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Variational Algorithms for Numerical Simulation of Collisionless Plasma with Point Particles Including Electromagnetic Interactions

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Energy- and charge-conserving algorithms for numerical simulation of collisionless plasma with point particles, including electromagnetic interactions, are derived from Hamilton's variational principle. The equations are put in a form suitable for advancing the electromagnetic potentials with a time-centered leapfrog difference scheme. An example is presented for a cartesian geometry.

I. INTRODUCTION

It has been shown [1, 2] that Hamilton's variational principle can be used in a systematic way to derive a wide class of numerical algorithms for studying collisionless plasmas. The simplest application of this method is when we consider a collection of point particles interacting purely electrostatically (vector potential equal to zero), and represent the scalar potential in periodic cartesian geometry as a continuous piecewise linear function of each coordinate. That is, we represent the scalar potential by its values at the points of a spatial grid with linear interpolation of the potential in each coordinate direction between the grid points. With point particles and this representation of the scalar potential, the approximation to Poisson's equation that is obtained from the variational principle is a system of equations that is in fact a particle-in-cell (or cloud-in-cell) method with "area-weighting" for the apportionment of charge to the different grid points [3–5]. The representation of the Laplacian implied by the variational derivation is the central difference approximation to d^2/dx^2 in one dimension [1, 2], and a particular nine-point scheme in two dimensions [1]. In the particle equations of motion that are deduced from the variational principle, the electric field is computed as the negative gradient of the assumed representation of the scalar potential without any interpolation or smoothing. To date, only limited analytical or numerical comparisons of the various methods currently in use for plasma

simulation have been made. However, it has been demonstrated that the variational prescription is advantageous with regard to numerical stability when the grid spacing is sufficiently large [6–8], and with regard to fluctuations in total energy for sufficiently large grid spacing and/or small time step [9]. No comparisons have been made in two or three dimensions.

In this paper, we use the variational principle to provide simulation algorithms for point particles interacting electromagnetically. Because of the common variational derivation, these algorithms are natural generalizations of the algorithms for electrostatic problems that were derived from the variational principle. As in the electrostatic case, the algorithms conserve energy exactly in the limit of zero time step. The variational method can be applied as easily in curvilinear geometry as in cartesian geometry, and it is applicable to more general representations of the potentials than, say, the piecewise linear representation that leads to "area-weighting" in electrostatic problems. The derivation and main results in this paper are given in curvilinear coordinates for a class of representations of the potentials, among which are included the piecewise linear and other representations that lead to generalized finite-difference approximations to the Maxwell equations. The final equations are written in matrix form, where the matrices are defined in terms of the representation and coordinate system that are to be used. Thus, the final equations can be specialized to a particular problem by evaluating the matrix elements appropriate to the representation and coordinate system chosen for that problem. This is generally a simple task; as an example, the matrix elements appropriate to a periodic cartesian geometry with two spatial variables and a piecewise linear representation of the scalar potential are presented at the end of the paper, and the final equations are rewritten specifically for that situation. It is not necessary to follow the derivation of the general equations in detail either to use those equations or to use the specific equations that are given for the cartesian example. The paper is a further application of the formalism presented in Ref. [1], with formulas that can be used in a variety of problems.

Of the schemes that have been proposed for simulating plasmas with electromagnetic interactions [10–17], the one most closely related to the schemes presented in this paper is one of the three used by Morse and Nielson in their simulation of the nonlinear Weibel instability [17]. They found it to be the most effective of the three. It is based on the scalar and vector potentials, as are the variational algorithms; and, except for quantities related to divergence-free currents, the spatial centering of the variables corresponds to the centering implied by the variational algorithm when a piecewise linear representation is used for the scalar potential. The geometry chosen for the example at the end of this paper is the same as that used by Morse and Nielson.

In principle, there need be no relation between the representation chosen for the scalar potential and that chosen for the vector potential, and none was assumed

in Ref. [1]. However, a special choice of representation of the vector potential in terms of the representation of the scalar potential has been made in deriving the final equations of this paper. With that choice, the final equations for the potentials can be viewed as a representation of the $\nabla \cdot \mathbf{E}$ Maxwell equation, a representation of the $\nabla \times \mathbf{B}$ Maxwell equation for that part of the current density that is divergence-free, and a representation of the divergence of the three vector components of the $\nabla \times \mathbf{B}$ equation for the part of the current density which has a nonzero divergence. As a result, the equations are consistent with a direct analog of the usual charge conservation theorem, and are redundant because of the charge conservation theorem, just as is true with the exact Maxwell equations. The redundancy is removed by imposition of a direct analog of one of the usual gauge conditions. It is possible for an analog of the usual charge conservation theorem to be satisfied by the numerical algorithms because a representation of the divergence of the current density enters the formulation.

The final equations are presented in a Hamiltonian form as well as in a Lagrangian form. With the Hamiltonian form, the dynamical variables, including those related to the vector potential, satisfy first-order differential equations in time, and the potentials can be advanced with a time-centered, time-reversible leapfrog scheme.

The notation used in this paper and in previous discussions of the variational method [1, 2] was chosen in a way that seemed appropriate to the generality of the method. For example, only for special choices of the basis functions are the expansion coefficients for the potentials equal to values of the potentials at points of a grid. Therefore, it seems inappropriate to use symbols for the expansion coefficients that are closely related to the usual symbols for the potentials. Instead, the symbols for the basis functions are chosen to correspond to the usual symbols for the potentials. It is hoped that the reader interested in a specific problem will bear with the generality of this treatment and a possibly unfamiliar notation.

In Section II the formulas for the numerical algorithms are derived and written in matrix form, and the charge conservation theorem is demonstrated. The gauge conditions are written for the Coulomb and Lorentz gauges. In Section III the Hamiltonian version of the equations is written and the leapfrog scheme for the potentials is specified. In Section IV the formulas are specialized to apply to the periodic two-dimensional cartesian geometry, and explicit formulas are presented assuming a piecewise linear representation of the scalar potential.

II. The Basic Equations

We consider point particles interacting self-consistently according to the Vlasov approximation either in a closed volume V or in a periodic system for which the

volume of the basic cell is V. The nomber of particles in V is N. The position vector, charge, and mass of particle i are $\mathbf{R}_i$, Q_i, and M_i, respectively. The coordinate system is that associated with three orthogonal unit vectors $\hat{\mathbf{e}}_j(\mathbf{r})$. The unit vectors form a right-handed set: $\hat{\mathbf{e}}_k = \hat{\mathbf{e}}_i \times \hat{\mathbf{e}}_j$ when (i, j, k) is a cyclic permutation of (1, 2, 3). The coordinate of $\mathbf{r}$ associated with $\hat{\mathbf{e}}_j$ is x_j. The derivative of $\mathbf{r}$ with respect to x_j is given as usual in terms of a function $h_j(\mathbf{r})$:

$$\frac{\partial \mathbf{r}}{\partial x_j} = h_j(\mathbf{r})\, \hat{\mathbf{e}}_j(\mathbf{r}).$$

The coordinate of $\mathbf{R}_i$ associated with $\hat{\mathbf{e}}_j$ is denoted by $\gamma_i^{(j)}$, and the time derivative of $\mathbf{R}_i$ is

$$\dot{\mathbf{R}}_i = \sum_{j=1}^{3} \hat{\mathbf{e}}_j(\mathbf{R}_i)\, h_j(\mathbf{R}_i)\, \dot{\gamma}_i^{(j)}.$$

The representations of the scalar and vector potentials that we consider are expressed by

$$\varphi(\mathbf{r}, t) = \varphi_0(\mathbf{r}, t) + \sum_n \alpha_n(t)\, \Phi_n(\mathbf{r}) \tag{1}$$

and

$$\mathbf{A}(\mathbf{r}, t) = \mathbf{A}_0(\mathbf{r}, t) + \sum_{j=1} \hat{\mathbf{e}}_j(\mathbf{r}) \sum_m \beta_m^{(j)}(t)\, \mathscr{A}_m^{(j)}(\mathbf{r}), \tag{2}$$

where the set of functions Φ_n and the three sets of functions $\mathscr{A}_m^{(j)}$, one for each j, are each linearly independent. The index n on the basis functions $\Phi_n(\mathbf{r})$ and $\mathscr{A}_n^{(j)}(\mathbf{r})$ is a shorthand notation for a set of three indices (n_1, n_2, n_3). If each basis function were a product of a function of x_1, a function of x_2, and a function of x_3, as is often the case, then n_j would label the functions of x_j. We need not specify the precise meaning of the three indices at this point, except to establish the convention that $n_j = 0$ implies no dependence on x_j:

if $n_j = 0$, then $\Phi_n(\mathbf{r}) = \Phi_{n_1 n_2 n_3}(\mathbf{r})$ does not depend on x_j and

$\mathscr{A}_n^{(j)}(\mathbf{r}) = \mathscr{A}_{n_1 n_2 n_3}^{(j)}(\mathbf{r})$ does not depend on x_j.

