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Recovery of Vectorial Fields and Currents in Multidimensional Simulation

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Abstract

In the context of 2-D and 3-D unstructured mixed-element meshes, a new method of recovering vectorial fields and currents in multidimensional simulation is introduced. The new method, called the method of edge elements, directly interpolates the projections of the vectors on the edges of an element into its interior. The new method is compared to two other recovery methods on the basis of resolution, consistency, and implementation ease.

1. Introduction

In the numerical simulation of semiconductor devices, the vectorial electric field and current density field (together: fields) are required throughout the domain of simulation to compute various physical models, such as mobility, impact ionization, and Joule heating. In finite-box simulations, the discretization and solution do not uniquely define the fields off of the edges joining the nodes. The fields are reconstructed from the projections of electric field or current density along the edges.

The recovery method should not only define a unique electric field and current density throughout the domain, but it should also specify how the recovered vectorial quantities should be used in the discretized equations. In general the parameter models may require the vectorial quantity along an edge, within an element, or at a node.

For accuracy, the ideal recovery method should be of high resolution and be consistent with the model and its discretization. Resolution measures the capability to distinguish between fields at adjacent locations. Inconsistency will introduce additional numerical errors. The recovery method should be consistent with the approximations of the Sharfetter-Gummel discretization, and the projections of the recovered field on the element edges should reproduce the original data.

For computer efficiency, the ideal recovery method should be easy to implement and be applicable to any 2-D or 3-D, unstructured, and mixed-element mesh. The implementation of the method should be computationally cheap, including calculation of the derivatives of the field for the Jacobian. Often, in order to apply a method only suitable for simplex meshes, nonsimplex elements are arbitrarily subdivided into simplices. However, it turns out that the numerical solutions are sensitive to the way elements are split. Splitting the elements introduces new edges ij with zero Voronoi cell areas A_{ij}, from which the field along the edge cannot be uniquely determined. Errors introduced in calculating the fields will feed back into the solution via the physical models, which may compromise the overall accuracy of the modeling effort.

2. Method of Edge Elements

The method of edge-elements (EEM) proposed below directly interpolates vectorial values defined on the edges of an element into the interior of the element. The vectorial interpolant $\mathbf{J}^k$ of the edge values F_{ij} into the interior of element k is

$$\mathbf{J}^k = \sum_{ij \in \mathcal{E}^k} F_{ij}\mathbf{e}_{ij}, \tag{1}$$

where $\mathbf{e}_{ij}$ is the basis function of edge ij and $\mathcal{E}^k$ is the set of edges of the element. The edge basis function is defined by

$$\mathbf{e}_{ij} = d_{ij}(\lambda_i \nabla \lambda_j - \lambda_j \nabla \lambda_i), \tag{2}$$

where d_{ij} is the length of edge ij and λ_i is the scalar finite-element shape function. The shape function λ_i for the element takes the value 1 at node i, the value 0 at all other nodes, and is linear between them. The basis function has the following characteristic properties: the tangential component of $\mathbf{e}_{ij}$ along the edge ij is equal to one, while the tangential components along all other edges are equal to zero. Reconstruction of the field using edge elements yields a non-constant vector function defined on the element which has the following properties: (1) The projection of the edge-element reconstruction on each edge of the element reproduces the original data. (2) The tangential components of the field are continuous from one element to the next. (3) The field is divergence-free. Property (2) is useful at internal interfaces between materials of different permittivities. Property (3) is consistent with the approximations made for the SG discretization of current.

To simplify the edge-element calculations, a coordinate transformation is applied to transform each element into its standard position. The coordinate transformation for an element with nodes at $\{\mathbf{r}_0, \mathbf{r}_1, \ldots\}$ into standard position is defined by $\mathbf{r}' = A^{-1}(\mathbf{r} - \mathbf{r}_0)$, where A is the Jacobian of the transformation. The edge elements transform according to

$$\mathbf{e}_{ij}(\mathbf{r}) = (A^{-1})^T \mathbf{e}_{ij}(\mathbf{r}'), \tag{3}$$

where the primed coordinates refer to the element in standard position.

Although the definition of the edge elements can be applied to non-simplex elements, the results are inaccurate due to the quadratic component in the direction normal to the edge. To rectify this, the modified edge-elements are introduced by removing one of the factors from each squared term. In this form, edge elements are suitable for 2-D and 3-D nonsimplex elements. The standard and modified 2-D edge-elements in standard position are listed in Table 1.

The vector quantity at a location required for a parameter model may be computed by averaging the interpolant function. For example, analytically averaging over the element k results in

$$< \mathbf{J}^k > = \frac{1}{V^k} \int_{V^k} \mathbf{J}^k \, dv. \tag{4}$$

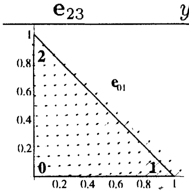
where V^k is the volume of the element k. On the other hand, the space-varying interpolant function may be directly evaluated at the location of interest.

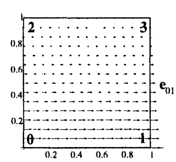
3. Method of Least-Squares Fitting

The method of least-squares (LSM) fitting treats the edge values in an element as measurements of the field. The recovered field is a constant field within the element

Table 1: The two-dimensional edge elements in standard position, each normalized by its length. A modified edge-element is shown in the vector plots, with node numbering indicated.

