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VARIATIONAL ALGORITHMS FOR NUMERICAL SIMULATION OF COLLISIONLESS PLASMA WITH POINT PARTICLES INCLUDING MAGNETIC INTERACTIONS

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VARIATIONAL ALGORITHMS FOR NUMERICAL SIMULATION OF COLLISIONLESS PLASMA WITH POINT PARTICLES INCLUDING MAGNETIC INTERACTIONS

by

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ABSTRACT

Energy- and charge-conserving algorithms for numerical simulation of collisionless plasma with point particles, including magnetic 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, exactly time-reversible difference scheme. An example is presented for a cartesian geometry.

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I. INTRODUCTION

It has been shown[1,2] that the usual particle-in-cell (PIC) or cloud-in-cell (CIC) scheme for Poisson's equation that is used for simulating electrostatic oscillations in collisionless plasma[3,4] can be derived as a special case from Hamilton's variational principle. This is achieved by simply requiring that the scalar potential be a piecewise linear function of each cartesian coordinate. The "area-weighting" feature of the PIC scheme and a particular finite-difference form of the Laplacian operator are then consequences of the variational principle. If the potential is computed from the variationally derived algorithm and the particles are moved in the exact electric field corresponding to that potential, then energy is conserved exactly in the limit of zero time step for any representation of the potential, piecewise linear or otherwise. That is, energy conservation is not destroyed by spatial differencing of Poisson's equation according to the variational prescription.

In this paper, the variational principle is used to obtain natural generalizations of the PIC scheme that are appropriate for numerically simulating collisionless plasma including magnetic interactions. This is motivated by the success of the linear PIC scheme for treating electrostatic oscillations. Morse and Nielson have also devised generalizations, which they used to study the nonlinear evolution of the Weibel instability[5]. The most effective of the three methods that they used, a method based on the electromagnetic potentials instead of on the electric and magnetic fields, is related to the variational algorithm given in this paper as an example.

There are three basic features of the variational algorithms for the full Maxwell's equations that should be noted. Firstly, spatial differencing of the Maxwell equations implied by these algorithms does not destroy energy conservation[1,2]. Secondly, by choosing the representation of the vector potential appropriately with respect to the representation of the scalar potential, we obtain a charge conservation theorem. Thirdly, the equations for the potentials can be cast into a system of first-order differential equations in time that are suitable for advancing the potentials with a time-centered, time-reversible difference scheme.

In Section II the formulas for numerical simulation with these charge-conserving algorithms are derived for curvilinear coordinates and the charge conservation is demonstrated. In Section III the equations appropriate for

the time-reversible difference scheme are derived. In Section IV the formulas are simplified to apply to the cartesian geometry considered by Morse and Nielson for the Weibel instability, 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 number of particles in V is N. The position vector, charge, and mass of particle i are $\underset{\sim}{R}_i$, Q_i, and M_i, respectively. The coordinate system is that associated with three orthogonal unit vectors $\hat{\underset{\sim}{e}}_j(\underset{\sim}{r})$. The unit vectors form a right-handed set: $\hat{\underset{\sim}{e}}_k = \hat{\underset{\sim}{e}}_i \times \hat{\underset{\sim}{e}}_j$ when (i, j, k) is a cyclic permutation of (1, 2, 3). The coordinate of $\underset{\sim}{r}$ associated with $\hat{\underset{\sim}{e}}_j$ is x_j. The derivative of $\underset{\sim}{r}$ with respect to x_j is given as usual in terms of a function $h_j(\underset{\sim}{r})$:

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

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

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

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

$$\varphi(\underset{\sim}{r},t) = \varphi_o(\underset{\sim}{r},t) + \sum_n \alpha_n(t)\Phi_n(\underset{\sim}{r}) \tag{1}$$

and

$$\underset{\sim}{A}(\underset{\sim}{r},t) = \underset{\sim}{A}_o(\underset{\sim}{r},t) + \sum_{j=1}^{3} \hat{\underset{\sim}{e}}_j(\underset{\sim}{r}) \sum_m \beta_m^{(j)}(t)\, G_m^{(j)}(\underset{\sim}{r}), \tag{2}$$

where the set of functions Φ_n and the three sets of functions $G_m^{(j)}$, one for each j, are linearly independent. The functions φ_o and $\underset{\sim}{A}_o$ 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 $\underset{\sim}{A}$, thus making $(\varphi - \varphi_0)$ and $(\underset{\sim}{A} - \underset{\sim}{A}_0)$ either vanish on the boundary or satisfy periodic boundary conditions. The specified charge and current densities associated with φ_0 and $\underset{\sim}{A}_0$ will be denoted by $\rho_0(\underset{\sim}{r},t)$ and $\underset{\sim}{j}_0(\underset{\sim}{r},t)$. The basis functions Φ_n and $G_m^{(j)}$ must separately either vanish on the boundary of V or satisfy periodic boundary conditions.

