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Simulation and Measurement of Interconnects and On-Chip Passives: Gauge Fields and Ghosts as Numerical Tools

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Summary. This paper describes the present status of using lattice gauge and ghost field methods for the simulation of on-chip interconnects and integrated passive components at low and high frequencies. Test structures have been developed and characterized in order to confront the simulation techniques with experimental data. The solution method gives results that are in agreement with the measurements.

Key words: Interconnects, Integrated Passives, Characterization, Simulation, Ghost Fields

1 Introduction

With the further downscaling of deep-submicron CMOS devices a continuous increase in transistors switching rates is achieved. This allows for faster circuits and as a consequence, more powerful products become available to consumers. The downscaling not only has an impact on the speed of information processing as a result of fast switching times. Moreover, per unit chip area a much larger number of active devices is encountered. In other words: the transistor density has continuously increased over the years. This evolution was captured in the famous Moore's law [Moore (1967)] predicting that every 18 months the performance of integrated circuits will double. Derivations of Moore's law are that the cost per transistor will drop exponentially
or that the clock frequency of the integrated circuits will grow exponentially. It should be emphasized that Moore's statement has been the driver behind the tremendous growth of the semiconductor industry, but it should also be stressed that Moore's law extrapolates an early observation, that at some instance will break down because physical laws will be violated or economical constraints will not release the required investments for the technology development and manufacturing. In the present work, we are primarily interested in the physical issues that will ultimately prevent us from sustaining in agreement with Moore's prediction. Actually, our approach is based on the very conventional attitude to keep in pace with the Moore's law. As a consequence, design methodologies that worked fine in the past have to be upgraded to incorporate the new physical phenomena that come with cranking up the frequencies and densifying the active devices. Moreover, new interconnect technology is needed to guarantee that the gain in switching speed is not annihilated by interconnects that suffer from too much delay and loss. In order to achieve these goals a number of challenges need to be addressed.

Which difficulties are to be expected?

The amount of difficulties coming with further downsampling of the integrated circuit is huge. The interested reader can find a detailed account in the annual revised International Technology Roadmap for Semiconductors [ITRS (2003)]. Just to mention a view: printing the small structures on Silicon, will require further research in lithography. Keeping the source and drain well separated and at the same time reducing the channel lengths of the transistors, will require increasing control over the activation and diffusion of the dopants. The engineering of the channel will require several modifications in order to suppress the short-channel effect (SCE). The latter corresponds to lowering of the threshold voltage and results into a less clearer distinction between the on and off state of the transistor. Apart from all the difficulties ("challenges") that one encounters inside the active devices or in-Silicon, there are also many issues to be dealt with for the interconnects or the on-Silicon architecture. The transistor densification requires that the interconnects have less spacing and cross talk becomes a serious issue. Not only do interconnects act as receivers for signals in neighboring runners, the currents in the runners are also re-distributed due to the presence of signals in neighboring lines. This is the proximity effect. These effects all occur at high-frequency. Of course, the well-known skin effect also plays an important role. Signal delay is an effect of major importance and the technological way to reduce it, is by reducing the resistance of the interconnects and to reduce the capacitances of the runners. The resistance can be lowered by choosing different metallic materials (Al → Cu) and the capacitances can be lowered by using dielectric materials with a lower permittivity (lowK materials). Here, a first hard limit is encountered from physics: the lowest permittivity that ever can be reached is $\varepsilon_r = 1$, being the permittivity of vac-
uum. The lowest values that are presently available are 1.7-2.3 and belong to porous materials that suffer from mechanical stability. Therefore it is not evident that these materials are suitable for use in the back-end processing. The difficulties that we will address in this paper deal with design. Whereas at low frequencies it suffices to characterize the interconnect layout by its lumped resistance and lumped capacitance parameters, at high frequencies the full electromagnetic characterization is required. It is desired that the designer still has access to compact models that characterize the structures, the building of the these compact models requires a full electromagnetic analysis in the frequency range of interest and in three spatial dimensions. Two-dimensional considerations are too restrictive since modern interconnect layouts are done in a multi-layer pattern. By inclusion of the frequency dependence, i.e. the physics of the electromagnetic fields, above mentioned effects are captured.

