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Abstract

Improved NGP and CIC particle-mesh schemes are suggested, and a NEC scheme proposed, to help reduce self forces in Monte Carlo semiconductor device simulation. An attempt to design a scheme with reduced self forces for unstructured triangular meshes is unsuccessful.

1. Introduction

A proper coupling between charged particles and Coulombic forces is required to maintain temporal stability and spatial accuracy in self-consistent Monte Carlo device modeling. Particle-mesh (PM) coupling can be broken into four steps[1]:

1. assign particle charge to the mesh;
2. solve the Poisson equation on the mesh;
3. calculate the mesh-defined forces; and
4. interpolate to find forces on the particles.

The usual charge assignment and force interpolation schemes employed are nearest-grid-point (NGP) or cloud-in-cell (CIC). Both schemes guarantee zero self force, *i.e.*, the force a charge exerts upon itself due to numerical artifacts. As stated in [1]:

> At best, the presence of the self force presents a nonphysical restriction on the time step and, at worst, it is disastrous.

The classical NGP and CIC schemes depend on two severe assumptions: (a) constant permittivity, and (b) tensor product mesh with uniform spacing in x- and y-axis directions. While it is straightforward to exercise NGP and CIC schemes for non-uniformly spaced tensor-product meshes and/or spatially dependent permittivity, it is also incorrect: self forces will not be zero, or even necessarily small.

After discussing the importance of self forces, this paper describes improvements to the NGP/CIC charge assignment/force interpolation schemes which do not require assumption (a) above, and a new nearest-element-center (NEC) scheme which, in addition, relaxes assumption (b). This leads naturally to a discussion of designing a scheme for unstructured triangular meshes, and how finding such a scheme remains an open question. The discussion here assumes two space dimensions throughout, although the extension to three dimensions is obvious.

2. Self-Forces and Their Importance

Discussing self forces is only relevant if the Coulombic forces are obtained self-consistently in time with particle position. Any smoothing of the electric field in time (*e.g.*, [2]) or using a time-invariant ("frozen") field (*e.g.*, [3]) renders a discussion of self forces irrelevant, as the force does not track instantaneous particle motion.

In its simplest embodiment, self-forces arise due to the failure of a non-uniformly spaced mesh to resolve symmetrically the potential singularity of a single charge (in 2D, a line charge). Differencing this potential and interpolating back to the charge position yields an erroneous, non-zero force exerted by the charge upon "itself". But note, self forces may locally be small compared to the total force. Self forces are expected to be most serious in regions of a device where internal fields are "low".

3. Improved NGP/CIC and the NEC Scheme

An improved NGP/CIC scheme can be obtained by altering step 3. These schemes (denoted NGP* and CIC*) pertain to the case when permittivity depends on position, yet the mesh spacing still obeys assumption (b). First, some notation is required: consider a uniformly-spaced, tensor product mesh with meshlines x_i, $i = 1, \ldots, \mathcal{N}_x$ and y_j, $j = 1, \ldots, \mathcal{N}_y$. Permittivities are considered constant within each mesh element (for simplicity only) and are denoted ϵ_{ij}.[1] Define centered finite-differences of the potential ψ in the x- and y-axis directions at element midpoints as follows:

$$\Delta^x_{k+\frac{1}{2},\ell} \doteq \frac{\psi_{k+1,\ell} - \psi_{k\ell}}{x_{k+1} - x_k}, \qquad \Delta^y_{k,\ell+\frac{1}{2}} \doteq \frac{\psi_{k,\ell+1} - \psi_{k\ell}}{y_{\ell+1} - y_\ell}.$$

For the NGP* and CIC* schemes, the new step 3 becomes:

3*. calculate the mesh-defined electric field at the four element vertices (k, ℓ), $\vec{E}_{k\ell} = [E^x_{k\ell}; E^y_{k\ell}]$, as $E^x_{k\ell} = (\epsilon_{k-1,j}\, \Delta^x_{k-\frac{1}{2},\ell} + \epsilon_{kj}\, \Delta^x_{k+\frac{1}{2},\ell})/(2\epsilon_{ij})$, $E^y_{k\ell} = (\epsilon_{i,\ell-1}\, \Delta^y_{k,\ell-\frac{1}{2}} + \epsilon_{i\ell}\, \Delta^y_{k,\ell+\frac{1}{2}})/(2\epsilon_{ij})$, for $k = i, i+1$ and $\ell = j, j+1$.

The standard NGP/CIC schemes use $E^x_{k\ell} = (\Delta^x_{k-\frac{1}{2},\ell} + \Delta^x_{k+\frac{1}{2},\ell})/2$ and $E^y_{k\ell} = (\Delta^y_{k,\ell-\frac{1}{2}} + \Delta^y_{k,\ell+\frac{1}{2}})/2$, which are incorrect if permittivity is spatially dependent.