The Lagrangian is [1]

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

where

$$A_{oj}(\underset{\sim}{r},t) = \hat{\underset{\sim}{e}}_j(\underset{\sim}{r}) \cdot \underset{\sim}{A}_0(\underset{\sim}{r},t).$$

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

$$
\begin{aligned}
& \frac{d}{dt} \left\{ M_i h_j^2(\underset{\sim}{R}_i)\, \dot{\gamma}_i^{(j)} + \frac{1}{c} Q_i\, h_j(\underset{\sim}{R}_i) A_j(\underset{\sim}{R}_i,t) \right\} \\
& = \frac{1}{2} M_i \sum_{k=1}^{3} (\dot{\gamma}_i^{(k)})^2 \frac{\partial}{\partial \gamma_i^{(j)}} h_k^2(\underset{\sim}{R}_i)
\end{aligned}
$$

$$- Q_i \frac{\partial}{\partial \gamma_i^{(j)}} \varphi(\underset{\sim}{R}_i,t) + \frac{1}{c} Q_i \sum_{k=1}^{3} \dot{\gamma}_i^{(k)} \frac{\partial}{\partial \gamma_i^{(j)}} \left[h_k(\underset{\sim}{R}_i) A_k(\underset{\sim}{R}_i,t) \right], \qquad (4)$$

where

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

The Euler-Lagrange equation for α_n is

$$\int_V d^3\underset{\sim}{r} \left[\sum_m \alpha_m \underset{\sim}{\nabla} \Phi_m(\underset{\sim}{r}) + \frac{1}{c} \sum_{j,m} \dot{\beta}_m^{(j)} \hat{\underset{\sim}{e}}_j(\underset{\sim}{r}) G_m^{(j)}(\underset{\sim}{r}) \right] \cdot \underset{\sim}{\nabla} \Phi_n(\underset{\sim}{r})$$

$$= 4\pi \sum_{i=1}^{N} Q_i \Phi_n(\underset{\sim}{R}_i), \qquad (5)$$

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

$$\int_V d^3\underset{\sim}{r} \left[\underset{\sim}{\nabla} \times \sum_{k,m} \beta_m^{(k)} \hat{\underset{\sim}{e}}_k(\underset{\sim}{r}) G_m^{(k)}(\underset{\sim}{r}) \right] \cdot \underset{\sim}{\nabla} \times \left[\hat{\underset{\sim}{e}}_j(\underset{\sim}{r}) G_n^{(j)}(\underset{\sim}{r}) \right]$$

$$= \frac{4\pi}{c} \sum_{i=1}^{N} Q_i \dot{\gamma}_i^{(j)} h_j(\underset{\sim}{R}_i) G_n^{(j)}(\underset{\sim}{R}_i)$$

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

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

The next step is to interpret Eqs.(5) and (6) by analogy with Maxwell's equations and to derive a charge conservation theorem. Equations (5) and (6) can be derived directly from the Maxwell $\underset{\sim}{\nabla} \cdot \underset{\sim}{E}$ equation,

$$- \underset{\sim}{\nabla} \cdot \left[\sum_m \alpha_m \underset{\sim}{\nabla} \Phi_m(\underset{\sim}{r}) + \frac{1}{c} \sum_{j,m} \dot{\beta}_m^{(j)} \hat{\underset{\sim}{e}}_j(\underset{\sim}{r}) G_m^{(j)}(\underset{\sim}{r}) \right]$$

$$= 4\pi \sum_{i=1}^{N} Q_i \delta(\underset{\sim}{r} - \underset{\sim}{R}_i), \qquad (7)$$

