ON-CHIP INTERCONNECT SIMULATION OF PARASITIC CAPACITANCES IN PERIODIC STRUCTURES

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ABSTRACT

Parasitic capacitances determine significantly the performance of todays complex on-chip interconnect structures. This article handles the implementation of periodic boundary conditions for electrical field calculation and parasitic capacitance extraction in interconnect structures. Various examples show the impact of these convenient boundary conditions.

INTRODUCTION

The numerical capacitance calculation uses commonly the energy method $C = \frac{U^2}{2W}$, where U is the voltage applied between the conductors and W is the electric energy stored in the interior of the dielectric $\mathcal{V}_D$. W can be derived from the electric field $\vec{E}$:

$$W = \int_{\mathcal{V}_D} \vec{E} \cdot \vec{D} \mathrm{d}V = \epsilon_0 \int_{\mathcal{V}_D} \vec{E} \cdot (\underset{\sim}{\epsilon_r} \cdot \vec{E}) \mathrm{d}V.$$

$\vec{E}$ is given by $\vec{E} = -\vec{\nabla}\varphi$ and φ is the solution of the equation:

$$\vec{\nabla} \cdot (\underset{\sim}{\epsilon_r} \cdot \vec{\nabla}\varphi) = -\frac{\rho}{\epsilon_0} \tag{1}$$

The insulators are free of electric charge ($\rho = 0$). Therefore, the solution of (1) is completely extracted from the data, defined on the boundary $\partial\mathcal{V}_D$. On one part of this boundary Dirichlet conditions ($\varphi(\vec{r}) = \varphi_0$) are applied and on the other part homogeneous Neumann conditions ($\vec{n}.\vec{\nabla}\varphi(\vec{r}) = 0$) [1]. For the numerical solution of the involved partial differential equation (1) the finite element method (FEM) [2] is applied. The simulation area is discretized in tetrahedrons. The algorithm for the linear algebraic equations arising from the finite element discretization is based on the iterative conjugate gradient method, which uses incomplete Cholesky preconditioning technique to speed up the iteration convergence [3]. The accurate numerical calculation of boundary value problems such as (1) requires an appropriately fine discretization. In large areas this leads to generation of a lot of simulation nodes, which means sizeable memory consumption and unacceptably long duration of the simulation process.

Often the interconnects represent regular structures (i.e. on-chip interconnect buses, DRAM cells) which can be described through mirroring and periodic spatial continuation of a given subspace [4]. A large simulation domain can be composed from numerous sub-domains [5]. A smart simplification is to simulate only in this small sub-domain by applying boundary conditions corresponding to the way how the whole domain is composed from the sub-domain pattern (by mirroring or periodic extension). Therefore the simulation duration and memory consumption are decreased heavily. To use this feature the simulation software has to provide mirroring and periodic functionality. The mirroring can be easily accomplished by applying homogeneous Neumann boundary conditions at the mirroring surface. However, the periodic boundaries require special treatment.
We define two faces $\mathcal{A}_{1p} \subset \partial\mathcal{V}$ and $\mathcal{A}_{2p} \subset \partial\mathcal{V}$ as periodic boundary, if:

- Each node from $\mathcal{A}_{1p}$ is uniquely mapped to another node from $\mathcal{A}_{2p}$.
- If $\vec{r}_{1i}$ is the position pointer to a simulation point of $\mathcal{A}_{1p}$ and $\vec{r}_{2i}$ is the position pointer to the corresponding simulation point of $\mathcal{A}_{2p}$ then $\varphi(\vec{r}_{1i}) = \varphi(\vec{r}_{2i})$ for each point of $\mathcal{A}_{1p}$ and $\mathcal{A}_{2p}$.
- Each node of $\mathcal{A}_{1p}$ has its own neighbor nodes and the neighbor nodes of the corresponding node from $\mathcal{A}_{2p}$.

Although each two corresponding periodic points are separated in the space, due to the periodic condition, they should behave as if they were attached to each other.