The functions φ_0 and $\mathbf{A}_0$ are specified external potentials that may be required by the physical problem or that are included for mathematical convenience. They must satisfy the boundary conditions that are imposed on φ and the tangential component of $\mathbf{A}$[1], thus making $(\varphi - \varphi_0)$ and the tangential component of $(\mathbf{A} - \mathbf{A}_0)$

[1] See Ref. [1, Eqs. (24) and (29)].

either vanish on the boundary or satisfy periodic boundary conditions. The specified charge and current densities associated with φ_0 and $\mathbf{A}_0$ will be denoted by $\rho_0(\mathbf{r}, t)$ and $\mathbf{j}_0(\mathbf{r}, t)$. The functions Φ_n and the tangential component of $\hat{\mathbf{e}}_j \mathscr{A}_m^{(j)}$ must separately either vanish on the boundary of V or satisfy periodic boundary conditions. (If there are periodic boundary conditions for one or more coordinates, then they must be satisfied the normal component of $\hat{\mathbf{e}}_j \mathscr{A}_m^{(j)}$ as well.)

The Lagrangian is [1]

$$
\begin{aligned}
L = \sum_{i=1}^{N} \Bigg\{ & \frac{1}{2} M_i \sum_{j=1}^{3} h_j^2(\mathbf{R}_i)(\dot{\gamma}_i^{(j)})^2 - Q_i \left[\varphi_0(\mathbf{R}_i, t) + \sum_n \alpha_n(t)\, \Phi_n(\mathbf{R}_i) \right] \\
& + \frac{1}{c} Q_i \sum_{j=1}^{3} h_j(\mathbf{R}_i)\, \dot{\gamma}_i^{(j)} \left[A_{0j}(\mathbf{R}_i, t) + \sum_m \beta_m^{(j)}(t)\, \mathscr{A}_m^{(j)}(\mathbf{R}_i) \right] \Bigg\} \\
& + \int_V d^3\mathbf{r} \Bigg\{ \frac{1}{8\pi} \left[\nabla \varphi_0(\mathbf{r}, t) + \sum_n \alpha_n(t)\, \nabla \Phi_n(\mathbf{r}) + \frac{1}{c} \dot{\mathbf{A}}_0(\mathbf{r}, t) + \frac{1}{c} \sum_{j,m} \hat{\mathbf{e}}_j(\mathbf{r}) \dot{\beta}_m^{(j)} \mathscr{A}_m^{(j)}(\mathbf{r}) \right]^2 \\
& - \frac{1}{8\pi} \left[\nabla \times \mathbf{A}_0(\mathbf{r}, t) + \nabla \times \sum_{j,m} \hat{\mathbf{e}}_j(\mathbf{r})\, \beta_m^{(j)}(t)\, \mathscr{A}_m^{(j)}(\mathbf{r}) \right]^2 \\
& - \rho_0(\mathbf{r}, t) \left[\varphi_0(\mathbf{r}, t) + \sum_n \alpha_n(t)\, \Phi_n(\mathbf{r}) \right] \\
& + \frac{1}{c} \mathbf{j}_0(\mathbf{r}, t) \cdot \left[\mathbf{A}_0(\mathbf{r}, t) + \sum_{j,m} \hat{\mathbf{e}}_j(\mathbf{r})\, \beta_m^{(j)}(t)\, \mathscr{A}_m^{(j)}(\mathbf{r}) \right] \Bigg\},
\end{aligned}
\tag{3}
$$

where

$$
A_{0j}(\mathbf{r}, t) = \hat{\mathbf{e}}_j(\mathbf{r}) \cdot \mathbf{A}_0(\mathbf{r}, t).
$$

The Euler–Lagrange equation for $\gamma_i^{(j)}$ is the usual particle equation of motion,

$$
\begin{aligned}
& \frac{d}{dt} \left\{ M_i h_j^2(\mathbf{R}_i)\, \dot{\gamma}_i^{(j)} + \frac{1}{c} Q_i h_j(\mathbf{R}_i)\, A_j(\mathbf{R}_i, t) \right\} \\
& \quad = \frac{1}{2} M_i \sum_{k=1}^{3} (\dot{\gamma}_i^{(k)})^2 \frac{\partial}{\partial \gamma_i^{(j)}} h_k^2(\mathbf{R}_i) \\
& \quad - Q_i \frac{\partial}{\partial \gamma_i^{(j)}} \varphi(\mathbf{R}_i, t) + \frac{1}{c} Q_i \sum_{k=1}^{3} \dot{\gamma}_i^{(k)} \frac{\partial}{\partial \gamma_i^{(j)}} [h_k(\mathbf{R}_i)\, A_k(\mathbf{R}_i, t)],
\end{aligned}
\tag{4}
$$

where

$$
A_j(\mathbf{r}, t) = \hat{\mathbf{e}}_j(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}, t).
$$

The Euler–Lagrange equation for α_n is

$$
\int_V d^3\mathbf{r} \left[\sum_m \alpha_m \nabla \Phi_m(\mathbf{r}) + \frac{1}{c} \sum_{j,m} \dot{\beta}_m^{(j)} \hat{\mathbf{e}}_j(\mathbf{r})\, \mathscr{A}_m^{(j)}(\mathbf{r}) \right] \cdot \nabla \Phi_n(\mathbf{r}) = 4\pi \sum_{i=1}^{N} Q_i \Phi_n(\mathbf{R}_i),
\tag{5}
$$

and that for $\beta_m^{(j)}$ is

$$\int_V d^3\mathbf{r}\left[\nabla \times \sum_{k,m} \beta_m^{(k)} \hat{\mathbf{e}}_k(\mathbf{r})\, \mathscr{A}_m^{(k)}(\mathbf{r})\right] \cdot \nabla \times [\hat{\mathbf{e}}_j(\mathbf{r})\, \mathscr{A}_n^{(j)}(\mathbf{r})]$$

$$= \frac{4\pi}{c} \sum_{i=1}^{N} Q_i \dot{\gamma}_i^{(j)} h_j(\mathbf{R}_i)\, \mathscr{A}_n^{(j)}(\mathbf{R}_i)$$

$$- \frac{1}{c} \int_V d^3\mathbf{r}\left[\sum_m \dot{\alpha}_m \nabla \Phi_m(\mathbf{r}) + \frac{1}{c} \sum_{k,m} \ddot{\beta}_m^{(k)} \hat{\mathbf{e}}_k(\mathbf{r})\, \mathscr{A}_m^{(k)}(\mathbf{r})\right] \cdot \hat{\mathbf{e}}_j(\mathbf{r})\, \mathscr{A}_n^{(j)}(\mathbf{r}). \quad (6)$$

The external potentials and sources do not appear in Eqs. (5) and (6) because they satisfy Maxwell's equations and because of the boundary conditions imposed on the basis functions.