and the Maxwell $\nabla \times B$ equation,

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

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

by forming the inner product of the $\nabla \cdot E$ equation with Φ_n and the inner product of the $\nabla \times B$ equation with $\hat{e}_j G_n^{(j)}$. That is, Eq.(5) can be obtained by multiplying the $\nabla \cdot E$ equation by $\Phi_n(r)$ and integrating over V, and Eq.(6) can be obtained by scalar multiplying the $\nabla \times B$ equation with $\hat{e}_j(r) G_n^{(j)}(r)$ and integrating over V. However, this is unsatisfactory from the standpoint of achieving a unified interpretation of the terms of Eqs. (5) and (6) by associating them with terms in the $\nabla \cdot E$ and $\nabla \times B$ equations. The reason is that the inner product of the $\nabla \times B$ equation is not taken with the same function as the inner product of the $\nabla \cdot E$ equation, so that the representation of the $\nabla \times B$ equation provided by Eq.(6) is not in the same space as the representation of the $\nabla \cdot E$ equation provided by Eq.(5); there is not a simple connection between terms in Eq.(6) and terms in Eq.(5). A remedy for this that leads to a charge conservation theorem is to define $G_n^{(j)}$ in terms of Φ_n by

$$G_n^{(j)}(r) = \hat{e}_j(r) \cdot \nabla \Phi_n(r)$$

$$= \frac{1}{h_j(r)} \frac{\partial}{\partial x_j} \Phi_n(r). \qquad (9)$$

With $G_n^{(j)}$ so defined, Eq.(6) can be viewed as a representation of the divergence of that part of the $\nabla \times B$ equation which is parallel to $\hat{e}_j$, and the representation is in the same space in which Eq.(5) is a representation of the $\nabla \cdot E$ equation. The divergence of that part of the $\nabla \times B$ equation parallel to $\hat{e}_j$ is

$$\nabla \cdot \left\{ e_j(r) \hat{e}_j(r) \cdot \left[\nabla \times \nabla \times \sum_{k,m} \beta_m^{(k)} \hat{e}_k(r) G_m^{(k)}(r) \right] \right\}$$

$$= \frac{4\pi}{c} \underset{\sim}{\nabla} \cdot \left[\hat{\underset{\sim}{e}}_j(\underset{\sim}{r})\hat{\underset{\sim}{e}}_j(\underset{\sim}{r}) \cdot \sum_{i=1}^{N} Q_i \dot{\underset{\sim}{R}}_i \delta(\underset{\sim}{r}-\underset{\sim}{R}_i) \right]$$

$$- \frac{1}{c} \underset{\sim}{\nabla} \cdot \left\{ \hat{\underset{\sim}{e}}_j(\underset{\sim}{r})\hat{\underset{\sim}{e}}_j(\underset{\sim}{r}) \cdot \left[\sum_{m} \dot{\alpha}_m \underset{\sim}{\nabla} \Phi_m(\underset{\sim}{r}) + \frac{1}{c} \sum_{k,m} \ddot{\beta}_m^{(k)} \hat{\underset{\sim}{e}}_k(\underset{\sim}{r}) \Gamma_m^{(k)}(\underset{\sim}{r}) \right] \right\}. \quad (10)$$

To obtain Eq.(6) we multiply Eq.(10) by $\Phi_n(\underset{\sim}{r})$, integrate over V, and use the partial integration formulas

$$\int_V d^3\underset{\sim}{r}\, \Phi_n \underset{\sim}{\nabla} \cdot [\hat{e}_j \hat{e}_j \cdot \underset{\sim}{D}] = - \int_V d^3\underset{\sim}{r}\, [\hat{e}_j \cdot \underset{\sim}{D}]\, G_n^{(j)}$$

and

$$\int_V d^3\underset{\sim}{r}\, \underset{\sim}{B} \cdot \underset{\sim}{\nabla} \times \underset{\sim}{G} = \int_V d^3\underset{\sim}{r}\, \underset{\sim}{G} \cdot \underset{\sim}{\nabla} \times \underset{\sim}{B} \ .$$

The expression for the vector potential is now

$$\underset{\sim}{A}(\underset{\sim}{r},t) = \underset{\sim}{A}_0(\underset{\sim}{r},t) + \sum_{j=1}^{3} \hat{\underset{\sim}{e}}_j(\underset{\sim}{r}) \sum_{m} \beta_m^{(j)}(t) \frac{1}{h_j(\underset{\sim}{r})} \frac{\partial}{\partial x_j} \Phi_m(\underset{\sim}{r}), \quad (11)$$

and its curl is

$$\underset{\sim}{\nabla} \times \underset{\sim}{A}(\underset{\sim}{r},t) = \underset{\sim}{\nabla} \times \underset{\sim}{A}_0(\underset{\sim}{r},t)$$
$$+ \sum_{i=1}^{3} \hat{\underset{\sim}{e}}_i(\underset{\sim}{r}) \left[\beta_m^{(k)} - \beta_m^{(j)} \right] \frac{1}{h_j(\underset{\sim}{r}) h_k(\underset{\sim}{r})} \frac{\partial^2}{\partial x_j \partial x_k} \Phi_m(\underset{\sim}{r}), \quad (12)$$