DOMAIN DISCRETIZATION

The discretization of the volume of interest is usually the first step of the finite element analysis. In this case the simulation domain is subdivided into a number of small volume elements, in our case tetrahedral elements. Therefore the surface is broken into a number of triangular elements.
For the sake of clarity this paragraph is restricted to parallelepiped structures. Of course periodic boundary conditions can be applied to an arbitrary pair of faces with unique bidirectional node mapping. If at two opposite parallel faces periodic boundary conditions are applied, the grid generated has to guarantee that the surface grids at these faces

are identical. Two different three-dimensional grid generation approaches are used in our interconnect simulation software *Smart Analysis Programs*. The first one is a fully unstructured grid generation approach which uses the program delink [6, 7]. The second approach is a layered based method which extends two-dimensional grid generator [8] into the third dimension by means of linear extrusion. Both approaches do not fulfill the above mentioned requirements for periodic boundaries a priori. To extend the grid generator for periodic boundaries an iterative approach is used. At first the simulation domain is meshed without any special treatment for periodic boundaries. Afterwards the periodic boundary faces are checked for conformity. If they are not conform the periodic nodes are merged. Therefore at the periodic surfaces new points are generated which are fed into the grid generator as additional input. These steps are repeated until conformity is reached. In the layer based meshing approach this iteration procedure must only be applied to the two-dimensional grid generation process. The conformity of the side walls is preserved by the following extrusion step. In the fully unstructured meshing method the conformity of the nodes on the periodic faces is not sufficient, because the same set of boundary nodes can lead to different boundary meshes (at least for cospherical points). Therefore also edge conformity has to be guaranteed. Because of these additional difficulties the layer based grid generation method is preferred for problems with periodic boundaries.

ASSEMBLING

If due to the discretization N points are created, the electric potential φ in $\mathcal{V}_D$ is approximated by the sum:

$$\varphi \approx \tilde{\varphi} = \sum_{j=1}^{NU} c_j N_j(\vec{r}) + \sum_{j=NU+1}^{N} c_j N_j(\vec{r}). \qquad (2)$$

The shape function N_j has the value 1 only on the node j (for $\vec{r} = \vec{r_j}$). N_j is different from 0 only in the elements directly attached to the node j and is 0 otherwise. Therefore the weighting factor c_j represents the potential on the node j. The points which do not belong to $\partial\mathcal{V}_{D1}$ are the unknown nodes and are numbered by $1 \leq j \leq NU$. The Dirichlet (known) nodes (at $\partial\mathcal{V}_{D1}$) are numbered by $NU + 1 \leq j \leq N$. Using (2) FEM leads to a linear equation system for the unknown c_j.

In general the grid generation software does not order the simulation nodes as in (2). To implement the desired node ordering a supplemental auxiliary index array with the length N is allocated. This additional index array is used by the assembling procedure. The first NU entries of this index array refer to the nodes in $\mathcal{V}_D$ without $\partial\mathcal{V}_{D1}$. The remaining entries refer to the nodes on the Dirichlet boundary $\partial\mathcal{V}_{D1}$ (from $NU + 1$ till N). The additional index assignment of the simulation nodes gives advantages to the implementation of the periodic boundary conditions. Each two corresponding points of the plains $\mathcal{A}_{1p}$ and $\mathcal{A}_{2p}$ get the same index in the additional index array. Thus, they are assembled to the same row in the linear equation system. Due to the element-by-element processing of the simulation volume each periodic point has not only its neighbor nodes but it is also connected to the neighbor nodes of the corresponding periodic point.

CONCEPTUAL FORMULATION

In the presented example which is considered part of a representative on-chip bus structure the simulation area consists of a SiO_2 rectangular parallelepiped with two parallel conductors inside as shown in Fig. <1>. The z axis is oriented such that the x y and z axes build a right aligned coordinate system. On one conductor a voltage of 1 V is applied, while the other is set to 0 V. The conductors in this simulation area are shown from another viewing angle in Fig. <2>.

On the interface between the dielectric and the electrodes Dirichlet conditions are applied, which comply with the potential of the electrodes. At the boundaries parallel to the xy plane homogeneous Neumann conditions are applied. For the remaining outer faces different combinations of homogeneous Neumann conditions and periodic boundaries are investigated. Homogeneous Neumann conditions influence the electric field in the simulation domain, as if the simulation domain would be mirrored with respect to the face, at which the homogeneous Neumann conditions are applied. It is convenient to combine opposite faces to periodic boundaries. In this case the electric field in the simulation area is influenced as if the simulation area would be shifted along the direction perpendicular to these faces by the corresponding length of the simulation area. That way the simulation domain appears as if it could be a part of a structure, which is constructed by mirroring of the simulation domain along the z direction and by periodic or mirrored spatial continuation of the simulation domain along the x and y directions. Such a structure could be for instance an interconnect bus. The total capacitance is the sum of the capacitances from all parts.