Choice of $\mathscr{A}_n^{(j)}$ and Interpretation of the Equations

Equation (5) can be viewed as the representation of the Maxwell $\nabla \cdot \mathbf{E}$ equation in the space of functions Φ_n, and Eq. (6) can be viewed as the representation of the Maxwell $\nabla \times \mathbf{B}$ equation in the space of functions $\hat{\mathbf{e}}_j \mathscr{A}_n^{(j)}$. In terms of the representations of the potentials given by Eqs. (1) and (2), the Maxwell $\nabla \cdot \mathbf{E}$ and $\nabla \times \mathbf{B}$ equations for point particles are, respectively,

$$-\nabla \cdot \left[\sum_m \alpha_m \nabla \Phi_m(\mathbf{r}) + \frac{1}{c} \sum_{j,m} \dot{\beta}_m^{(j)} \hat{\mathbf{e}}_j(\mathbf{r})\, \mathscr{A}_m^{(j)}(\mathbf{r})\right] = 4\pi \sum_{i=1}^{N} Q_i\, \delta(\mathbf{r} - \mathbf{R}_i), \quad (7)$$

and

$$\nabla \times \nabla \times \sum_{k,m} \beta_m^{(k)} \hat{\mathbf{e}}_k(\mathbf{r})\, \mathscr{A}_m^{(k)}(\mathbf{r}) = \frac{4\pi}{c} \sum_{i=1}^{N} Q_i \dot{\mathbf{R}}_i\, \delta(\mathbf{r} - \mathbf{R}_i)$$

$$- \frac{1}{c}\left[\sum_m \dot{\alpha}_m \nabla \Phi_m(\mathbf{r}) + \frac{1}{c} \sum_{k,m} \ddot{\beta}_m^{(k)} \hat{\mathbf{e}}_k(\mathbf{r})\, \mathscr{A}_m^{(k)}(\mathbf{r})\right]. \quad (8)$$

The representations of these equations are the systems of equations obtained by forming the inner product of the $\nabla \cdot \mathbf{E}$ equation with each of the functions Φ_n and the inner product of the $\nabla \times \mathbf{B}$ equation with each of the functions $\hat{\mathbf{e}}_j \cdot \mathscr{A}_n^{(j)}$. That is, Eq. (5) can be obtained by multiplying the $\nabla \cdot \mathbf{E}$ equation by $\Phi_n(\mathbf{r})$ and integrating over V, and Eq. (6) can be obtained by scalar multiplying the $\nabla \times \mathbf{B}$ equation by $\hat{\mathbf{e}}_j(\mathbf{r})\, \mathscr{A}_n^{(j)}(\mathbf{r})$ and integrating over V. Equations (7) and (8) can usually be satisfied only if the basis functions are complete. Nevertheless, even if the basis

functions are incomplete, Eqs. (5) and (6) can still be thought of as representations of the $\nabla \cdot \mathbf{E}$ and $\nabla \times \mathbf{B}$ equations in the spaces of the functions Φ_n and $\hat{\mathbf{e}}_j \cdot \mathscr{A}_n^{(j)}$.

So far we have not assumed a connection between the basis functions for the vector potential and those for the scalar potential. As long as the two sets of basis functions are complete, this does not present a problem in principle because Eqs. (5) and (6) are then equivalent to the $\nabla \cdot \mathbf{E}$ and $\nabla \times \mathbf{B}$ equations. All manipulations with the differential equations have exact analogs with the representations, and general properties of the differential equations are also general properties of the representations. However, when the basis functions are incomplete, as is generally the case when we think of numerical computations, the situation is different. Then, Eqs. (5) and (6) are only approximately equivalent to the $\nabla \cdot \mathbf{E}$ and $\nabla \times \mathbf{B}$ equations. Manipulations with the differential equations do not necessarily have exact analogs with the representations, and general properties of the differential equations are not necessarily general properties of the representations. The energy conservation theorem is always valid regardless of what the basis functions are [1]. On the other hand, the charge conservation theorem, which is obtained by adding $1/c$ times the time derivative of the $\nabla \cdot \mathbf{E}$ equation to the divergence of the $\nabla \times \mathbf{B}$ equation, is not usually valid for the representations unless there is an appropriate connection between the basis functions for the vector and scalar potentials.

In this paper we choose a connection between the basis functions that always ensures a charge conservation theorem for the representations. We define $\mathscr{A}_n^{(j)}$ in terms of Φ_n by

$$\mathscr{A}_n^{(j)}(\mathbf{r}) = \begin{cases} \hat{\mathbf{e}}_j(\mathbf{r}) \cdot \nabla\Phi_n(\mathbf{r}) = \dfrac{1}{h_j(\mathbf{r})} \dfrac{\partial}{\partial x_j} \Phi_n(\mathbf{r}), & \text{for} \quad n_j \neq 0, \\ \dfrac{1}{h_j(\mathbf{r})} \Phi_n(\mathbf{r}), & \text{for} \quad n_j = 0. \end{cases} \tag{9}$$

With $\mathscr{A}_n^{(j)}$ so defined, we can interpret Eq. (6) in terms of the space of functions Φ_n, so that Eqs. (5) and (6) together can be interpreted in a unified way in terms of the same space. The cases $n_j = 0$ and $n_j \neq 0$ must be considered separately. For $n_j \neq 0$, Eq. (6) is the representation of the divergence of that part of the $\nabla \times \mathbf{B}$ equation that is parallel to $\hat{\mathbf{e}}_j$; that is, it is a representation of

$$\begin{aligned} &\nabla \cdot \left\{ \hat{\mathbf{e}}_j(\mathbf{r})\, \hat{\mathbf{e}}_j(\mathbf{r}) \cdot \left[\nabla \times \nabla \times \sum_{k,m} \beta_m^{(k)} \hat{\mathbf{e}}_k(\mathbf{r})\, \mathscr{A}_m^{(k)}(\mathbf{r}) \right] \right\} \\ &\quad = \frac{4\pi}{c} \nabla \cdot \left[\hat{\mathbf{e}}_j(\mathbf{r})\, \hat{\mathbf{e}}_j(\mathbf{r}) \cdot \sum_{i=1}^{N} Q_i \dot{\mathbf{R}}_i\, \delta(\mathbf{r} - \mathbf{R}_i) \right] \\ &\quad - \frac{1}{c} \nabla \cdot \left\{ \hat{\mathbf{e}}_j(\mathbf{r})\, \hat{\mathbf{e}}_j(\mathbf{r}) \cdot \left[\sum_m \dot{\alpha}_m \nabla\Phi_m(\mathbf{r}) + \frac{1}{c} \sum_{k,m} \dot{\beta}_m^{(k)} \hat{\mathbf{e}}_k(\mathbf{r})\, \mathscr{A}_m^{(k)}(\mathbf{r}) \right] \right\}. \end{aligned} \tag{10}$$

To obtain Eq. (6) from Eq. (10) for $n_j \neq 0$, multiply Eq. (10) by $\Phi_n(\mathbf{r})$, integrate over V, and use the partial integration formulas

$$\int_V d^3\mathbf{r}\Phi_n \nabla \cdot [\hat{\mathbf{e}}_j \hat{\mathbf{e}}_j \cdot \mathbf{D}] = -\int_V d^3\mathbf{r}[\hat{\mathbf{e}}_j \cdot \mathbf{D}]\, \mathscr{A}_n^{(j)} \qquad (\text{for } n_j \neq 0)$$

and

$$\int_V d^3\mathbf{r}\mathbf{B} \cdot \nabla \times \mathscr{A} = \int_V d^3\mathbf{r}\mathscr{A} \cdot \nabla \times \mathbf{B}.$$

[For $n_j = 0$, the inner product of Eq. (10) with Φ_n vanishes because then $\hat{\mathbf{e}}_j(\mathbf{r}) \cdot \nabla\Phi_n(\mathbf{r}) = 0$.] Clearly, that part of the current density that is parallel to $\hat{\mathbf{e}}_j$ and divergence-free is ignored in Eq. (10), and is also ignored in Eq. (6) for $n_j \neq 0$. That part of the current density is taken into account in Eq. (6) when $n_j = 0$. For $n_j = 0$, Eq. (6) is the representation of $[1/h_j(\mathbf{r})]$ times the part of the $\nabla \times \mathbf{B}$ equation that is parallel to $\hat{\mathbf{e}}_j$. This representation is in the space of functions Φ_n such that $n_j = 0$. [The functions $\Phi_n(\mathbf{r})$ such that $n_j = 0$ are those that do not depend on x_j.]