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

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

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

and

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

where

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

$$J_n^{(\ell)} = - \sum_{i=1}^{N} Q_i \, \dot{\gamma}_i^{(\ell)} \, h_\ell(\underset{\sim}{R}_i) \, G_n^{(\ell)}(\underset{\sim}{R}_i)$$

$$= - \sum_{i=1}^{N} Q_i \boldsymbol{\gamma}_i^{(\ell)} \frac{\partial}{\partial \boldsymbol{\gamma}_i^{(\ell)}} \Phi_n(\underset{\sim}{R}_i) \, , \tag{15b}$$

$$T_{n;m}^{(j)} = - \int_V d^3 \underset{\sim}{r} [\underset{\sim}{\nabla} \Phi_n(\underset{\sim}{r})] \cdot \hat{\underset{\sim}{e}}_j(\underset{\sim}{r}) \hat{\underset{\sim}{e}}_j(\underset{\sim}{r}) \cdot [\underset{\sim}{\nabla} \Phi_m(\underset{\sim}{r})] \, , \tag{15c}$$

$$T_{n;m} = \sum_{j=1}^{3} T_{n;m}^{(j)} \, , \tag{15d}$$

and

$$S_{n;m}^{(\ell,k)} = - \int_V d^3 \underset{\sim}{r} \left\{ \underset{\sim}{\nabla} \times [\hat{\underset{\sim}{e}}_\ell(r) G_n^{(\ell)}(\underset{\sim}{r})] \right\} \cdot \left\{ \underset{\sim}{\nabla} \times [\hat{\underset{\sim}{e}}_k(\underset{\sim}{r}) G_m^{(k)}(\underset{\sim}{r})] \right\}$$

$$= - \int_V d^3 \underset{\sim}{r} \left\{ \underset{\sim}{\nabla} \times [\hat{\underset{\sim}{e}}_\ell(\underset{\sim}{r}) \hat{\underset{\sim}{e}}_\ell(\underset{\sim}{r}) \cdot \underset{\sim}{\nabla} \Phi_n(\underset{\sim}{r})] \right\} \cdot \left\{ \underset{\sim}{\nabla} \times [\hat{\underset{\sim}{e}}_k(\underset{\sim}{r}) \hat{\underset{\sim}{e}}_k(\underset{\sim}{r}) \cdot \underset{\sim}{\nabla} \Phi_m(\underset{\sim}{r})] \right\} \cdot \tag{15e}$$

The sum over ℓ of $S_{n;m}^{(\ell,k)}$ vanishes because $\underset{\sim}{\nabla} \times \underset{\sim}{\nabla} \Phi_n(\underset{\sim}{r})$ vanishes.

Equations (13) and (14) are representations of Eqs. (5) and (10), respectively. The set of coefficients α_n is a representation of the self-consistent scalar potential $[\varphi(\underset{\sim}{r},t) - \varphi_o(\underset{\sim}{r},t)]$, and the set of coefficients $\beta_n^{(j)}$ is a representation of

$$\int_{\underset{\sim}{r}_o}^{\underset{\sim}{r}} d\underset{\sim}{r}' \cdot [\underset{\sim}{A}(\underset{\sim}{r}',t) - \underset{\sim}{A}_o(\underset{\sim}{r}',t)]$$

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

$$= \sum_n \beta_n^{(j)}(t) \, [\Phi_n(\underset{\sim}{r}) - \Phi_n(\underset{\sim}{r}_o)] \, , \tag{16}$$

where the integral is a line integral taken between a fixed point $\underset{\sim}{r}_o$ to a variable point $\underset{\sim}{r}$ along a path parallel to $\hat{\underset{\sim}{e}}_j(\underset{\sim}{r}')$. It is to be noted that the numbers $\beta_n^{(j)}$ do not represent $[\underset{\sim}{A}(\underset{\sim}{r},t) - \underset{\sim}{A}_o(\underset{\sim}{r},t)]$ in this space, and