2 The Maxwell Equations and the Drift-Diffusion Equations

After having described the problem under consideration, we will give in this section the physical equations corresponding to it. As was stated above, we want to obtain compact models for given structures in three dimensions that describe their current-voltage characteristics accurately. These characteristics are the results of an interplay between electromagnetic fields and their sources being the charge and current densities. The latter are described by the Maxwell equations that are summarized below:

\[
\begin{align*}
\nabla \cdot D &= \rho \\
\nabla \cdot B &= 0 \\
\n\nabla \times E &= -\frac{\partial B}{\partial t} \\
\n\nabla \times H &= J + \frac{\partial D}{\partial t}.
\end{align*}
\]

In here, \(D, E, B, H, J\) and \(\rho\) denote the electrical induction, the electric field, the magnetic induction, the magnetic field, the current density and the charge density. The following constitutive equations relate the inductances to the field strengths.

\[
B = \mu H, \quad D = \varepsilon E.
\]

The permittivity, \(\varepsilon\), and permeability, \(\mu\) and the constitutive equation that relates the current \(J\) to the electric field and the carrier densities, are determined by the medium under consideration. For a conductor the current \(J\) is given by Ohm's law:

\[
J = \sigma E.
\]
At metallic contact, we assume that the contact is such a high quality conductor, that the tangential electric field in the contact pad vanishes. In other words at the contact, we have

\[ n \times E(x, t) = 0, \quad x \in \text{contact}. \] (7)

Furthermore, at the metallic contact pad it is assumed that the perpendicular component of the magnetic induction \( B \) vanishes:

\[ B \cdot n = 0, \quad x \in \text{contact}. \] (8)

Outside the contact pads different boundary conditions can be explored. The precise implementation depends on the problem under consideration and the frequencies of interest. It should be stressed that the failure or success of a high-frequency simulation strongly depends on the proper choice and treatment of the boundary conditions. In the semiconducting regions, the current \( J \) consists of negatively and positively charged carrier currents obeying the current continuity equations.

\[ \nabla \cdot J_n - q \frac{\partial n}{\partial t} = U(n, p) \] (9)

\[ \nabla \cdot J_p + q \frac{\partial p}{\partial t} = -U(n, p) . \] (10)

In here, the charge and current densities are

\[ \rho = q(p - n + N_D - N_A) \] (11)

\[ J_n = q \mu_n n E + kT \mu_n \nabla n \] (12)

\[ J_p = q \mu_p p E - kT \mu_p \nabla p , \] (13)

and \( U(n, p) \) is the generation/recombination rate of charged carriers. The current continuity equations provide the solution of the variables \( n \) and \( p \). Up to this point we have not faced the need for introducing the Fermi potentials as well as the Poisson potential. These variables enter the description through the boundary conditions. At ohmic contacts it is assumed that charge neutrality is valid and that the applied bias is equal to the Fermi potential. In particular, in the drift-diffusion model, the carrier densities are given in terms of the Poisson and Fermi potential as

\[ p = n_s \exp \frac{q}{k_B T} (\phi_p - V) \]

\[ p = n_s \exp \frac{q}{k_B T} (V - \phi_n) . \] (14)

Using the charge neutrality, the contacts are characterized by \( p - n + N_D - N_A = 0 \) and \( \phi_p = \phi_n = V_{app} \), where the latter is the applied voltage. Since the boundary conditions are formulated in terms of potentials, it makes sense to
introduce the magnetic vector potential $A$ next to the electric scalar potential $V$ in the following way: The magnetic induction $B$ is given by

$$B = \nabla \times A$$

and using (3), the electric field is given by

$$E = -\nabla V - \frac{\partial A}{\partial t}.$$  

The Maxwell equations are expressed in terms of the potential formulation as follows:

$$-\nabla \cdot \varepsilon \left( \nabla V + \frac{\partial A}{\partial t} \right) = \rho$$

$$\nabla \times \nabla \times A = \mu_0 J - \mu_0 \varepsilon \frac{\partial}{\partial t} \left( \nabla V + \frac{\partial A}{\partial t} \right).$$