The expression for the vector potential is now

$$\mathbf{A}(\mathbf{r}, t) = \mathbf{A}_0(\mathbf{r}, t) + \sum_{j=1}^{3} \hat{\mathbf{e}}_j(\mathbf{r}) \frac{1}{h_j(\mathbf{r})} \left[\sum_{\substack{m \\ (m_j \neq 0)}} \beta_m^{(j)}(t) \frac{\partial}{\partial x_j} \Phi_m(\mathbf{r}) + \sum_{\substack{m \\ (m_j = 0)}} \beta_m^{(j)}(t)\, \Phi_m(\mathbf{r}) \right] \tag{11}$$

and its curl is

$$\nabla \times \mathbf{A}(\mathbf{r}, t) = \nabla \times \mathbf{A}_0(\mathbf{r}, t) + \sum_{i=1}^{3} \hat{\mathbf{e}}_i(\mathbf{r}) \sum_{\substack{m \\ (m_j \neq 0 \\ m_k \neq 0)}} [\beta_m^{(k)} - \beta_m^{(j)}] \frac{1}{h_j(\mathbf{r})\, h_k(\mathbf{r})} \frac{\partial^2}{\partial x_j\, \partial x_k} \Phi_m(\mathbf{r})$$

$$+ \sum_{i=1}^{3} \hat{\mathbf{e}}_i(\mathbf{r}) \frac{1}{h_j(\mathbf{r})\, h_k(\mathbf{r})} \left[\sum_{\substack{m \\ (m_k = 0 \\ m_j \neq 0)}} \beta_m^{(k)} \frac{\partial}{\partial x_j} \Phi_m(\mathbf{r}) - \sum_{\substack{m \\ (m_j = 0 \\ m_k \neq 0)}} \beta_m^{(j)} \frac{\partial}{\partial x^k} \Phi_m(\mathbf{r}) \right], \tag{12}$$

where (i, j, k) is a cyclic permutation of $(1, 2, 3)$.

The Final Equations in Matrix Notation and Charge Conservation

By introducing matrix notation we can write Eqs. (5) and (6) in a more transparent form as

$$-\sum_m \left[T_{n;m}\alpha_m + \frac{1}{c} \sum_{j=1}^{3} T_{n;m}^{(j)} \dot{\beta}_m^{(j)} \right] = 4\pi P_n \tag{13}$$

and

$$\sum_m \sum_{k=1}^{3} S_{n;m}^{(l,k)} \beta_m^{(k)} = \frac{4\pi}{c} J_n^{(l)} - \frac{1}{c} \sum_m \left[\dot{\alpha}_m T_{m;n}^{(l)} + \frac{1}{c} W_{n;m}^{(l)} \ddot{\beta}_m^{(l)} \right] \tag{14}$$

where

$$P_n = \sum_{i=1}^{N} Q_i \Phi_n(\mathbf{R}_i), \tag{15a}$$

$$J_n^{(l)} = - \sum_{i=1}^{N} Q_i \dot{\gamma}_i^{(l)} h_l(\mathbf{R}_i) \mathscr{A}_n^{(l)}(\mathbf{R}_i) \qquad \text{(for all } n\text{)} \tag{15b}$$

$$= - \sum_{i=1}^{N} Q_i \dot{\gamma}_i^{(l)} \frac{\partial}{\partial \gamma_i^{(l)}} \Phi_n(\mathbf{R}_i) \qquad \text{(for } n_l \neq 0\text{)}, \tag{15c}$$

$$T_{n;m}^{(j)} = - \int_V d^3\mathbf{r} [\nabla \Phi_n(\mathbf{r})] \cdot \hat{\mathbf{e}}_j(\mathbf{r}) \mathscr{A}_m^{(j)}(\mathbf{r}) \qquad \text{(for all } m\text{)} \tag{15d}$$

$$= - \int_V d^3\mathbf{r} [\nabla \Phi_n(\mathbf{r})] \cdot \hat{\mathbf{e}}_j(\mathbf{r}) \hat{\mathbf{e}}_j(\mathbf{r}) \cdot [\nabla \Phi_m(\mathbf{r})] \qquad \text{(for } m_j \neq 0\text{)}, \tag{15e}$$

$$T_{n;m} = - \int_V d^3\mathbf{r} [\nabla \Phi_n(\mathbf{r})] \cdot [\nabla \Phi_m(\mathbf{r})] \tag{15f}$$

$$= \sum_{j=1}^{3} T_{n;m}^{(j)} (1 - \delta_{0,m_j}),$$

$$W_{n;m}^{(j)} = - \int_V d^3\mathbf{r} \mathscr{A}_n^{(j)}(\mathbf{r}) \mathscr{A}_m^{(j)}(\mathbf{r}) \tag{15g}$$

$$= T_{n;m}^{(j)} \qquad \text{for} \quad n_j \neq 0,$$

$$S_{n;m}^{(l,k)} = - \int_V d^3\mathbf{r} \{\nabla \times [\hat{\mathbf{e}}_l(\mathbf{r}) \mathscr{A}_n^{(l)}(\mathbf{r})]\} \cdot \{\nabla \times [\hat{\mathbf{e}}_k(\mathbf{r}) \mathscr{A}_m^{(k)}(\mathbf{r})]\} \qquad \text{(for all } n \text{ and } m\text{)} \tag{15h}$$

$$= - \int_V \{d^3\mathbf{r} \nabla \times [\hat{\mathbf{e}}_l(\mathbf{r}) \hat{\mathbf{e}}_l(\mathbf{r}) \cdot \nabla \Phi_n(\mathbf{r})]\} \cdot \{\nabla \times [\hat{\mathbf{e}}_k(\mathbf{r}) \hat{\mathbf{e}}_k(\mathbf{r}) \cdot \nabla \Phi_m(\mathbf{r})]\}.$$

$$\text{(for } n_l \neq 0 \text{ and } m_k \neq 0\text{)} \tag{15i}$$

The relation

$$\sum_{l=1}^{3} S_{n;m}^{(l,k)} (1 - \delta_{0,n_l}) = 0$$

holds because $\nabla \times \nabla \Phi_n(\mathbf{r})$ vanishes.

The equations and quantities that have been introduced can all be interpreted as representations in the space of functions Φ_n. The interpretation of Eqs. (13) and (14) was discussed in connection with the choice of $\mathscr{A}_n^{(j)}$. Equation (13) represents the $\nabla \cdot \mathbf{E}$ equation. For $n_l \neq 0$, Eq. (14) represents the divergence of that part of the $\nabla \times \mathbf{B}$ equation that is parallel to $\hat{\mathbf{e}}_l$. For $n_l = 0$, Eq. (14) represents $-[1/h_l(\mathbf{r})]$ times the part of the $\nabla \times \mathbf{B}$ equation that is parallel to $\hat{\mathbf{e}}_l$ in the subspace of functions $\Phi_n(\mathbf{r})$ that do not depend on x_l. The coefficients α_n and $\beta_n^{(j)}$ represent the functions for which they are the expansion coefficients in a linear combination of the basis functions Φ_n. The coefficients α_n represent the self-consistent scalar potential $[\varphi(\mathbf{r}, t) - \varphi_0(\mathbf{r}, t)]$. For $n_j = 0$, the coefficients $\beta_n^{(j)}$ represent the part of $h_j(\mathbf{r})\,\hat{\mathbf{e}}_j(\mathbf{r}) \cdot [\mathbf{A}(\mathbf{r}, t) - \mathbf{A}_0(\mathbf{r}, t)]$ that does not depend on x_j. For $n_j \neq 0$, the coefficients $\beta_n^{(j)}$ represent an integral of the part of $h_j(\mathbf{r})\,\hat{\mathbf{e}}_j(\mathbf{r}) \cdot [\mathbf{A}(\mathbf{r}, t) - \mathbf{A}_0(\mathbf{r}, t)]$ that does depend on x_j; that is, they represent

$$\int_{\mathbf{r}_0}^{\mathbf{r}} d\mathbf{r}' \cdot \left\{ [\mathbf{A}(\mathbf{r}', t) - \mathbf{A}_0(\mathbf{r}', t)] - \hat{\mathbf{e}}_j(\mathbf{r}') \frac{1}{h_j(\mathbf{r}')} \sum_{\substack{n \\ (n_j = 0)}} \beta_n^{(j)}(t)\, \Phi_n(\mathbf{r}') \right\}$$