Before describing the NEC scheme, a short digression is necessary: unfortunately, the NEC scheme only yields "approximately zero" self forces. To understand this, consider the canonical self force Gedanken experiment: a single line change Q is placed upon a two-dimensional mesh of infinite extent ($-\infty < x, y < \infty$). With no other charges present, no boundaries where induced charges may reside, and a constant permittivity everywhere, this charge should not experience any acceleration (the force on Q, *i.e.*, the self force, should be zero). This requires the charge assignment/force interpolation schemes be the same *and* forces be equal and opposite between two charges[1]. This latter condition can be restated: if Q is located on a mesh node p, then the force at any other mesh node o depends only on the directed distance separating p and o. This is obvious, and can be rigorously proven for a tensor-product mesh with uniform spacings in the x- and y-axis direction[1]. Physically the force behaves exactly this way; for this category of meshes the discrete case reproduces this behavior. To my knowledge this is not rigorously true for unstructured meshes nor for non-uniformly spaced tensor-product meshes; however, *assume this is* approximately *true for all two-dimensional meshes in what follows*[2]. The extent to which it is not true in the

[1]Elements, and elemental quantities like permittivity, are indexed by the minimum i and j indices of the element.

[2]Computations indicate this "approximation" is remarkably true, to within a 1% error; can this be shown rigorously?

discrete case is responsible for nonzero instead of truly zero self forces. I shall call this the "well-behaved forces" assumption (WBF).

The nearest element center (NEC) charge assignment/force interpolation scheme will now be described. This scheme attempts to reduce self forces in the presence of non-uniformly spaced tensor-product meshes and/or spatially-dependent permittivity. In addition, the NEC scheme can be utilized in one axis direction (where local mesh spacing is non-uniform) and the CIC* scheme can be utilized in the other (where local mesh spacing is uniform). Such hybrid schemes, dubbed NEC-x–CIC*-y or NEC-y–CIC*-x, offer smoother assignment/interpolation on the mesh compared to pure NEC.

Consider a line charge ρ residing at (x, y) in a rectangular mesh element (i,j) with permittivity ϵ_{ij}. The new steps of the (pure-)NEC PM scheme are:

1′. assign the line charge *equally* to the four mesh points of the element (i, j);

3′. calculate the fields $\Delta^x_{i+\frac{1}{2},\ell}$, $\ell = j, j+1$, and $\Delta^y_{k,j+\frac{1}{2}}$, $k = i, i+1$;

4′. interpolate the field $\vec{E}(x, y) = [E^x;\ E^y]$, according to $E^x = (\Delta^x_{i+\frac{1}{2},j} + \Delta^x_{i+\frac{1}{2},j+1})/2$, $E^y = (\Delta^y_{i,j+\frac{1}{2}} + \Delta^y_{i+1,j+\frac{1}{2}})/2$.

The NEC designation derives from the appearance, in step 1′, of moving the charge to the center of its element and applying a CIC assignment scheme. The NEC scheme involves *only* one mesh element and its four nodal values of potential. This locality makes the method well-suited to non-uniform mesh spacings and permittivity.

The NEC-x–CIC*-y scheme involves only (i, j) elemental quantities for x-directed fields, but not for y-directed fields. The new steps of the NEC-x–CIC*-y scheme are:

1″. conceptually move the charge from its location (x, y) to $(0.5(x_i + x_{i+1}), y)$ and apply the CIC charge weighting scheme (denote these CIC weights as w_{ij}, $w_{i+1,j}$, $w_{i,j+1}$ and $w_{i+1,j+1}$; note $w_{ij} = w_{i+1,j}$ and $w_{i,j+1} = w_{i+1,j+1}$);

3″. calculate fields $\Delta^x_{i+\frac{1}{2},j}$ and $\Delta^x_{i+\frac{1}{2},j+1}$ as in pure-NEC; calculate fields $E^y_{k\ell}$, $k = i, i+1$ and $\ell = j, j+1$ as in CIC*;

4″. interpolate the field $\vec{E}(x, y) = [E^x;\ E^y]$ according to $E^x = (w_{ij} + w_{i+1,j})\Delta^x_{i+\frac{1}{2},j} + (w_{i,j+1} + w_{i+1,j+1})\Delta^x_{i+\frac{1}{2},j+1}$, $E^y = \sum_{k=i,i+1;\,\ell=j,j+1} w_{k\ell}E^y_{k\ell}$, where the w_{ij} are the CIC weights from step 1″.

The other mixed scheme, NEC-y–CIC*-x, is defined analogously.

The mixed schemes provide for smoother assignment and interpolation in the "CIC" direction. In a device simulation context, the decision whether to apply NEC or CIC* in the x-axis direction (for example) in the vicinity of element (i, j) is: *if* the local x-axis mesh spacing is constant (*i.e.*, $x_i - x_{i-1} = x_{i+1} - x_i = x_{i+2} - x_{i+1}$), *and* the local permittivity is constant (*i.e.*, $\epsilon_{i-1,j} = \epsilon_{ij} = \epsilon_{i+1,j}$), *and* none of the nodes (k, ℓ), $k = i-1, \ldots, i+2$ and $\ell = j, j+1$ are contact nodes, *then* CIC* should be used; *otherwise*, NEC should be employed. Applying analogous rules in the y-axis direction leads to four outcomes for element (i, j): pure NEC or CIC*, or the two hybrid schemes.