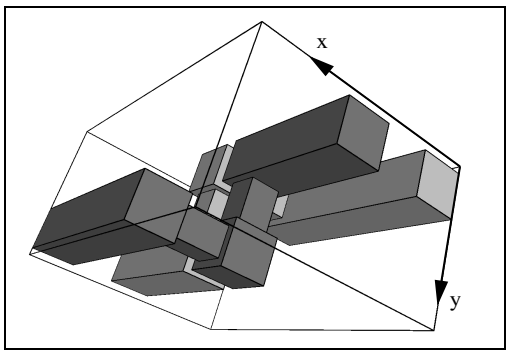

Figure 1: The Simulation Area.

THE ELECTRIC FIELD

The simulation results are evaluated by visualization of the electric field using VTK[9]. The differences between the investigated cases are well shown by the potential iso faces

and by the angles between these potential iso faces and the outer boundaries. The simulated potential distribution confirms with the expected one under consideration of the corresponding boundary conditions.

Mirroring along the x and y axes

At the boundary faces of the simulation area parallel to yz and xz planes homogeneous Neumann conditions are specified. Therefore the simulation domain is mirrored in $\vec{x}$, $-\vec{x}$, $\vec{y}$ and $-\vec{y}$ directions. The mirror planes are the planes, at which homogeneous Neumann conditions are defined. The potential distribution and the corresponding iso faces are shown in Fig. <3> and Fig. <4>. As expected the potential iso faces are perpendicular to the outer bounds. The iso faces should wrap round an electrode and its imaginary mirror images. Therefore iso faces can be seen only between the two electrodes in the simulation area. The other cases should be compared to this one to indicate the changes caused by the substitution of the Neumann boundaries for the periodic boundaries.

Periodicity along the x and mirroring along the y axis

In this case, at the boundary faces of the simulation area parallel to the yz plane a periodic condition is defined. That is as if the simulation domain would be moved in $\vec{x}$ and $-\vec{x}$ direction by the length of its x dimension. In $-\vec{y}$ and $\vec{y}$ direction the simulation domain is mirrored. This behavior can be observed in Fig. <5> and Fig. <6>. The electric field looks like, as if the one boundary parallel to yz would be directly connected to the opposite one. The stamp of the one of the electrodes which is lying on the one of the periodic faces can be seen on the other periodic face. The iso faces are not any more perpendicular to the boundaries parallel to the yz plane. Of course they are still perpendicular to the boundaries parallel to the xz plane.

Mirroring along the x and periodicity along the y axis

An interconnect bus structure is modeled, which is built by mirroring the simulation domain from Fig. <1> along the x axis and by periodic spatial iteration along the y axis. This case is similar to the previous one. As shown in Fig. <7> and Fig. <8> the potential iso faces are not perpendicular to the boundaries parallel to the xz plane, but are still perpendicular to the boundaries parallel to the yz plane. This time the boundaries parallel to the xz plane seem to be connected to each other.

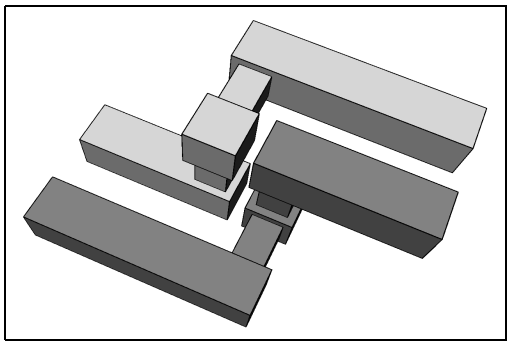

Figure 2: The Electrodes.

Periodicity along the x and y axes

In this case periodic boundaries are applied at the faces parallel to the xz and yz planes. That way the structure of Fig. <1> is spatially continued periodically in $\vec{x}$, $-\vec{x}$, $\vec{y}$ and $-\vec{y}$ directions. The potential distribution and the corresponding iso faces are shown in Fig. <9> and Fig. <10>. Each boundary parallel to the z axis looks so as if it would be connected to the opposite one. They also lie not any more perpendicular to the potential iso faces. Each electrode is placed among the second electrode in the simulation area and the imaginary periodic images. The iso faces in the simulation area look correspondingly.

As mentioned above the periodic boundary condition is not applied at the faces parallel to the xy plane. For the specific simulation domain of Fig. <1> in order to have a continuous interconnect structure in z direction only mirroring (homogeneous Neumann boundary) can be applied.

CAPACITANCE

Table <1> shows the extracted capacitance values depending on the different boundary conditions applied. C_0 is the capacitance between the conductors of Fig. <1> if at all boundary faces homogeneous Neumann conditions are applied. The capacitance of the three other cases is relative to it.