	Standard EE		Modified EE		Element averaged
Element	$\hat{\mathbf{a}}_x$	$\hat{\mathbf{a}}_y$	$\hat{\mathbf{a}}_x$	$\hat{\mathbf{a}}_y$	
Triangle					$<\mathbf{J}_x^k>= \frac{1}{3}(2d_{01}F_{01} + d_{02}F_{02} - d_{12}F_{12})$
$\mathbf{e}_{01}$	$1-y$	x	$1-y$	x	
$\mathbf{e}_{02}$	y	$1-x$	y	$1-x$	$<\mathbf{J}_y^k>= \frac{1}{3}(d_{01}F_{01} + 2d_{02}F_{02} + d_{12}F_{12})$
$\mathbf{e}_{12}$	$-y$	x	$-y$	x	
Rectangle					$<\mathbf{J}_x^k>= \frac{1}{2}(d_{01}F_{01} + d_{23}F_{23})$
$\mathbf{e}_{01}$	$(1-y)^2$	0	$1-y$	0	
$\mathbf{e}_{02}$	0	$(1-x)^2$	0	$1-x$	$<\mathbf{J}_y^k>= \frac{1}{2}(d_{01}F_{01} + d_{23}F_{23})$
$\mathbf{e}_{13}$	0	x^2	0	x	
$\mathbf{e}_{23}$	y^2	0	y	0	





that minimizes the error along each edge, that is, the field $\mathbf{J}^k$ that minimizes $f(\mathbf{J}^k)$,

$$f(\mathbf{J}^k) = \sum_{ij \in \mathcal{E}^k} (\mathbf{J}^k \cdot \hat{\mathbf{a}}_{ij} - F_{ij})^2, \tag{5}$$

where $\hat{\mathbf{a}}_{ij}$ is a unit vector from node i to node j. The LSM can be applied uniformly to edge-, element-, or cell-field recoveries.

4. Method of Corner Averages

The method of corner averages (CAM) partitions the domain into "corners" and calculates a constant vector value in each corner. The volume V_i^k associated with the corner of element k at node i, where node i belongs to the element, is defined by the intersection of element k with the Voronoi cell at i. The corner value $\mathbf{J}_i^k$ in V_i^k is calculated by solving the system of equations

$$\mathbf{J}_i^k \cdot \hat{\mathbf{a}}_{ij} = F_{ij},\ j \in \mathcal{N}_i^k, \tag{6}$$

where $\mathcal{N}_i^k$ is the set of nodal neighbors of i within element k.

The field at a location required for a parameter model is computed through a suitably weighted average of corner values. The original CAM [1] was proposed for triangular or prismatic elements, and it is difficult to generalize their averaging scheme to other elements. Here, a more general averaging scheme is proposed which is suitable for other elements. The generalized average is defined by

$$< \mathbf{J} > = \sum_{i,k} \mathbf{J}_i^k / V_i^k \Big/ \sum_{i,k} 1/V_i^k, \tag{7}$$

where the indices (i, k) take on different values depending on whether the average is for a node, an element, or along an edge.

5. Discussion

The EEM was compared to the LSM and the CAM. On the basis of resolution, the EEM is clearly superior since it can distinguish any two arbitrarily close points. The other methods produce fields which are constant over various zones. On the basis of consistency, the EEM is consistent with the SG discretization. The recovered field is also consistent with the solution, since the projections of the field along element edges reproduces the original data. However, the other methods do not have this property. On the basis of implementation ease, the EEM and LSM are computationally cheaper that the CAM. The work involved in recovering the field using the EEM or LSM involves evaluating a polynomial function in the number of edges and multiplying by a matrix for the coordinate transformation.

A detailed comparison between the element-averaged EEM and the LSM was made, since it can be argued that the LSM produces fields which are optimum. It was found that the two methods yield identical results for the rectangular faces of any element, so the differences were evaluated in triangular faces. For an equilateral triangle, with nodes at $(0,0)$, $(1,0)$, and $(1/2, \sqrt{3}/2)$, the recovered fields are identical and given by

$$\mathbf{J}^k = \{0.667F_{01} + 0.333F_{02} - 0.333F_{12}, 0.577F_{02} + 0.577F_{12}\}. \tag{8}$$

When the upper node was moved upward, from $(1/2, \sqrt{3}/2)$ to $(1/2, 10 + \sqrt{3}/2)$, the methods produced:

$$\mathbf{J}^k_{EEM} = \{0.667F_{01} + 3.62F_{02} - 3.62F_{12}, 0.501F_{02} + 0.501F_{12}\}, \tag{9}$$

$$\mathbf{J}^k_{LSM} = \{0.996F_{01} + 0.045F_{02} - 0.045F_{12}, 0.501F_{02} + 0.501F_{12}\}. \tag{10}$$

These methods differ in the reconstruction of the x-component of the field. Which is correct? The EEM uses the geometry of the figure when averaging over the area of the element. Longer edges dominate more of the figure and therefore weigh proportionately more in the averaging. On the other hand, the LSM ignores the geometry of the figure in which the field is computed; only the relative orientation of the measurements matters. In the elongated triangle, the upper legs are rotated toward the y-direction and thus the influence of these legs on J^k_x is smaller. This means that the LSM is inaccurate for element reconstructions. The use of the LSM should be restricted to field reconstructions where all the measurements are collected at one point, for example, to reconstruct the field at the center of the Voronoi cell.

In conclusion, the newly proposed method of edge-elements is an accurate and efficient vectorial field reconstruction method. The EEM has been installed in SIMASTER, a general purpose 2-D and 3-D device simulator using unstructed meshes [2]. The EEM has proven effective in many different types of simulations.

References

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