that $\hat{\underset{\sim}{e}}_j(\underset{\sim}{x}) \cdot [\underset{\sim}{A}(\underset{\sim}{x},t) - \underset{\sim}{A}_0(\underset{\sim}{x},t)]$ is obtained from the integral in Eq.(16) by operation with $\hat{\underset{\sim}{e}}_j(\underset{\sim}{r}) \cdot \underset{\sim}{\nabla}$. The matrices $T^{(j)}$, T, and $S^{(\ell,k)}$ are representations of differentiation operators according to the scheme

$$T^{(j)} \leftrightarrow \underset{\sim}{\nabla} \cdot \hat{\underset{\sim}{e}}_j \hat{\underset{\sim}{e}}_j \cdot \underset{\sim}{\nabla}, \tag{17a}$$

$$T \leftrightarrow \underset{\sim}{\nabla} \cdot \underset{\sim}{\nabla} , \tag{17b}$$

and

$$S^{(\ell,k)} \leftrightarrow \underset{\sim}{\nabla} \cdot \hat{\underset{\sim}{e}}_\ell \hat{\underset{\sim}{e}}_\ell \cdot \underset{\sim}{\nabla} \times \underset{\sim}{\nabla} \times \hat{\underset{\sim}{e}}_k \hat{\underset{\sim}{e}}_k \cdot \underset{\sim}{\nabla}. \tag{17c}$$

The set of numbers P_n represents the charge density due to the particles; and the set of numbers $J_n^{(\ell)}$ for fixed ℓ represents the divergence of that part of the current density due to the particles that is parallel to $\hat{\underset{\sim}{e}}_\ell$.

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

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

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 those equations as representations of the Maxwell equations. On the other hand, because it is obviously true as a result of the definition of P_n and $J_n^{(\ell)}$, 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 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.

The representation of the Coulomb gauge condition is

$$\int_V d^3\underset{\sim}{r}\, \Phi_n(\underset{\sim}{r})\, \underset{\sim}{\nabla} \cdot \sum_m \sum_{j=1}^{3} \beta_m^{(j)}\, \hat{\underset{\sim}{e}}_j(\underset{\sim}{r})\, G_m^{(j)}(\underset{\sim}{r}) = 0$$

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

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

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.

The Lorentz gauge condition is represented by

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

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

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

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:

$$L = \sum_{i=1}^{N} \left\{ \frac{1}{2} M_i \sum_{j=1}^{3} h_j^2(\underset{\sim}{R}_i)(\dot{\gamma}_i^{(j)})^2 - Q_i \varphi_o(\underset{\sim}{R}_i,t) + \frac{1}{c} Q_i \sum_{j=1}^{3} h_j(\underset{\sim}{R}_i)\, \dot{\gamma}_i^{(j)} A_{oj}(\underset{\sim}{R}_i,t) \right\}$$

$$- \sum_n \alpha_n P_n - \frac{1}{c} \sum_n \sum_{\ell=1}^{3} \beta_n^{(\ell)} J_n^{(\ell)}$$

$$- \frac{1}{8\pi} \sum_{n,m} \left\{ \alpha_n T_{n;m} \alpha_m + \sum_{j=1}^{3} \left[\frac{2}{c} \alpha_n T_{n;m}^{(j)} \dot{\beta}_m^{(j)} + \frac{1}{c^2} \dot{\beta}_n^{(j)} T_{n;m}^{(j)} \dot{\beta}_m^{(j)} \right] \right\}$$

$$+ \frac{1}{8\pi} \sum_{n,m} \sum_{j,k=1}^{3} \beta_n^{(j)} S_{n;m}^{(j,k)} \beta_m^{(k)}. \qquad (25)$$

The canonical momenta and Hamiltonian are

$$\tau_i^{(j)} = \frac{\partial L}{\partial \dot{\gamma}_i^{(j)}}$$

$$= M_i h_j^2(\underset{\sim}{R}_i)\, \dot{\gamma}_i^{(j)} + \frac{1}{c} Q_i h_j(\underset{\sim}{R}_i) A_j(\underset{\sim}{R}_i,t), \qquad (26a)$$

$$\sigma_n^{(\ell)} = \frac{\partial L}{\partial \dot{\beta}_n^{(\ell)}}$$

$$= - \frac{1}{4\pi c} \sum_m T_{n;m}^{(j)} \left[\frac{1}{c} \dot{\beta}_m^{(\ell)} + \alpha_m \right], \qquad (26b)$$

and

$$H = \sum_{i=1}^{N} \sum_{j=1}^{3} \dot{\gamma}_i^{(j)} \tau_i^{(j)} + \sum_n \sum_{\ell=1}^{3} \dot{\beta}_n^{(\ell)} \sigma_n^{(\ell)} - L$$