Table 1: The Capacitance Values Extracted Using Different Boundary Conditions.

x mirroring and y mirroring	C_0
x periodic and y mirroring	$1.33C_0$
x mirroring and y periodic	$1.07C_0$
x periodic and y periodic	$1.69C_0$

The smallest capacitance occurs if no periodic boundaries are specified. The biggest capacitance is in the case of x and y periodicity. The calculated capacitance values refer only to the small simulation area as defined in Fig. <1>. This simulation area is used to construct the whole domain. The capacitance of the whole area is the capacitance of the small simulation domain multiplied by the number of all small simulation domains needed to construct the complete structure.

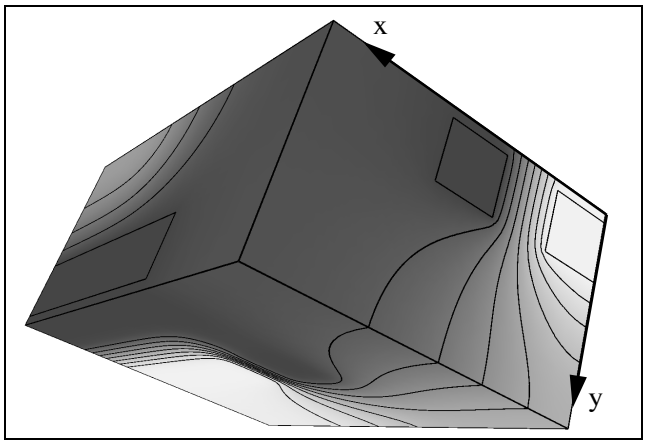

Figure 3: The Potential Distribution without Periodicity.

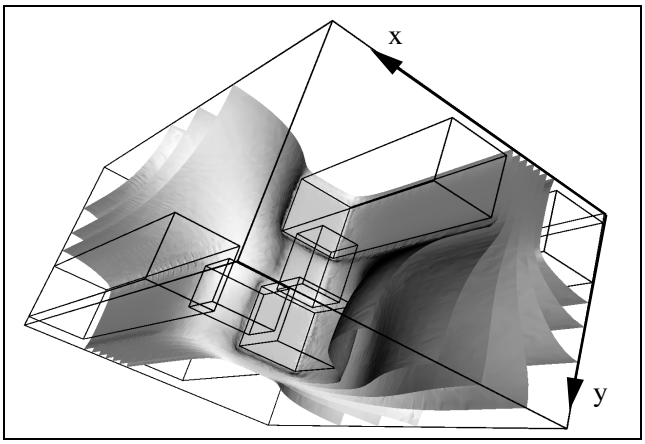

Figure 4: The Iso Faces of the Potential Distribution without Periodicity.

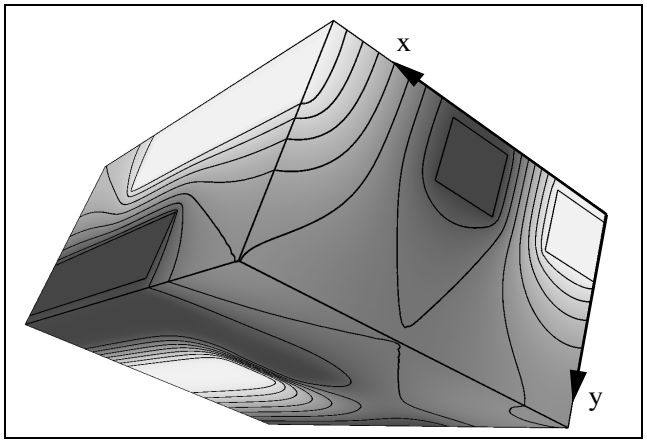

Figure 5: The Potential Distribution with x Periodicity.

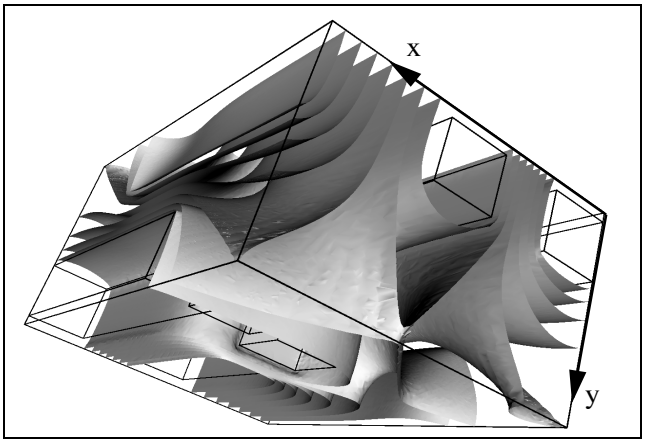

Figure 6: The Iso Faces of the Potential Distribution with x Periodicity.

