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Energy and Momentum Conservation Theorems for Electrostatic Simulations

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An energy and momentum conservation theorem is derived for electrostatic particle simulations. These allow verification of how well a code is conserving energy and momentum in the presence of external sources.

I. INTRODUCTION

Electrostatic particle simulations, which retain only the Coulomb force of interaction between particles, are useful approximations in many problems. From the complete set of Maxwell's equations, one can derive [1, 2] an energy and momentum flux theorem for the fields

$$\nabla \cdot \mathbf{S} + \frac{\partial}{\partial t}\left(\frac{E^2 + B^2}{8\pi}\right) = -\mathbf{j} \cdot \mathbf{E} \tag{1}$$

$$\nabla \cdot \mathbf{T} - \frac{\partial}{\partial t}\left(\frac{\mathbf{S}}{c^2}\right) = \rho\mathbf{E} + \mathbf{j} \times \mathbf{B}/c \tag{2}$$

where $\mathbf{S} \equiv (c/4\pi)\,\mathbf{E} \times \mathbf{B}$ is the Poynting vector, and

$$\mathbf{T} \equiv \frac{1}{4\pi}\left[\mathbf{EE} + \mathbf{BB} - \frac{1}{2}\,(\mathbf{E} \cdot \mathbf{E} + \mathbf{B} \cdot \mathbf{B})\mathbf{I}\right] \tag{3}$$

is the Maxwell stress tensor and $\mathbf{I}$ is the unit tensor.

Since in electrostatics, $\mathbf{B}$ does not appear in the field equations, it is not immediately clear if the Poynting vector has any meaning. In an earlier paper [3], it was shown that one could indeed derive an energy flux vector in the electrostatic limit. In this paper, an analogous momentum conservation theorem will be derived. These two laws, when combined with the flow of particle energy and momentum, allow one to account completely for energy and momentum flow in electrostatic systems. One can therefore determine if a simulation model is properly conserving these quantities even in the presence of external sources, such as one may have in the

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simulation of RF heating or current drive. This is important because even in models using momentum or energy conserving algorithms [4], these quantities are not conserved when external sources are driving the system. Unlike much of the earlier work on energy and power [5, 6], no linearization has been employed.

II. Energy and Momentum Flow in Electrostatic Fields

The energy flow relation for electrostatic fields can be derived by defining a vector $\boldsymbol{\imath}$, equal to the total current, conduction plus displacement,

$$\boldsymbol{\imath} \equiv \mathbf{j} - \frac{1}{4\pi} \nabla \frac{\partial \Phi}{\partial t} \tag{4}$$

and the vector

$$\mathbf{V} \equiv \boldsymbol{\imath} \Phi, \tag{5}$$

where the electric field is related to the electrostatic potential according to $\mathbf{E} = -\nabla \Phi$. By making use of Poisson's equation $\nabla^2 \Phi = -4\pi\rho$ and the equation of continuity, $\nabla \cdot \mathbf{j} + \partial\rho/\partial t = 0$, one can readily show that

$$\nabla \cdot \boldsymbol{\imath} = \nabla \cdot \mathbf{j} - \frac{1}{4\pi} \frac{\partial}{\partial t} (\nabla^2 \Phi) = 0. \tag{6}$$

It follows that $\nabla \cdot \mathbf{V} = \boldsymbol{\imath} \cdot \nabla \Phi$, and therefore

$$\nabla \cdot \mathbf{V} + \frac{\partial}{\partial t} \left(\frac{E^2}{8\pi} \right) = -\mathbf{j} \cdot \mathbf{E}. \tag{7}$$

Thus, the vector $\mathbf{V}$ is the required energy flux vector, and Eq. (7) is the electrostatic analogue of Eq. (1).

Expressions for energy flow in electrostatic fields similar to equation (7) have appeared recently [3, 7–9]. The energy flux vector $\mathbf{V}$ is not uniquely defined. Only the divergence of $\mathbf{V}$ has physical significance, so that another vector with equal divergence can also be used [8]. It is less well known [10] that the energy density has the same type of arbitrariness. For example, if one defines electrostatic energy by the quantity $\rho\Phi/2$, then the vector

$$\mathbf{V}' \equiv \mathbf{j}\Phi + \frac{1}{8\pi} \left[\frac{\partial \Phi}{\partial t} \nabla \Phi - \Phi \nabla \frac{\partial \Phi}{\partial t} \right] \tag{8}$$

satisfies the equation

$$\nabla \cdot \mathbf{V}' + \frac{\partial}{\partial t} \left(\frac{1}{2} \rho \Phi \right) = -\mathbf{j} \cdot \mathbf{E} \tag{9}$$

and thus $\mathbf{V}'$ and $\rho\Phi/2$ could also be used to describe energy flow in electrostatic fields. The form of Eq. (7) is, however, convenient, since it is simple to calculate in a particle code, and will be used here.