$$= \sum_{i=1}^{N} \left\{ \frac{1}{2M_i} \sum_{j=1}^{3} \left[\frac{1}{h_j(\underset{\sim}{R}_i)} \tau_i^{(j)} - \frac{1}{c} Q_i A_{oj}(\underset{\sim}{R}_i,t) - \frac{1}{c} Q_i \sum_n \beta_n^{(j)} G_n^{(j)}(\underset{\sim}{R}_i) \right]^2 + Q_i \varphi_o(\underset{\sim}{R}_i,t) + Q_i \sum_n \alpha_n \Phi_n(\underset{\sim}{R}_i) \right\}$$

$$- 2\pi c^2 \sum_{n,m} \sum_{j=1}^{3} \sigma_n^{(j)} T_{n;m}^{(j)-1} \sigma_m^{(j)} - c \sum_n \sum_{j=1}^{3} \alpha_n \sigma_n^{(j)}$$

$$- \frac{1}{8\pi} \sum_{n,m} \sum_{j,k=1}^{3} \beta_n^{(j)} S_{n;m}^{(j,k)} \beta_m^{(k)} , \qquad (27)$$

where

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

The Hamiltonian equations are

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

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

$$c \sum_{j=1}^{3} \sigma_n^{(j)} = P_n , \qquad (29)$$

$$\sum_m T_{n;m}^{(\ell)} \dot{\beta}_m^{(\ell)} = - 4\pi c^2 \sigma_n^{(\ell)} - c \sum_m T_{n;m}^{(\ell)} \alpha_m , \qquad (30a)$$

and

$$\dot{\sigma}_n^{(\ell)} = \frac{1}{4\pi} \sum_m \sum_{k=1}^{3} S_{n;m}^{(\ell,k)} \beta_m^{(k)} - \frac{1}{c} J_n^{(\ell)} . \qquad (30b)$$

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 reversible 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 $\beta_n^{(\ell)}$ and $\sigma_n^{(\ell)}$. The quantities P_n, α_n, and $\sigma_n^{(\ell)}$ are defined at integral multiples of the time step, whereas $J_n^{(\ell)}$ and $\beta_n^{(\ell)}$ 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 $\beta_n^{(\ell)}$ and $\sigma_n^{(\ell)}$ in time, and the scheme will be exactly reversible. If the particle transport, either with Eq. (4) or Eqs. (28a) and (28b), is performed with a reversible scheme as Morse and Nielson have done[5], 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 cartesian geometry that was used for simulating the Weibel instability[5]. Each function $h_j(\underset{\sim}{r})$ 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 $\underset{\sim}{\nabla}\cdot\underset{\sim}{E}$ equation is

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

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

$$(-1)^\ell \frac{\partial^2}{\partial x_1^2}\,\frac{\partial^2}{\partial x_2^2}\left[\int^{x_1} dx_1'\, A_1(x_1', x_2, t) - \int^{x_2} dx_2'\, A_2(x_1, x_2', t)\right]$$

$$= \frac{4\pi}{c}\frac{\partial}{\partial x_\ell} \sum_{i=1}^{N} Q_i\, \dot{\gamma}_i^{(\ell)}\ \delta(x_1 - \gamma_i^{(1)})\,\delta\,(x_2 - \gamma_i^{(2)})$$

$$-\frac{1}{c}\,\frac{\partial^2}{\partial x_\ell^2}\left[\dot{\varphi}(x_1, x_2, t) + \delta_{1,\ell}\frac{1}{c}\int^{x_1} dx_1'\,\ddot{A}_1(x_1', x_2, t) + \delta_{2,\ell}\frac{1}{c}\int^{x_2} dx_2'\,\ddot{A}_2(x_1, x_2', t)\right] \qquad (32)$$

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

The basis functions $\Phi_n(\underset{\sim}{r})$ depend on x_1 and x_2, but not on x_3. Since nothing depends on x_3, we consider the system to be periodic in x_3 with unit period, so that all integrals over x_3 simply give a factor of unity and can be ignored. The matrices associated with the x_3 coordinate vanish:

$$T_{n;m}^{(3)} = S_{n;m}^{(3,k)} = S_{n;m}^{(k,3)} = J_n^{(3)} = 0. \qquad (33)$$