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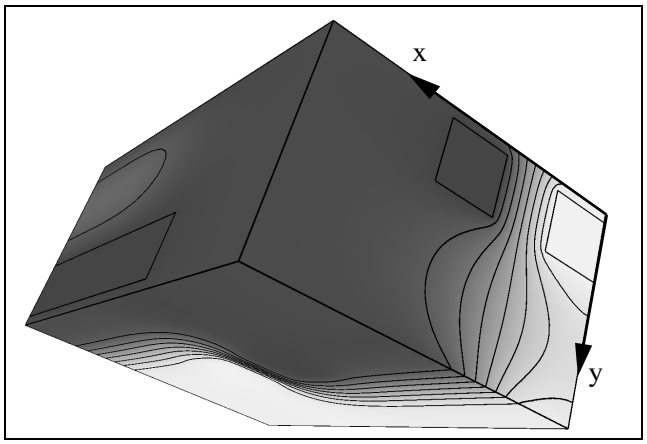

Figure 7: The Potential Distribution with y Periodicity.

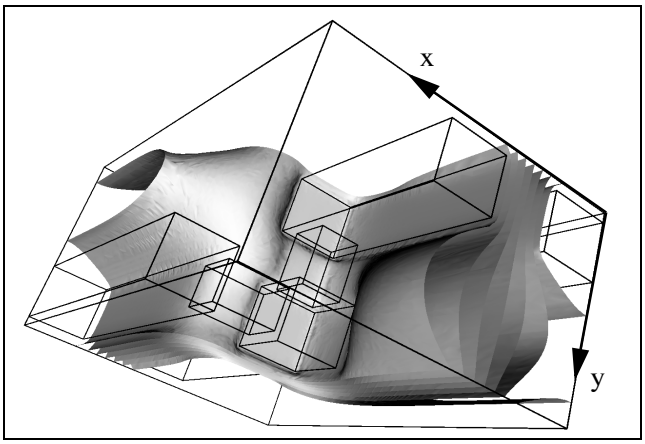

Figure 8: The Iso Faces of the Potential Distribution with y Periodicity.

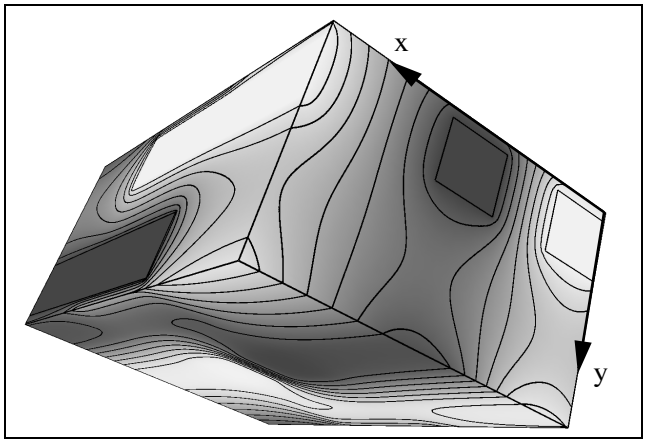

Figure 9: The Potential Distribution with xy Periodicity.

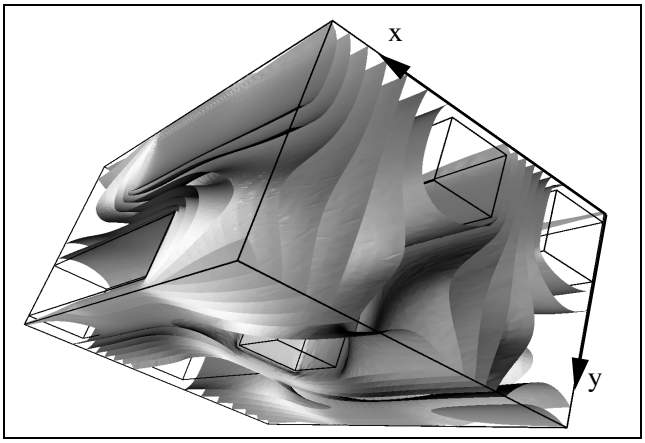

Figure 10: The Iso Faces of the Potential Distribution with xy Periodicity.

BIOGRAPHY

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