In a similar manner one can derive the momentum flux relation for electrostatics. The electrostatic force density is given by

$$\rho\mathbf{E} = \frac{1}{4\pi}\,\mathbf{E}(\nabla\cdot\mathbf{E}). \tag{10}$$

Since for an electrostatic system $\nabla\times\mathbf{E}=0$, one can show that

$$-\mathbf{E}\times(\nabla\times\mathbf{E}) = (\mathbf{E}\cdot\nabla)\mathbf{E} - \tfrac{1}{2}\nabla(\mathbf{E}\cdot\mathbf{E}) = 0. \tag{11}$$

Therefore by adding Eqs. (10) and (11) one obtains the relation between momentum flux and force density

$$\rho\mathbf{E} = \frac{1}{4\pi}\left[\mathbf{E}(\nabla\cdot\mathbf{E}) + (\mathbf{E}\cdot\nabla)\mathbf{E} - \frac{1}{2}\,\nabla(\mathbf{E}\cdot\mathbf{E})\right] = \nabla\cdot\mathsf{T}. \tag{12}$$

Where

$$\mathsf{T} = \frac{1}{4\pi}\left[\mathbf{E}\mathbf{E} - \frac{1}{2}\,(\mathbf{E}\cdot\mathbf{E})\mathsf{I}\right] \tag{13}$$

is the Maxwell stress tensor in the limit $c\to\infty$. Equation (12) is the electrostatic analogue of Eq. (2). Note that electrostatic fields do not carry momentum and there is no electrostatic analogue to the electromagnetic momentum vector $\mathbf{S}/c^2$, even though there is an analogue to the Poynting vector $\mathbf{S}$.

III. Energy and Momentum Flux Carried by Particles

In order to account fully for energy and momentum flow in electrostatic particle simulations, one needs to take into account the flow of energy and momentum carried by particles. For finite-size particles with shape function $S(r)$, one can define the kinetic energy flux vector

$$\mathbf{K} \equiv \tfrac{1}{2}\sum_i m_i v_i^2(t)\,\mathbf{v}_i(t)\,S[\mathbf{r}-\mathbf{r}_i(t)] \tag{14}$$

and the kinetic energy density,

$$U \equiv \tfrac{1}{2}\sum_i m_i v_i^2(t)\,S[\mathbf{r}-\mathbf{r}_i(t)] \tag{15}$$

where the subscript i refers to particle number, $\mathbf{r}$ is the spatial variable, and $\mathbf{r}_i$ is the position of the center of the ith particle. By differentiation of these quantities, one can show that

$$\nabla \cdot \mathbf{K} + \frac{\partial U}{\partial t} = \sum_i m_i \mathbf{v}_i(t) \cdot \frac{d\mathbf{v}_i(t)}{dt} S[\mathbf{r} - \mathbf{r}_i(t)]. \tag{16}$$

In a similar manner one can show that

$$\nabla \cdot \mathbf{M} + \frac{\partial \mathbf{P}}{\partial t} = \sum_i m_i \frac{d\mathbf{v}_i(t)}{dt} S[\mathbf{r} - \mathbf{r}_i(t)] \tag{17}$$

where

$$\mathbf{M} \equiv \sum_i m_i \mathbf{v}_i(t) \mathbf{v}_i(t) S[\mathbf{r} - \mathbf{r}_i(t)] \tag{18}$$

is the particle momentum flux tensor and

$$\mathbf{P} \equiv \sum_i m_i \mathbf{v}_i(t) S[\mathbf{r} - \mathbf{r}_i(t)] \tag{19}$$

is the particle momentum density vector.

