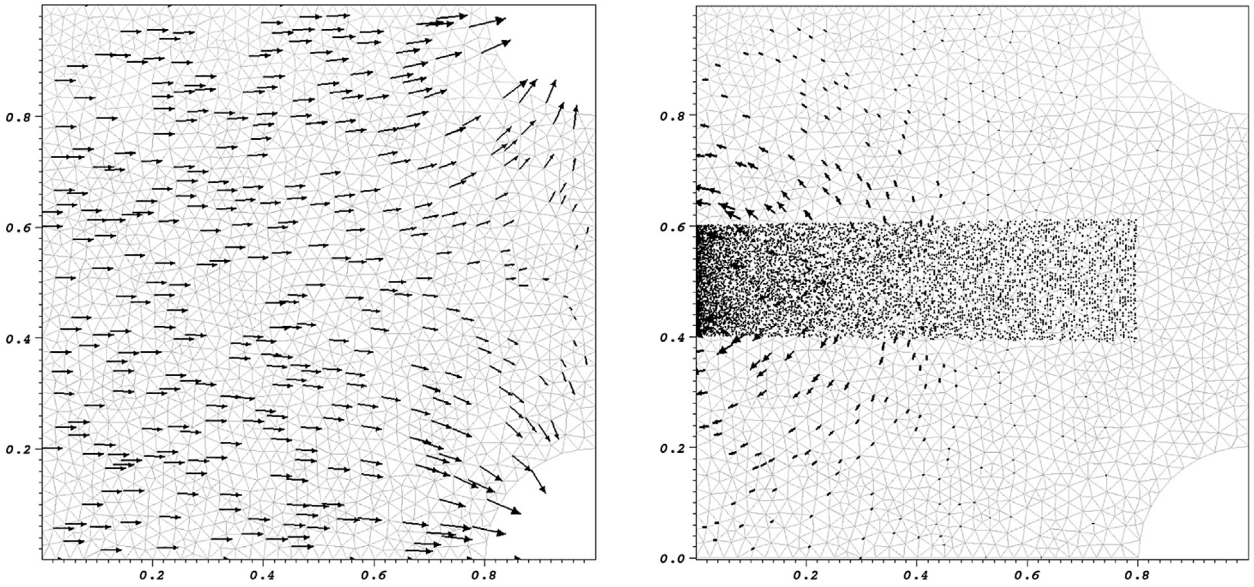

Fig. 2. Start of the beam test case: external field E_{ext} created by the boundary conditions (left), and particles positions with self-consistent field $E_{\text{self}} := E - E_{\text{ext}}$ after about 300 iterations (right).

4. A numerical validation

4.1. The diode test case

To validate the above algorithm we have implemented, a 2D diode test case, which is known to strongly rely on the Gauss law being satisfied, see for instance [28]. In this test case the domain $\Omega := [0,1]^2 \setminus (B_+ \cup B_-)$ consists of a square minus two disks of radius 0.2 that are respectively centered in $(1,1)$ and $(1,0)$. It is meshed with triangles. In order to accelerate a bunch of electrons that is emitted with slow positive horizontal speed on a segment $\{0\} \times [0.4, 0.6]$ of the left edge, the boundary conditions are as follows. The left boundary, as well as the two arcs, are perfect electric conductors with fixed potentials that simulate a cathode and an anode. The other boundary conditions are absorbing. The resulting external field is plotted in Fig. 2, left.

We compare two runs, one using the inconsistent current density source $\underline{J}_i^{n+1/2} := \sum_{k=1}^{N_{\text{part}}} w_k v_k^{n+1/2} \cdot \varphi_i^\varepsilon(x_k^{n+1/2})$, $i = 1, \ldots, N^\varepsilon$, that corresponds to evaluating the particle current density in (34) at the time $t^{n+1/2}$, and one using the charge-conserving Algorithm 3.4. Both runs implement Nédélec finite elements of order 1 and leap-frog time discretizations for the Maxwell system and the particles trajectories. In Fig. 2, right, we have plotted the bunch of particles after about 300 iterations, that is, before it has reached the right boundary of the domain. At this time, the two runs are very similar. Differences become visible after a large number of iterations, when unphysical filaments appear in the run that implements the inconsistent coupling. In Fig. 3, we have plotted the particles' positions after about 10,000 iterations, which correspond to around 20 crossing times of the beam (alone on top, and together with the self-consistent electric field on the bottom). On the left, the beam resulting from the inconsistent coupling is clearly non-physical, as particles of the same charge should not concentrate into thin filaments. Moreover the self-consistent electric field shows spurious oscillations (bottom left). On the right, we see that Algorithm 3.4 prevents such unphysical behavior. Moreover we have checked that the finite-element Gauss law (15) was satisfied up to machine accuracy, as formally established by combining Lemmas 2.3 and 3.3.