(path parallel to $\hat{\mathbf{e}}_j$)

$$= \sum_{\substack{n \\ (n_j \neq 0)}} \beta_n^{(j)}(t)[\Phi_n(\mathbf{r}) - \Phi_n(\mathbf{r}_0)], \tag{16}$$

where the integral is a line integral taken between a fixed point $\mathbf{r}_0$ to a variable point $\mathbf{r}$ along a path parallel to $\hat{\mathbf{e}}_j(\mathbf{r}')$. It is to be noted that the numbers $\beta_n^{(j)}$ for $n_j \neq 0$ do not represent $[\mathbf{A}(\mathbf{r}, t) - \mathbf{A}_0(\mathbf{r}, t)]$ in this space, and that the part of $\hat{\mathbf{e}}_j(\mathbf{r}) \cdot [\mathbf{A}(\mathbf{r}, t) - \mathbf{A}_0(\mathbf{r}, t)]$ that depends on x_j is obtained from the integral in Eq. (16) by operation with $\hat{\mathbf{e}}_j(\mathbf{r}) \cdot \nabla$.

The numbers P_n represent the charge density due to the particles. The numbers $J_n^{(l)}$ for fixed l and $n_l \neq 0$ represent the divergence of that part of the current density due to the particles that is parallel to $\hat{\mathbf{e}}_l$. The numbers $J_n^{(l)}$ for fixed l and $n_l = 0$ represent $-[1/h_l(\mathbf{r})]$ times the lth component of the current density due to the particles in the subspace of functions $\Phi_n(\mathbf{r})$ that do not depend on x_l. The matrices $T^{(j)}$, T, $W^{(j)}$, and $S^{(l,k)}$ represent differentiation operators according to the scheme

$$T_{n;m}^{(j)} = W_{n;m}^{(j)} \leftrightarrow \nabla \cdot \hat{\mathbf{e}}_j \hat{\mathbf{e}}_j \cdot \nabla \qquad (\text{for } n_j \neq 0,\ m_j \neq 0), \tag{17a}$$

$$T_{n;m}^{(j)} \leftrightarrow \nabla \cdot \hat{\mathbf{e}}_j \frac{1}{h_j} \qquad (\text{for } m_j = 0), \tag{17b}$$

$$T_{n;m} \leftrightarrow \nabla \cdot \nabla, \tag{17c}$$

$$W_{n;m}^{(j)} \leftrightarrow -\frac{1}{h_j^2} \qquad (\text{for } n_j = 0,\ m_j = 0), \tag{17d}$$

and

$$S^{(l,k)}_{n;m} \leftrightarrow \begin{cases} \nabla \cdot \hat{\mathbf{e}}_l \hat{\mathbf{e}}_l \cdot \nabla \times \nabla \times \hat{\mathbf{e}}_k \hat{\mathbf{e}}_k \cdot \nabla & (\text{for } n_l \neq 0,\ m_k \neq 0), \\ \nabla \cdot \hat{\mathbf{e}}_l \hat{\mathbf{e}}_l \cdot \nabla \times \nabla \times \hat{\mathbf{e}}_k \dfrac{1}{h_k} & (\text{for } n_l \neq 0,\ m_k = 0), \\ -\dfrac{1}{h_l} \hat{\mathbf{e}}_l \cdot \nabla \times \nabla \times \hat{\mathbf{e}}_k \hat{\mathbf{e}}_k \cdot \nabla & (\text{for } n_l = 0,\ m_k \neq 0), \\ -\dfrac{1}{h_l} \hat{\mathbf{e}}_l \cdot \nabla \times \nabla \times \hat{\mathbf{e}}_k \dfrac{1}{h_k} & (\text{for } n_l = 0,\ m_k = 0). \end{cases} \tag{17e}$$

The charge conservation theorem can be demonstrated by adding $1/c$ times the time derivative of Eq. (13) to the sum over l of $(1 - \delta_{0,n_l})$ times Eqs. (14). The sum over l is the representation of the divergence of the $\nabla \times \mathbf{B}$ equation, and the left-hand side vanishes because the sum over l of $(1 - \delta_{0,n_l}) S^{(l,k)}_{n;m}$ vanishes. The result is

$$\frac{d}{dt} P_n + \sum_{l=1}^{3} J_n^{(l)}(1 - \delta_{0,n_l}) = 0, \tag{18}$$

which is the representation of the usual charge conservation theorem. The fact that it can be derived from Eqs. (13) and (14) reflects the consistency of our interpretation of these equations in terms of the Maxwell equations. On the other hand, because it is obviously true as a result of the definitions of P_n and $J_n^{(l)}$, it also shows the redundancy of Eqs. (13) and (14). That is, we can use it to derive the time derivative of Eq. (13) from the sum over l of $(1 - \delta_{0,n_l})$ times Eq. (14), so that Eq. (13) is automatically valid at all times if it is satisfied at any one time. To remove this redundancy, we introduce a Coulomb or Lorentz gauge condition in analogy to the usual treatment of Maxwell's equations.

Coulomb Gauge

The representation of the Coulomb gauge condition is

$$\int_V d^3\mathbf{r} \Phi_n(\mathbf{r})\, \nabla \cdot \sum_m \sum_{j=1}^{3} \beta_m^{(j)} \hat{\mathbf{e}}_j(\mathbf{r})\, \mathscr{A}_m^{(j)}(\mathbf{r}) = 0$$

or

$$\sum_m \sum_{j=1}^{3} T^{(j)}_{n;m} \beta_m^{(j)} = 0. \tag{19}$$

This simplifies Eq. (13) to

$$-\sum_m T_{n;m} \alpha_m = 4\pi P_n\,, \tag{20}$$

which is the representation of Poisson's equation. The potential coefficients can be determined from this equation. Their time derivatives, which appear in Eq. (14), can be determined from

$$\sum_m T_{n;m}\dot{\alpha}_m = 4\pi \sum_{l=1}^{3} J_n^{(l)}(1 - \delta_{0,n_l}), \tag{21}$$

which is the time derivative of Eq. (20) rewritten by use of the charge conservation theorem. Therefore, the problem can be treated in the Coulomb gauge by solving Eqs. (20), (21), and (14). Solution of Eq. (21) for the coefficients $\dot{\alpha}_m$ can be avoided by using the Hamiltonian formulation presented in Section III.

Lorentz Gauge

The Lorentz gauge condition is represented by

$$\int_V d^3\mathbf{r}\Phi_n(\mathbf{r}) \sum_m \left[\frac{1}{c}\dot{\alpha}_m \Phi_m(\mathbf{r}) + \nabla \cdot \sum_{j=1}^{3} \beta_m^{(j)} \hat{\mathbf{e}}_j(\mathbf{r})\, \mathscr{A}_m^{(j)}(\mathbf{r})\right] = 0$$

or

$$\frac{1}{c}\sum_m G_{n;m}\dot{\alpha}_m = -\sum_m \sum_{j=1}^{3} T_{n;m}^{(j)} \beta_m^{(j)}, \tag{22}$$

where

$$G_{n;m} = \int_V d^3\mathbf{r}\Phi_n(\mathbf{r})\, \Phi_m(\mathbf{r}). \tag{23}$$

The quantities $\dot{\alpha}_m$ appearing in Eq. (14) are then determined from Eq. (22), and Eq. (13) is rewritten as

$$\sum_m \left[\frac{1}{c^2} G_{n;m}\ddot{\alpha}_m - T_{n;m}\alpha_m\right] = 4\pi P_n \tag{24}$$

Therefore, in the Lorentz gauge, the equations to be solved are Eqs. (24), (22), and (14).