IV. Energy and Momentum Balance

The particle quantities and field quantities are related by Newton's law

$$m_i \frac{d\mathbf{v}_i(t)}{dt} = q_i \langle \mathbf{E}[\mathbf{r}_i(t)] \rangle + q_i \mathbf{v}_i(t) \times \mathbf{B}_{\mathrm{ext}}/c, \tag{20}$$

where

$$\langle \mathbf{E}[\mathbf{r}_i(t)] \rangle \equiv -\int_v S[\mathbf{r}' - \mathbf{r}_i(t)] \; \nabla \Phi(\mathbf{r}') \, d^3r' \tag{21}$$

is the net electric field accelerating the particle and $\mathbf{B}_{\mathrm{ext}}$ is any non-self-consistent external magnetic field one may wish to impose in the particle equation of motion. Combining Eqs. (7) and (16) and substituting Eq. (20) allows one to write the overall energy balance equation

$$\nabla \cdot (\mathbf{K} + \mathbf{V}) + \frac{\partial}{\partial t} \left[U + \frac{E^2}{8\pi} \right] = \sum_i q_i \mathbf{v}_i(t) \cdot \{ \langle \mathbf{E}[\mathbf{r}_i(t)] \rangle - \mathbf{E}(\mathbf{r}) \} S[\mathbf{r} - \mathbf{r}_i(t)] \tag{22}$$

where we have used the expression

$$\mathbf{j}(\mathbf{r}) \equiv \sum_i q_i \mathbf{v}_i(t) S[\mathbf{r} - \mathbf{r}_i(t)]. \tag{23}$$

The term on the right-hand side of Eq. (22) represents the work done by the internal tension force which is constraining an extended particle to move together as a unit, when different parts of the particle feel a different electric field. When integrated over a particle, the net work done on the particle by this tension force vanishes, and in the limit of a vanishingly small particle, the right-hand side also approaches zero.

The energy flow associated with this internal tension force is, of course, of no physical interest in most simulations, but its presence reminds one that one should not attempt to account for energy flow on scale lengths less than the particle size. In any case, for fields which do not vary rapidly on the scale of the particle, the right-hand side of Eq. (22) is small and point particle result is approximately valid:

$$\nabla \cdot (\mathbf{K}+\mathbf{V})+\frac{\partial}{\partial t}\left[U+\frac{E^2}{8\pi}\right]=0. \tag{24}$$

In a similar manner one can combine Eqs. (12) and (17) and substitute Eq. (20) to obtain the overall momentum balance equation

$$\begin{aligned}\nabla \cdot \mathbf{M}+\frac{\partial \mathbf{P}}{\partial t}=&\nabla \cdot \mathbf{T}+\mathbf{j}\times\mathbf{B}_{\text{ext}}/c\\ &+\sum_i q_i\{\langle\mathbf{E}[\mathbf{r}_i(t)]\rangle-\mathbf{E}(\mathbf{r})\}\,S[\mathbf{r}-\mathbf{r}_i(t)],\end{aligned} \tag{25}$$

where we have used the expression

$$\rho(\mathbf{r})\equiv\sum_i q_i S[\mathbf{r}-\mathbf{r}_i(t)]. \tag{26}$$

As before, the last term of the right-hand side of Eq. (25) represents the momentum flow associated with the internal tension force. The point particle result is

$$\nabla \cdot \mathbf{M}+\frac{\partial \mathbf{P}}{\partial t}=\nabla \cdot \mathbf{T}+\mathbf{j}\times\mathbf{B}_{\text{ext}}/c. \tag{27}$$

To obtain a global energy conservation theorem for simulation, one can express Eq. (22) in integral form by making use of the divergence theorem

$$\oint_S (\mathbf{K}+\mathbf{V})\cdot d\mathbf{a}+\frac{\partial}{\partial t}(W_E+W_K)=0, \tag{28}$$

where $W_E=\int_V (E^2/8\pi)\,dV$ is the total electrostatic energy inside the simulation volume V, which is enclosed by surface S and $W_K=\sum_i m_i v_i^2/2$ is the total kinetic energy. Note that the volume integral of the right-hand side of Eq. (22) vanishes identically for all particles inside the volume V.

An expression similar to Eq. (28) was recently derived by Swift and Ambrosiano [9]. Their derivation was based on the Vlasov equation, an assumption which is not necessary, although generally adequate for particle simulations. More importantly, however, they neglected the longitudinal displacement current $-(1/4\pi)\,\nabla(\partial\Phi/\partial t)$ in their expression for the energy flow (compare Eq. (28) with Eq. (14) in [9]). Although the energy flow associated with this term is zero for the boundary conditions they considered, it is not generally true. And for the case of antennas on the boundary, this term is crucial, as is shown in the next section.

A similar expression exists for the momentum

$$\oint_S (\mathbf{M}-\mathbf{T})\cdot d\mathbf{a}+\frac{\partial\mathbf{\Pi}}{\partial t}=\int_V (\mathbf{j}\times\mathbf{B}_{\mathrm{ext}}/c)\,dV, \tag{29}$$

where $\mathbf{\Pi}\equiv\sum_i m_i\mathbf{v}_i$ is the total momentum content inside the simulation volume.