We now let $\Phi_n(x_1, x_2)$ be a product of a function of x_1 with a function of x_2 in the form

$$\Phi_n(x_1, x_2) \rightarrow g_{n_1}(x_1) g_{n_2}(x_2), \tag{34}$$

and modify the notation by replacing the indices n and m on α_n, $\beta_n^{(j)}$, $\sigma_n^{(\ell)}$, P_n, $J_n^{(\ell)}$, $T_{n;m}^{(j)}$, $T_{n;m}$, $S_{n;m}^{(\ell,k)}$ and $G_{n;m}$ by $n_1 n_2$ and $m_1 m_2$, respectively. The matrices are then defined by

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

$$J_{n_1 n_2}^{(\ell)} = - \sum_{i=1}^{N} Q_i \, \dot{\gamma}_i^{(\ell)} \, \frac{\partial}{\partial \gamma_i^{(\ell)}} g_{n_1}(\gamma_i^{(1)}) \, g_{n_2}(\gamma_i^{(2)}), \tag{35b}$$

$$T_{n_1 n_2; m_1 m_2}^{(j)} = - \int dx_1 dx_2 \left[\frac{\partial}{\partial x_j} g_{n_1}(x_1) \; g_{n_2}(x_2) \right] \left[\frac{\partial}{\partial x_j} g_{m_1}(x_1) g_{m_2}(x_2) \right], \tag{35c}$$

$$T_{n_1 n_2; m_1 m_2} = T_{n_1 n_2; m_1 m_2}^{(1)} + T_{n_1 n_2; m_1 m_2}^{(2)}, \tag{35d}$$

$$S_{n_1 n_2; m_1 m_2}^{(\ell,k)}$$

$$= - \int dx_1 \, dx_2 \left[\underset{\sim}{\nabla} \times \hat{\underset{\sim}{e}}_\ell \frac{\partial}{\partial x_\ell} \; g_{n_1}(x_1) \; g_{n_2}(x_2) \right] \cdot \left[\underset{\sim}{\nabla} \times \hat{\underset{\sim}{e}}_k \frac{\partial}{\partial x_k} g_{m_1}(x_1) g_{m_2}(x_2) \right], \tag{35e}$$

and

$$G_{n_1 n_2; m_1 m_2} = \int dx_1 \, dx_2 \, g_{n_1}(x_1) \, g_{n_2}(x_2) g_{m_1}(x_1) g_{m_2}(x_2). \tag{35f}$$

with the symmetry relations

$$T_{n_1 n_2; m_1 m_2}^{(j)} = T_{m_1 m_2; n_1 n_2}^{(j)}, \tag{36a}$$

$$T_{n_1 n_2; m_1 m_2}^{(1)} = T_{n_2 n_1; m_2 m_1}^{(2)}, \tag{36b}$$

$$S_{n_1 n_2; m_1 m_2}^{(\ell,k)} = S_{m_1 m_2; n_1 n_2}^{(k,\ell)} = S_{n_2 n_1; m_2 m_1}^{(\ell,k)}, \tag{36c}$$

$$S_{n_1 n_2; m_1 m_2}^{(1,1)} = S_{n_1 n_2; m_1 m_2}^{(2,2)}, \tag{36d}$$

and

$$S^{(1,2)}_{n_1 n_2;m_1 m_2} = - S^{(1,1)}_{n_1 n_2;m_1 m_2} \quad . \tag{36e}$$

With this notation, the basic equations for the problem, Eqs. (20), (14), (30a), and (30b), can be written as

$$- \sum_{m_1,m_2} T_{n_1 n_2;m_1 m_2} \alpha_{m_1 m_2} = 4\pi P_{n_1 n_2}, \tag{37}$$

$$(-1)^{\ell} \sum_{m_1 m_2} S^{(1,1)}_{n_1 n_2;m_1 m_2} \left[\beta^{(2)}_{m_1 m_2} - \beta^{(1)}_{m_1 m_2} \right]$$

$$= \frac{4\pi}{c} J^{(\ell)}_{n_1 n_2} - \frac{1}{c} \sum_{m_1,m_2} T^{(\ell)}_{n_1 n_2;m_1 m_2} \left[\dot{\alpha}_{m_1 m_2} + \frac{1}{c} \ddot{\beta}^{(\ell)}_{m_1 m_2} \right], \tag{38}$$

$$\sum_{m_1,m_2} T^{(\ell)}_{n_1 n_2;m_1 m_2} \dot{\beta}^{(\ell)}_{m_1 m_2} = - 4\pi c^2 \sigma^{(\ell)}_{n_1 n_2} - c \sum_{m_1,m_2} T_{n_1 n_2;m_1 m_2} \alpha_{m_1 m_2}, \tag{39a}$$

and

$$\dot{\sigma}^{(\ell)}_{n_1 n_2} = (-1)^{\ell} \frac{1}{4\pi} \sum_{m_1,m_2} S^{(1,1)}_{n_1 n_2;m_1 m_2} \left[\beta^{(2)}_{m_1 m_2} - \beta^{(1)}_{m_1 m_2} \right] - \frac{1}{c} J^{(\ell)}_{n_1 n_2} \quad . \tag{39b}$$