III. Hamiltonian Formulation and a Reversible Difference Scheme

By using a Hamiltonian formulation, the representation of Maxwell's equations can be recast into a system of first-order differential equations that are amenable

to a reversible, time-centered difference scheme. We begin again with the Lagrangian, rewritten in terms of the matrices introduced in the previous section:

$$
\begin{aligned}
L = & \sum_{i=1}^{N} \left\{ \frac{1}{2} M_i \sum_{j=1}^{3} h_j^2(\mathbf{R}_i)(\dot{\gamma}_i^{(j)})^2 - Q_i \varphi_0(\mathbf{R}_i, t) + \frac{1}{c} Q_i \sum_{j=1}^{3} h_j(\mathbf{R}_i)\, \dot{\gamma}_i^{(j)} A_{0j}(\mathbf{R}_i, t) \right\} \\
& - \sum_n \alpha_n P_n - \frac{1}{c} \sum_n \sum_{l=1}^{3} \beta_n^{(l)} J_n^{(l)} \\
& - \frac{1}{8\pi} \sum_{n,m} \left\{ \alpha_n T_{n;m} \alpha_m + \sum_{j=1}^{3} \left[\frac{2}{c} \alpha_n T_{n;m}^{(j)} \dot{\beta}_m^{(j)} + \frac{1}{c^2} \dot{\beta}_n^{(j)} W_{n;m}^{(j)} \dot{\beta}_m^{(i)} \right] \right\} \\
& + \frac{1}{8\pi} \sum_{n,m} \sum_{j,k=1}^{3} \beta_n^{(j)} S_{n;m}^{(j,k)} \beta_m^{(k)}.
\end{aligned} \tag{25}
$$

The canonical momenta and Hamiltonian are

$$
\begin{aligned}
\tau_i^{(j)} &= \frac{\partial L}{\partial \dot{\gamma}_i^{(j)}} \\
&= M_i h_j^2(\mathbf{R}_i)\, \dot{\gamma}_i^{(j)} + \frac{1}{c} Q_i h_j(\mathbf{R}_i)\, A_j(\mathbf{R}_i, t),
\end{aligned} \tag{26a}
$$

$$
\begin{aligned}
\sigma_n^{(l)} &= \frac{\partial L}{\partial \dot{\beta}_n^{(l)}} \\
&= -\frac{1}{4\pi c} \sum_m \left[\frac{1}{c} W_{n;m}^{(l)} \dot{\beta}_m^{(l)} + \alpha_m T_{m;n}^{(l)} \right],
\end{aligned} \tag{26b}
$$

and

$$
\begin{aligned}
H = & \sum_{i=1}^{N} \sum_{j=1}^{3} \dot{\gamma}_i^{(j)} \tau_i^{(j)} + \sum_n \sum_{l=1}^{3} \dot{\beta}_n^{(l)} \sigma_n^{(l)} - L \\
= & \sum_{i=1}^{N} \frac{1}{2} M_i \sum_{j=1}^{3} h_j^2(\mathbf{R}_i)(\dot{\gamma}_i^{(j)})^2 + \left[\sum_{i=1}^{N} Q_i \varphi(\mathbf{R}_i, t) + \frac{1}{8\pi} \sum_{n,m} \alpha_n T_{n;m} \alpha_m \right] \\
& + \frac{1}{8\pi} \sum_{n,m} \left[-\frac{1}{c^2} \sum_{j=1}^{3} \dot{\beta}_n^{(j)} W_{n;m}^{(j)} \dot{\beta}_m^{(j)} - \sum_{j,k=1}^{3} \beta_n^{(j)} S_{n;m}^{(j,k)} \beta_m^{(k)} \right] \\
= & \sum_{i=1}^{N} \left\{ \frac{1}{2M_i} \sum_{j=1}^{3} \left[\frac{1}{h_j(\mathbf{R}_i)} \tau_i^{(j)} - \frac{1}{c} Q_i A_{0j}(\mathbf{R}_i, t) - \frac{1}{c} Q_i \sum_n \beta_n^{(j)} \mathscr{A}_n^{(j)}(\mathbf{R}_i) \right]^2 \right. \\
& \left. + Q_i \varphi_0(\mathbf{R}_i, t) + Q_i \sum_n \alpha_n \Phi_n(\mathbf{R}_i) \right\} \\
& - 2\pi c^2 \sum_{n,m} \sum_{j=1}^{3} \sigma_n^{(j)} W_{n;m}^{(j)-1} \sigma_m^{(j)} - c \sum_n \sum_{j=1}^{3} \alpha_n \sigma_n^{(j)} (1 - \delta_{0,n_j}) \\
& - \frac{1}{8\pi} \sum_{n,m} \sum_{j,k=1}^{3} \beta_n^{(j)} S_{n;m}^{(j,k)} \beta_m^{(k)},
\end{aligned} \tag{27}
$$

where

$$\sum_r W^{(j)^{-1}}_{n;r} W^{(j)}_{r;m} = \delta_{n,m} .$$

The Hamiltonian equations are

$$\dot{\gamma}_i^{(j)} = \frac{1}{M_i h_j^2(\mathbf{R}_i)} \tau_i^{(j)} - \frac{1}{c} \frac{Q_i}{M_i} \frac{1}{h_j(\mathbf{R}_i)} A_j(\mathbf{R}_i , t), \tag{28a}$$

$$\dot{\tau}_i^{(j)} = -\frac{1}{M_i} \sum_{k=1}^{3} \left[\frac{1}{h_k(\mathbf{R}_i)} \tau_i^{(k)} - \frac{1}{c} Q_i A_k(\mathbf{R}_i , t)\right]\left[\tau_i^{(k)} \frac{\partial}{\partial \gamma_i^{(j)}} \frac{1}{h_k(\mathbf{R}_i)} - \frac{1}{c} Q_i \frac{\partial}{\partial \gamma_i^{(j)}} A_k(\mathbf{R}_i , t)\right] - Q_i \frac{\partial}{\partial \gamma_i^{(j)}} \varphi(\mathbf{R}_i , t), \tag{28b}$$

$$c \sum_{j=1}^{3} \sigma_n^{(j)}(1 - \delta_{0,n_j}) = P_n , \tag{29}$$

$$\sum_m W^{(l)}_{n;m} \dot{\beta}^{(l)}_m = -4\pi c^2 \sigma_n^{(l)} - c \sum_m \alpha_m T^{(l)}_{m;n} , \tag{30a}$$

and

$$\dot{\sigma}_n^{(l)} = \frac{1}{4\pi} \sum_m \sum_{k=1}^{3} S^{(l,k)}_{n;m} \beta^{(k)}_m - \frac{1}{c} J_n^{(l)}. \tag{30b}$$

Equations (28a) and (28b) are the Hamiltonian form of Eq. (4), and Eq. (29) is identical to Eq. (13). Equations (30a) and (30b) are equivalent to Eq. (14).

To obtain a time-centered difference scheme we use the Coulomb gauge, so that the electromagnetic equations to be solved are Eq. (20) for α_n, and Eqs. (30a) and (30b) for $\beta_n^{(l)}$ and $\sigma_n^{(l)}$. The quantities P_n, α_n, and $\sigma_n^{(l)}$ are defined at integral multiples of the time step, whereas $J_n^{(l)}$ and $\beta_n^{(l)}$ are defined at half-integral multiples of the time step. With this convention, the usual leapfrog scheme may be used with Eqs. (30a) and (30b) to advance $\beta_n^{(l)}$ and $\sigma_n^{(l)}$ in time, and the scheme will be exactly reversible insofar as the potentials are concerned. If the particle transport, either with Eq. (4) or Eqs. (28a) and (28b), is performed with a reversible scheme, then the time evolution of the entire system will be reversible.