So far this development has been in terms of continuous spatial variables. In practice, the field quantities in a particle simulation are defined on a grid. Conceptually, this presents no problem, since the only place the grid quantities enter is in the final evaluation of Eqs. (28) and (29), where one must replace the field integrals by discrete sums over the field quantities. Volume integrals of particle quantities, such as W_K and $\mathbf{\Pi}$, reduce to summations over particle quantities.

V. Application

The surface integrals involving only particle quantities, $\oint_S \mathbf{K}\cdot d\mathbf{a}$ and $\oint_S \mathbf{M}\cdot d\mathbf{a}$, measure the rate of energy and momentum increase, respectively, due to particles entering or leaving the computation region. If particles which leave through one boundary are reintroduced on the opposite side, then these terms will vanish. The surface integrals involving $\oint_S \mathbf{V}\cdot d\mathbf{a}$ and $\oint \mathbf{T}\cdot d\mathbf{a}$ measure the rate of energy and momentum change due to the fields. If the simulations have periodic boundary conditions for both particles and fields, then these terms will vanish. If only the particles are periodic but not the fields, such as the case considered in [9], then the term involving mixed particle and field quantites, $\mathbf{j}\Phi$ in $\mathbf{V}$, will not vanish in general. If specular reflection is used for the particles, then those particle quantities which involve odd powers of $\mathbf{v}\cdot\hat{n}$, such as $\mathbf{j}\cdot\hat{n}$, and $\mathbf{K}\cdot\hat{n}$, where $\hat{n}$ is the unit normal, will vanish at the boundaries. Other cases have to be considered individually by keeping track of the amount of energy or momentum flux in the particles crossing the boundaries.

An example where these conservation equations proved useful was in the simulation of plasma heating by launching electrostatic lower hybrid waves from an antenna at one boundary [11]. Specular reflection was used so that when Eq. (28) was integrated one obtained the result

$$W_E+W_K-\frac{1}{4\pi}\int_0^t dt\oint_S \Phi\nabla\frac{\partial\Phi}{\partial t}\cdot d\mathbf{a}=\text{constant}. \tag{30}$$

The last term on the left-hand side of this equation can be interpreted as the work done on the plasma by the antenna. In our example, furthermore, the model was periodic in one direction ($\hat{y}$) and the Neumann boundary condition was used at $x = L_x$ (that is, $(\partial\Phi/\partial x)\ (x = L_x) = 0$), so that only the surface at $x = 0$ contributed to the integral. Numerically, the time integration was done by using the trapezoidal rule, so that

$$W_E + W_K + \frac{1}{8\pi} \sum_{n=0}^{N-1} \int_0^{L_y} [\Phi(t_{n+1}) + \Phi(t_n)] \left[\frac{\partial\Phi}{\partial x}(t_{n+1}) - \frac{\partial\Phi}{\partial x}(t_n) \right] \bigg|_{x=0} dy$$
$$= \text{constant}. \tag{31}$$

Since the quantities Φ and $\partial\Phi/\partial x$ at the boundaries had to be calculated anyway [12] in order to solve Poisson's equation, calculation of Eq. (31) involved negligible computer time and only slightly more storage.

When Eq. (31) was applied to these heating simulations, we obtained the same energy conservation (0.5% for 6000 time steps) for all amplitudes of the exciting field, even though the plasma energy doubled in some cases. This provided a valuable check on the integrity of the simulation.

An example where the momentum conservation equations proved useful was in the simulation of current drive [13]. We were primarily interested in accounting for the momentum increase along $\mathbf{B}_{\text{ext}} = B_0\mathbf{y}$, to be sure it was not due to some nonphysical effect. With specularly reflecting particles Eq. (29) can be integrated to give

$$\Pi_y - \int_0^t dt \oint_S \mathbf{T}_y \cdot d\mathbf{a} = \text{constant}, \tag{32}$$

where

$$\mathbf{T}_y = \frac{1}{4\pi} \left[E_y\mathbf{E} - \frac{1}{2}(\mathbf{E}\cdot\mathbf{E})\hat{y} \right]. \tag{33}$$

For the same geometry as before, Eq. (32) reduces to

$$\Pi_y + \frac{1}{4\pi} \sum_{n=0}^{N-1} \Delta t_n \int_0^{L_y} E_x(t_n)\, E_y(t_n) \bigg|_{x=0} dy = \text{constant}. \tag{34}$$

Starting with an electron drift equal to 30% of the thermal velocity, $\langle v\rangle/v_e = 0.3$, we found momentum was conserved to within a few tenths of a percent after 12,000 time steps, even when the plasma momentum doubled.

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