The matrices $T^{(\ell)}$, T, and $S^{(1,1)}$ represent operators according to the scheme

$$T^{(\ell)} \longleftrightarrow \frac{\partial^2}{\partial x_\ell^2} \quad , \tag{40a}$$

$$T \longleftrightarrow \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \quad , \tag{40b}$$

and

$$S^{(1,1)} \longleftrightarrow - \frac{\partial^2}{\partial x_1^2} \frac{\partial^2}{\partial x_2^2} \quad . \tag{40c}$$

As the last step we specialize to the case of periodic boundary conditions in x_1 and x_2 over a square the length of whose side is λ, and represent the scalar potential as a piecewise bilinear function on a square mesh. The edge length of the elementary cell is Δ. The one-dimensional local basis functions for this representation are [6]

$$g_n(x) \quad \text{for } 1 \leq n \leq \frac{\lambda}{\Delta} - 1 = \begin{cases} \frac{1}{\Delta}\,[x - (n-1)\Delta], & \text{if } (n-1)\Delta \leq x \leq n\Delta \\ \frac{1}{\Delta}\,[(n+1)\Delta - x], & \text{if } n\Delta \leq x \leq (n+1)\Delta \end{cases} \tag{41a}$$

$$g_{\lambda/\Delta}(x) = \begin{cases} \frac{1}{\Delta}\,(\Delta - x), & \text{if } 0 \leq x \leq \Delta \\ \frac{1}{\Delta}\,(x - \lambda + \Delta), & \text{if } (\lambda - \Delta) \leq x \leq \lambda. \end{cases} \tag{41b}$$

$g_n(x)$ vanishes for other values of x. The matrices $T^{(1)}$, T, $S^{(1,1)}$, and G are then given by:

$$T^{(1)}_{n_1 n_2; m_1 m_2} = -\left[2\delta_{n_1 m_1} - (\delta_{n_1, m_1+1} + \delta_{n_1+1, m_1})\right]\left[\frac{2}{3}\,\delta_{n_2 m_2} + \frac{1}{6}\,(\delta_{n_2, m_2+1} + \delta_{n_2+1, m_2})\right], \tag{42a}$$

$$T_{n_1 n_2; m_1 m_2} = -\left[3\delta_{n_1 m_1}\delta_{n_2 m_2} - \frac{1}{3}\,(\delta_{n_1 m_1} + \delta_{n_1, m_1+1} + \delta_{n_1+1, m_1})(\delta_{n_2 m_2} + \delta_{n_2, m_2+1} + \delta_{n_2+1, m_2})\right], \tag{42b}$$

$$S^{(1,1)}_{n_1 n_2; m_1 m_2} = -\frac{1}{\Delta^2}\left[2\delta_{n_1 m_1} - (\delta_{n_1, m_1+1} + \delta_{n_1+1, m_1})\right]\left[2\delta_{n_2 m_2} - (\delta_{n_2, m_2+1} + \delta_{n_2+1, m_2})\right], \tag{42c}$$

$$G_{n_1 n_2; m_1 m_2} = \Delta^2\left[\frac{2}{3}\,\delta_{n_1 m_1} + \frac{1}{6}\,(\delta_{n_1, m_1+1} + \delta_{n_1+1, m_1})\right]\left[\frac{2}{3}\,\delta_{n_2 m_2} + \frac{1}{6}\,(\delta_{n_2, m_2+1} + \delta_{n_2+1, m_2})\right]. \tag{42c}$$

These formulas are valid for all values of n_1, n_2, m_1, and m_2 between 1 and λ/Δ, inclusive, if $\delta_{n,(\lambda/\Delta)+1}$ and $\delta_{(\lambda/\Delta)+1,n}$ are replaced by $\delta_{n,1}$ and $\delta_{1,n}$, respectively. A useful schematic representation of the matrices in the interior of the mesh 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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6 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.