4. What About Unstructured Triangular Meshes?

Consider a triangular element $\mathcal{T}$ with nodes i, j, k in an unstructured triangular mesh of infinite spatial extent. A line charge ρ resides at (x, y) within $\mathcal{T}$. Assume the potential is a linear function of position within $\mathcal{T}$, *i.e.*, $\psi(x, y) = \psi_i N_i(x, y) + \psi_j N_j(x, y) + \psi_k N_k(x, y)$, where the $N_\ell(x, y)$ are the linear shape functions associated with $\mathcal{T}$.[3] Will

[3] Linear shape functions on triangular elements are the simplest shape functions which are local to the element, making them a natural choice[4].

any charge assignment scheme yield a PM coupling with zero self force (in the WBF sense) for a simple PM scheme? Consider the four steps:

$1^\triangle$. Charge assignment is left unspecified; assign charge to nodes as $\varrho \doteq [\rho_i, \rho_j, \rho_k]^T = \rho[c_i, c_j, c_k]^T \doteq \rho\mathbf{c}$, where $\sum_{\ell=i,j,k} c_\ell = 1$ by charge conservation.

$2^\triangle$. Solve the Poisson equation; the charges at the nodes will result in a potential $\varphi = \mathbf{G}\varrho$, where $\varphi = [\psi_i, \psi_j, \psi_k]^T$ and $\mathbf{G} = (g_{ij})$ is a 3×3 matrix extracted from the inverse of the Laplacian on the infinite mesh. The WBF assumption dictates the form of $\mathbf{G}$: diagonal entries are all equal and the matrix is symmetric. Therefore,

$$\mathbf{G} = \begin{pmatrix} g_{ii} & g_{ij} & g_{ik} \\ g_{ji} & g_{jj} & g_{jk} \\ g_{ki} & g_{kj} & g_{kk} \end{pmatrix} \overset{\text{from WBF}}{=} \begin{pmatrix} g_{ii} & g_{ij} & g_{ik} \\ g_{ij} & g_{ii} & g_{jk} \\ g_{ik} & g_{jk} & g_{ii} \end{pmatrix} = g_{ii} \begin{pmatrix} 1 & \alpha & \beta \\ \alpha & 1 & \gamma \\ \beta & \gamma & 1 \end{pmatrix} \doteq g_{ii}\tilde{\mathbf{G}},$$

where $0 < \alpha, \beta, \gamma < 1$ and α, β and γ are not equal in general.

$3^\triangle$–$4^\triangle$. The electric field in $\mathcal{T}$ is the constant vector $\vec{E} = -\nabla\psi = -\sum \psi_\ell \nabla N_\ell$. Since the field in $\mathcal{T}$ is everywhere the same, field interpolation is automatically accomplished.

A *zero* field on the original line charge $\rho(x, y)$ is sought; therefore, the field in step $4^\triangle$ should be zero. Obtaining $\vec{E} = \vec{0}$ can only occur if $\psi_i = \psi_j = \psi_k$ (straightforward to show, but not proven here). A charge weighting scheme $\mathbf{c}$ that gives equal nodal potentials obeys:

$$\mathbf{G}\varrho = g_{ii}\rho\tilde{\mathbf{G}}\mathbf{c} = \varphi \propto [1\,1\,1]^T \rightarrow\ \tilde{\mathbf{G}}\mathbf{c} \propto [1\,1\,1]^T\,.$$

This has a complicated solution ($\mathbf{c} \propto \tilde{\mathbf{G}}^{-1}[1\,1\,1]^T$) and a simple solution ($c_i = c_j = c_k = \frac{1}{3}$, if $\alpha = \beta = \gamma$). To be useful, the charge weights $\mathbf{c}$ should be local functions of the element $\mathcal{T}$; since α, β and γ are global functions of the entire mesh, $\mathbf{c}$ should be independent of α, β and γ. This requires the complicated solution be discarded. The simple solution obtains $\mathbf{c}$ independent of α, β and γ as required, but only when $\alpha = \beta = \gamma$. This implies the mesh be composed of identically-sized equilateral triangles, which is not a very useful "unstructured" triangular mesh! Can a useful PM coupling for unstructured triangular meshes be designed which yields zero self forces (in the WBF sense)? To my knowledge this important question remains unanswered.

5. Conclusions

The NEC*, CIC* and NEC PM schemes are proposed to reduce self forces. Hybrid combinations of these methods are described. An attempt to design a PM scheme for unstructured triangular meshes is successful only for meshes of equilateral triangles.

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