IV. An Example

To give a specific instance of the formulas that have been derived, we take the simplified periodic cartesian geometry that was used for simulating the Weibel instability by Morse and Nielson [17]. We assume periodic boundary conditions

with period L in the x_1 and x_2 directions and unit period in the x_3 direction. (No confusion should arise because of using the symbol L both for the period and the Lagrangian.) Each function $h_j(\mathbf{r})$ is unity and the coordinates (x_1, x_2, x_3) correspond to (x, y, z). The potentials are allowed to depend on x_1 and x_2, but not on x_3, and the third component (z component) of the vector potential is identically zero. Correspondingly, the charge and current densities may depend on x_1 and x_2, but not on x_3, and the third component of the current density vanishes identically. There are no external potentials and we work in the Coulomb gauge. The $\nabla \cdot \mathbf{E}$ equation is

$$-\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^2}\right)\varphi(x_1, x_2, t)=4\pi\sum_{i=1}^{N} Q_i\,\delta(x_1-\gamma_i^{(1)})\,\delta(x_2-\gamma_i^{(2)}). \tag{31}$$

The $\nabla \times \mathbf{B}$ equation is

$$\hat{\mathbf{e}}_1\left(\frac{\partial^2 A_2}{\partial x_1\,\partial x_2}-\frac{\partial^2 A_1}{\partial x_2^2}\right)+\hat{\mathbf{e}}_2\left(\frac{\partial^2 A_1}{\partial x_1\,\partial x_2}-\frac{\partial^2 A_2}{\partial x_1^2}\right)$$
$$=\sum_{j=1}^{2}\hat{\mathbf{e}}_j\left[\frac{4\pi}{c}\sum_{i=2}^{N} Q_i\dot{\gamma}_i^{(j)}\,\delta(x_1-\gamma_i^{(1)})\,\delta(x_2-\gamma_i^{(2)})-\frac{1}{c}\frac{\partial}{\partial x_j}\dot{\varphi}-\frac{1}{c^2}\ddot{A}_j\right]; \tag{32}$$

and the divergence of that part of the $\nabla \times \mathbf{B}$ equation that is parallel to $\hat{\mathbf{e}}_l$ ($l = 1$ or 2) can be written as

$$(-1)^l\frac{\partial^2}{\partial x_1^2}\frac{\partial^2}{\partial x_2^2}\left[\int^{x_1}dx_1' A_1(x_1', x_2, t)-\int^{x_2}dx_2' A_2(x_1, x_2', t)\right]$$
$$=\frac{4\pi}{c}\frac{\partial}{\partial x_l}\sum_{i=1}^{N} Q_i\dot{\gamma}_i^{(l)}\,\delta(x_1-\gamma_i^{(1)})\,\delta(x_2-\gamma_i^{(2)})$$
$$-\frac{1}{c}\frac{\partial^2}{\partial x_l^2}\left[\dot{\varphi}(x_1, x_2, t)+\delta_{1,l}\frac{1}{c}\int^{x_1}dx_1'\ddot{A}_1(x_1', x_2, t)+\delta_{2,l}\frac{1}{c}\int^{x_2}dx_2'\ddot{A}_2(x_1, x_2', t)\right]. \tag{33}$$

The relation $\nabla \cdot \mathbf{A} = 0$ has been used to simplify the $\nabla \cdot \mathbf{E}$ equation, but it has not been used in Eq. (32) to replace $\nabla \times \nabla \times \mathbf{A}$ by $-\nabla^2\mathbf{A}$. The reason is that, although the Coulomb gauge condition expressed by Eq. (19) makes the representation of $\nabla \cdot \mathbf{A}$ vanish, it does not make the representation of $\nabla \cdot \hat{\mathbf{e}}_j\hat{\mathbf{e}}_j \cdot \nabla\nabla \cdot \mathbf{A}$ vanish as it would if the basis functions formed a complete set. The form in which Eq. (33) is written stresses the relation of that equation to Eq. (14) for $n_l \neq 0$.

We now take $\Phi_n(x_1, x_2) = \Phi_{n_1 n_2}(x_1, x_2)$ to be the product of a function of x_1 and a function of x_2,

$$\Phi_{n_1 n_2}(x_1, x_2) = g_{n_1}(x_1)\,h_{n_2}(x_2), \tag{34a}$$

where

$$g_0(x) = h_0(x) \equiv 1.$$

The basis functions for the vector potential are then

$$\mathscr{A}^{(1)}_{n_1 n_2}(x_1, x_2) = \begin{cases} g'_{n_1}(x_1)\, h_{n_2}(x_2), & n_1 \neq 0, \\ h_{n_2}(x_2), & n_1 = 0, \end{cases} \tag{34b}$$

and

$$\mathscr{A}^{(2)}_{n_1 n_2}(x_1, x_2) = \begin{cases} g_{n_1}(x_1)\, h'_{n_2}(x_2), & n_2 \neq 0, \\ g_{n_1}(x_1), & n_2 = 0. \end{cases} \tag{34c}$$

The indices n and m on all matrix quantities will be replaced by $n_1 n_2$ and $m_1 m_2$, respectively.

The representations of the charge and current densities are defined in accordance with Eqs. (15a)–(15c) as

$$P_{n_1 n_2} = \sum_{i=1}^{N} Q_i g_{n_1}(\gamma_i^{(1)})\, h_{n_2}(\gamma_i^{(2)}), \tag{35a}$$

$$J^{(1)}_{n_1 n_2} = -\sum_{i=1}^{N} Q_i \dot{\gamma}_i^{(1)} \frac{\partial}{\partial \gamma_i^{(1)}} g_{n_1}(\gamma_i^{(1)})\, h_{n_2}(\gamma_i^{(2)}) \qquad \text{for} \quad n_1 \neq 0, \tag{35b}$$

$$J^{(1)}_{0, n_2} = -\sum_{i=1}^{N} Q_i \dot{\gamma}_i^{(1)} h_{n_2}(\gamma_i^{(2)}), \tag{35c}$$

$$J^{(2)}_{n_1, 0} = -\sum_{i=1}^{N} Q_i \dot{\gamma}_i^{(2)} g_{n_1}(\gamma_i^{(1)}). \tag{35d}$$

Because each basis function is the product of a function of x_1 and a function of x_2, each of the matrix elements defined by Eqs. (15d)–(15i) and Eq. (23) is the product of a factor related to x_1 and a factor related to x_2. The expressions for the matrix elements will look simpler and be clearer if we take the factorization into account explicitly at this point. There are in fact only *four* distinct factors that are combined in various ways to form the matrix elements. The four distinct factors are

$$u^{(1)}_{nm} = \int dx\, g_n(x)\, g_m(x), \tag{36a}$$

$$u^{(2)}_{nm} = -\int dx\, g_n'(x)\, g_m'(x), \tag{36b}$$

$$v^{(1)}_{nm} = \int dx\, h_n(x)\, h_m(x), \tag{36c}$$

and

$$v^{(2)}_{nm} = -\int dx\, h_n'(x)\, h_m'(x). \tag{36d}$$

$u^{(1)}_{nm}$ and $u^{(2)}_{nm}$ are the representations of unity and d^2/dx^2, respectively, in the space of functions $g_n(x)$; $v^{(1)}_{nm}$ and $v^{(2)}_{nm}$ are the representations of unity and d^2/dx^2, respectively, in the space of functions $h_n(x)$. In terms of these factors, the matrix elements are:

