# Maxwell Current Is Conserved

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**Executive Summary**

**Including displacement current might make MD much easier and more powerful.**

## Maxwell Current

We start with ampere's law as generalized by Maxwell. $\mathbf{I}_{\text{particle}}$ is the total electric current carried by particles, i.e., anything with mass.

$$\nabla \times \mathbf{B} = \mu_0 \left( \mathbf{I}_{\text{particle}} + \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} \right); \quad \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} \text{ is often called the 'displacement current'} \qquad (1)$$

Note that equation (1) is true for the total electric current carried by particles $\mathbf{I}_{\text{particle}}$. It does not say anything about how that current $\mathbf{I}_{\text{particle}}$ is distributed between different chemical species, e.g. $\mathbf{I}_{\text{Na}^+}, \mathbf{I}_{\text{K}^+}, \mathbf{I}_{\text{Cl}^-}$.

Take the divergence of both sides and remember that the divergence of a curl is always zero.

$$\nabla \cdot \left( \nabla \times \mathbf{B} \right) = 0 = \nabla \cdot \left( \mu_0 \mathbf{I}_{\text{particle}} + \mu_0 \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} \right) \qquad (2)$$

I define **Maxwell Current** as $\mathbf{I}_{\text{Max}} = \mathbf{I}_{\text{particle}} + \varepsilon_0 \dfrac{\partial \mathbf{E}}{\partial t}$ (3)

**Maxwell Current** is an invariant. It is conserved because its divergence is zero,

$$\nabla \cdot \mathbf{I}_{\text{Max}} = 0 \qquad (4)$$

**Maxwell current is conserved and invariant wherever and whenever the Maxwell equations are valid.** Eq. (2) does not involve any property of matter so it is valid everywhere, in vacuums, inside solids, in liquids, in ionic solutions, even inside atoms. (Textbooks suggest Maxwell equations are valid to distances very much smaller than an atomic radius and to interstellar distances as well, although I cannot be the judge of either claim.)

‘Displacement current’ is sometimes defined (e.g., in membrane biophysics, Armstrong and Bezanilla) to include properties of dielectric materials. I do **not** include those properties in the definition here. $\mathbf{I}_{\text{Max}}$ is a property of space. It does not depend on any properties of matter.

## Relevance to Molecular Dynamics

**It would be useful if Molecular Dynamics simulations conserved Maxwell current**

The best way to enforce the requirement that Maxwell current is always conserved depends on the details of the MD code and I sadly am not an expert in that.

One way to enforce the requirement would be to introduce an auxiliary equation where the particle current (computed from the flux of charge carried by all the species, e.g., $Na^+$, $K^+$, and $Cl^-$ being careful to have the opposite sign current carried by anions and cations) is adjusted by the displacement current $\varepsilon_0 \dfrac{\partial \mathbf{E}}{\partial t}$ at each time step so eq. (4) is satisfied at each time step and $\mathbf{I}_{\text{Max}}$ is conserved at every time step. This requires computation of the flux, and the gradient of the potential and its time derivative at every time step. There are many ways to enforce auxiliary conditions in numerical calculations, e.g. using Lagrange multipliers, but what matters is what works easily and efficiently.

**Qualitative Effects.** It is very important to note that the displacement current $\varepsilon_0 \dfrac{\partial \mathbf{E}}{\partial t}$ term would be largest when fields are changing most rapidly, i.e., at short times and high frequencies.

The new term $\varepsilon_0 \dfrac{\partial \mathbf{E}}{\partial t}$ **damps rapid motions, perhaps quite dramatically** corresponding to the well-known experimental phenomenon that the noise in wide band current measurements decreases dramatically when a grounded plate is near the ionic solution. The grounded plate presumably acts like an $\varepsilon_r \varepsilon_0 \dfrac{\partial \mathbf{E}}{\partial t}$ term, where $\varepsilon_r$ is the (long time) relative dielectric coefficient, ~80 for distilled water.

Damping high frequency motions might make it much easier to perform long time simulations with atomic resolution. That is to say, **including displacement current might make MD much easier and more powerful.**