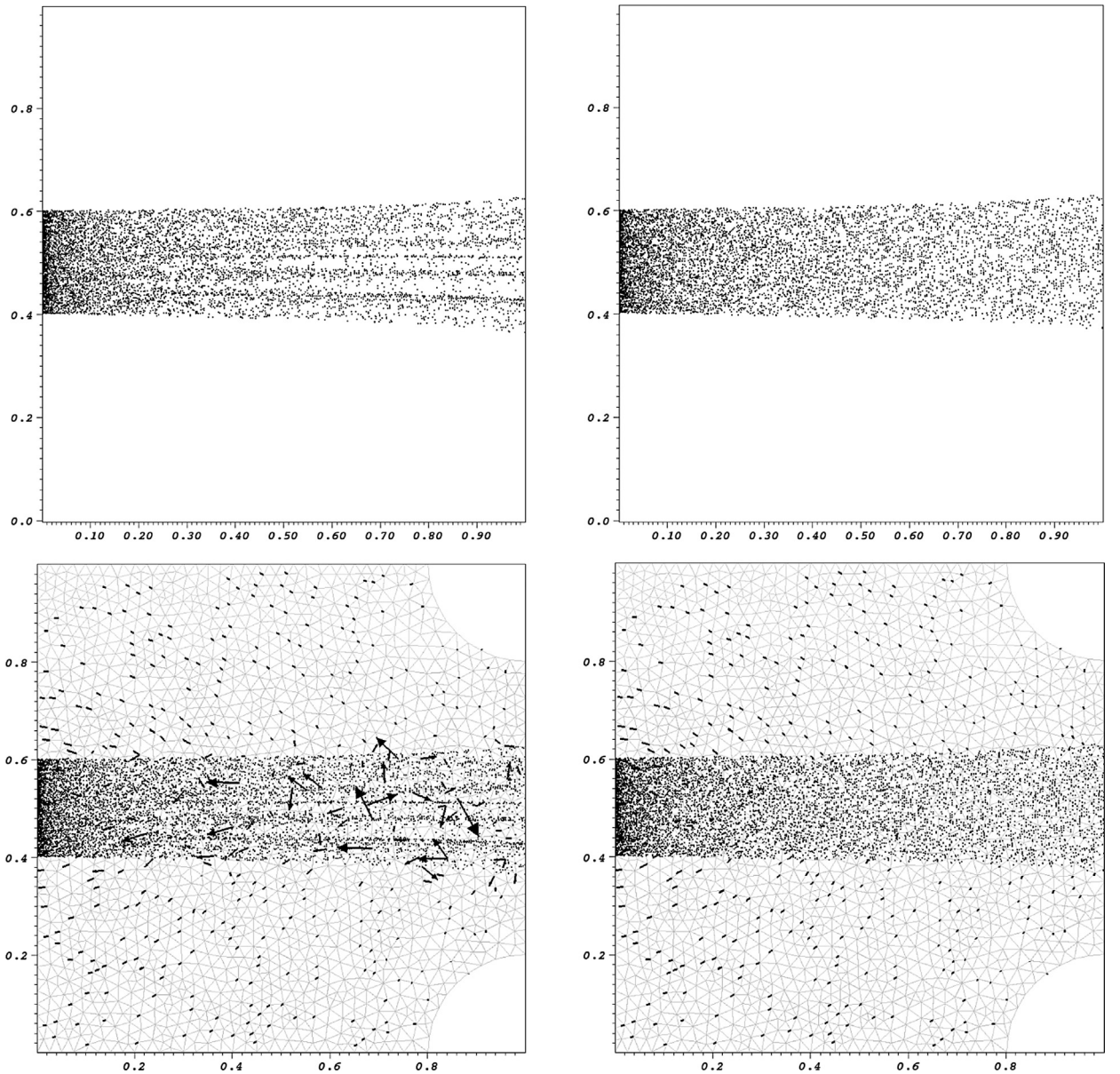

Fig. 3. Particle beams after about 10,000 iterations, computed with the inconsistent (nonconservative) current definition, left, and Algorithm 3.4, right. Top: particles alone. Bottom: together with self-consistent electric field (with the same scale for both runs).

4.2. The Landau damping problem

The Landau damping problem is a classical plasma physics phenomenon that is purely electrostatic and is quite hard to get right with the Vlasov–Maxwell equations: it absolutely requires the Gauss law to be well satisfied.

In Fig. 4 the decay of the potential energy with respect to time is represented. The theoretical decay rate is 0.1533. This decay is captured well in the initial phase with the new Algorithm 3.4 (left picture) and 10,000 particles per cell and second-order Nedelec elements. This could be improved with more particles or more efficiently using some variance reduction technique, but this is not the aim of this article. On the other hand, the non-conservative deposition scheme using exactly the same numerical data does not capture a decay at all (right picture).

5. Conclusion