$$T^{(1)}_{n_1n_2;m_1m_2} = u^{(2)}_{n_1m_1}v^{(1)}_{n_2m_2}, \tag{37a}$$

$$T^{(2)}_{n_1n_2;m_1m_2} = u^{(1)}_{n_1m_1}v^{(2)}_{n_2m_2}, \tag{37b}$$

$$T_{n_1n_2;m_1m_2} = u^{(2)}_{n_1m_1}v^{(1)}_{n_2m_2} + u^{(1)}_{n_1m_1}v^{(2)}_{n_2m_2}, \tag{37c}$$

$$W^{(1)}_{n_1n_2;m_1m_2} = u^{(2)}_{n_1m_1}v^{(1)}_{n_2m_2} \qquad \text{unless } n_1 = m_1 = 0, \tag{37d}$$

$$W^{(1)}_{0,n_2;0,m_2} = -Lv^{(1)}_{n_2m_2}, \tag{37e}$$

$$W^{(2)}_{n_1n_2;m_1m_2} = u^{(1)}_{n_1m_1}v^{(2)}_{n_2m_2} \qquad \text{unless } n_2 = m_2 = 0, \tag{37f}$$

$$W^{(2)}_{n_1,0;m_1,0} = -Lu^{(1)}_{n_1m_1}, \tag{37g}$$

$$S^{(l,k)}_{n_1n_2;m_1m_2} = -(-1)^{l+k}u^{(2)}_{n_1m_1}v^{(2)}_{n_2m_2} \qquad \text{unless } n_l = m_k = 0 \text{ and } l = k, \tag{37h}$$

$$S^{(1,1)}_{0,n_2;0,m_2} = Lv^{(2)}_{n_2m_2}, \tag{37i}$$

$$S^{(2,2)}_{n_1,0;m_1,0} = Lu^{(2)}_{n_1m_1}, \tag{37j}$$

$$G_{n_1n_2;m_1m_2} = u^{(1)}_{n_1m_1}v^{(1)}_{n_2m_2}. \tag{37k}$$

Remembering that matrices $u^{(1)}$ and $v^{(1)}$ are representations of unity and that $u^{(2)}$ and $v^{(2)}$ are representations of d^2/dx^2, it is easily verified that $T^{(j)}$, T, $W^{(j)}$, and $S^{(l,k)}$ represent operators of differentiation as stated in Eqs. (17a)–(17e).

For convenience, we rewrite the equations that determine the potentials in the Coulomb gauge. Equation (20) becomes

$$-\sum_{m_1,m_2} T_{n_1n_2;m_1m_2}\alpha_{m_1m_2} = 4\pi P_{n_1n_2}. \tag{38}$$

Equation (21) becomes

$$\sum_{m_1,m_2} T_{n_1n_2;m_1m_2}\dot{\alpha}_{m_1m_2} = 4\pi \sum_{l=1}^{2} J^{(l)}_{n_1n_2}(1 - \delta_{0,n_l}). \tag{39}$$

Equation (14) becomes

$$\sum_{m_1,m_2} \sum_{k=1}^{2} S^{(l,k)}_{n_1n_2;m_1m_2}\beta^{(k)}_{m_1m_2} = \frac{4\pi}{c} J^{(l)}_{n_1n_2} - \frac{1}{c} \sum_{m_1,m_2} \left[\dot{\alpha}_{m_1m_2} T^{(l)}_{m_1m_2;n_1n_2} + \frac{1}{c} W^{(l)}_{n_1n_2;m_1m_2}\ddot{\beta}^{(l)}_{m_1m_2}\right]. \tag{40}$$

Equations (30a) and (30b) become

$$\sum_{m_1,m_2} W^{(l)}_{n_1n_2;m_1m_2}\dot{\beta}^{(l)}_{m_1m_2} = -4\pi c^2\sigma^{(l)}_{n_1n_2} - c \sum_{m_1,m_2} \alpha_{m_1m_2} T^{(l)}_{m_1m_2;n_1n_2} \tag{41a}$$

and

$$\dot{\sigma}^{(l)}_{n_1n_2} = \frac{1}{4\pi} \sum_{m_1,m_2} \sum_{k=1}^{2} S^{(l,k)}_{n_1n_2;m_1m_2}\beta^{(k)}_{m_1m_2} - \frac{1}{c} J^{(l)}_{n_1n_2}. \tag{41b}$$

As was discussed before, either Eqs. (38)–(40) can be solved, or Eqs. (38), (41a), and (41b) can be solved. The gauge condition given by Eq. (19), which must be satisfied initially, is

$$\sum_{m_1,m_2} \sum_{j=1}^{2} T^{(j)}_{n_1n_2;m_1m_2}\beta^{(j)}_{m_1m_2} = 0. \tag{42}$$

As the last step in the example we specialize to a uniform square mesh and a piecewise bilinear representation of the scalar potential. This leads to "area-weighting" for the apportionment of charge. Let the edge length of the elementary cell be Δ, so that the number of cells in each direction is L/Δ. For the functions $g_n(x)$ and $h_n(x)$, we take the local basis functions for one-dimensional, periodic, continuous, piecewise linear functions.[2]

$$g_0(x) = h_0(x) = 1, \tag{43a}$$

$$g_n(x) = h_n(x) = \begin{cases} \frac{1}{\Delta}[x - (n-1)\Delta], & \text{if } (n-1)\Delta \leqslant x \leqslant n\Delta, \\ \frac{1}{\Delta}[(n+1)\Delta - x], & \text{if } n\Delta \leqslant x \leqslant (n+1)\Delta, \\ 0, & \text{otherwise.} \end{cases} \tag{43b}$$

$$\text{for } 1 \leqslant n \leqslant \frac{L}{\Delta} - 1$$

[2] See pp. 326–331 of Ref. [1]. There is a minor difference between the representation used here and that used in Ref. [1]. Here the potential is only assumed to satisfy periodic boundary conditions, whereas in Ref. [1] it is assumed to vanish on the boundary as well.

Note that $\varphi(n_1\Delta, n_2\Delta, t)$ is $(\alpha_{n_1 n_2} + \alpha_{0,n_2} + \alpha_{n_1,0} + \alpha_{0,0})$ with these basis functions, and that $\alpha_{0,0}$ may be set equal to zero. The matrices $u^{(1)}$, $u^{(2)}$, $v^{(1)}$, and $v^{(2)}$ are given by

$$u^{(1)}_{nm} = v^{(1)}_{nm} = \begin{cases} \dfrac{\Delta}{6}[4\delta_{nm} + (\delta_{n-1,m} + \delta_{n+1,m})], & \text{if } n \neq 0 \text{ and } m \neq 0, \\ \Delta, \text{ if } n = 0 \text{ and } m \neq 0, \text{ or if } n \neq 0 \text{ and } m = 0, \\ L, \text{ if } n = m = 0, \end{cases} \tag{44}$$

$$u^{(2)}_{nm} = v^{(2)}_{nm} = \begin{cases} \dfrac{1}{\Delta}[-2\delta_{nm} + (\delta_{n-1,m} + \delta_{n+1,m})], & \text{if } n \neq 0 \text{ and } m \neq 0, \\ 0, \quad \text{if } n = 0 \text{ or } m = 0. \end{cases} \tag{45}$$

An illustrative schematic representation of the matrices $T^{(1)}$, T, $S^{(1,1)}$, and G in the interior of the mesh when n_1, n_2, m_1, and m_2 are all nonzero is

$$T^{(1)} \to \frac{1}{6}\begin{pmatrix} 1 & -2 & 1 \\ 4 & -8 & 4 \\ 1 & -2 & 1 \end{pmatrix}, \qquad T \to \frac{1}{3}\begin{pmatrix} 1 & 1 & 1 \\ 1 & -8 & 1 \\ 1 & 1 & 1 \end{pmatrix},$$

$$S^{(1,1)} \to \frac{1}{\Delta^2}\begin{pmatrix} -1 & 2 & -1 \\ 2 & -4 & 2 \\ -1 & 2 & -1 \end{pmatrix}, \qquad G \to \frac{\Delta^2}{36}\begin{pmatrix} 1 & 4 & 1 \\ 4 & 16 & 4 \\ 1 & 4 & 1 \end{pmatrix}.$$

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