In this article, we have described a unified mathematical formulation for curl-conforming finite elements coupled with particle schemes, and we have shown that in order to yield charge-conserving schemes, the discrete current sources that

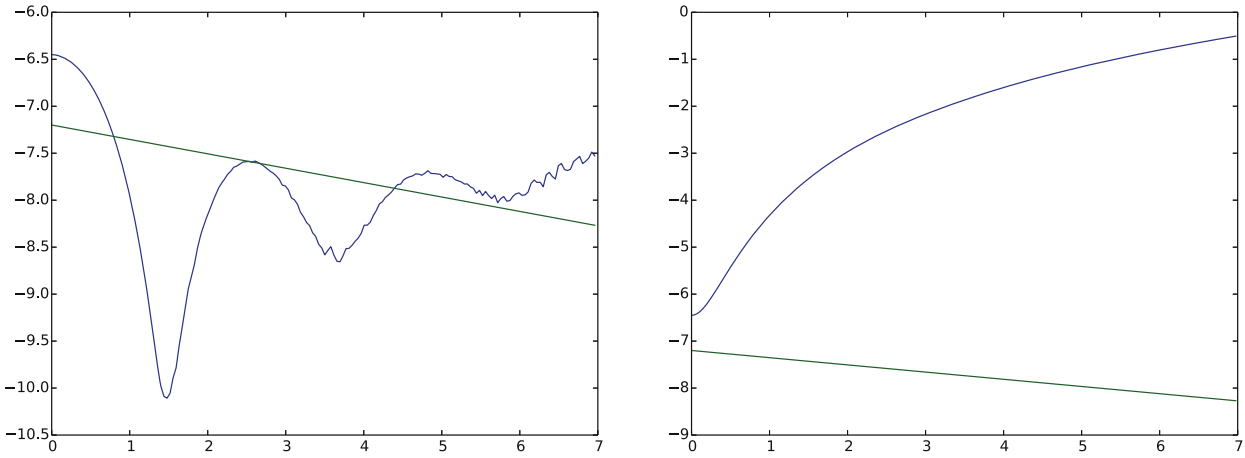

Fig. 4. (Color online.) Landau damping: log plot of the electric energy computed with the new Algorithm 3.4, left, and the inconsistent (nonconservative) current definition, right.

appear in several kind of time discretization schemes had to meet a consistency criterion that essentially amounts to a finite-element continuity equation. Moreover we have proposed a generic algorithm for computing such charge-conserving current sources, which extends the virtual particle method of Eastwood to the case of arbitrary shape factors and piecewise polynomial trajectories of arbitrary degree.

As they cover a large class of potential FEM–PIC solvers, and general grids in 2 and 3 dimensions, we believe that these results provide a useful roadmap in the design of high-order charge-conserving schemes.

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