Since the operator $\nabla \times \nabla \times$ has no inverse, the vector potential is not uniquely defined and a gauge condition should be added. It is very appealing to use the Coulomb gauge since in this gauge the Poisson equation remains unaltered. In other words: the Poisson equation has no frequency-dependent terms. Thus we obtain:

$$\nabla \cdot (\varepsilon A) = 0 \quad \text{and} \quad -\nabla \cdot (\varepsilon \nabla V) = \rho$$

From (16) it follows that $E$ and $A$ should be considered on equal level. As a consequence, since $E$ is assigned to links of the computational grids, this should also be the case for the variables $A$. This observation has far reaching consequences. In order to compute link variables as fundamental unknowns, the corresponding discretization should reflect this point. Setting up discretized equations for these variables amounts to assigning a pointer to every link in the grid.

### 3 Gauge Fields and Ghost Fields

The discretization of Ampère's equation (18) can be done by applying Stokes' theorem twice [Meuris et al. (2001)]. In Fig. 1, this method is illustrated. Each link of the grid provides one equation and one unknown, i.e. the projection of $A$ along the link: $A_{ij} = A \cdot e_{ij}$, where $e_{ij}$ is the unit vector pointing from node $i$ to node $j$. However, the singularity of the $\nabla \times \nabla \times$ operator pops up as redundancy in the system of equations, i.e. the equations are not independent. In fact, the discretization of the gauge condition by applying Gauss' theorem for each node results into an additional system of equations that just eliminates the redundancy. Although we could proceed with the system of equations (17, 18, 19), there is a serious drawback in this formulation:
the combined system of equations is not square, i.e. there are more equations for the link variables as $A_{ij}$ than there are unknowns. The mismatch in the counting of the number equations and the number of unknowns corresponds to the number of nodes in the grid [Schoenmaker (2002)]. The lack of having a square matrix corresponding to the system of equations for the the link variables obstructs the use of iterative linear solvers, that are nowadays the workhorses is simulation [Schenk et al. (2004)]. However, from the observation that the size of the mismatch is just equal to the number of nodes, suggests that we could recover a square formulation by adding additional degrees of freedom. To be more precise: for each node we need one additional unknown. This strategy lies at the heart of the solving techniques exploited by MAGWEL [www.magwel.com]. The feasibility of this approach was shown in [Schoenmaker (2002), Schoenmaker et al. (2002)]. The additional collection of unknowns has been named a ghost field $\chi$. Just as the quantum ghost particles that are indispensable to formulate the problem in a mathematical consistent and computable way, this ghost field has a classical (non-quantum) basis and is also indispensable to formulate the problem in an attractive numerical scheme. Whereas in the past, only analytical efforts shaped our language to describe a physical problem we now enter into an era in which the desire to address computational methods also contributes to the language of physics. After inclusion of the ghost field, the equations (17, 18, 19) become

$$-\nabla \cdot (\varepsilon \nabla V) = \rho$$  \hspace{1cm} (20)

$$\nabla \times \nabla \times A + \nabla \chi = \mu_0 J - \mu_0 \varepsilon \frac{\partial}{\partial t} \left( \nabla V + \frac{\partial A}{\partial t} \right)$$ \hspace{1cm} (21)

$$\nabla^2 \chi + \nabla \cdot A = 0$$ \hspace{1cm} (22)
Finally, after applying a small-signal analysis by setting all variables $X = X_0 + (X_R + iX_I) \exp(i\omega t)$ we finally arrive at the system of equations that may formally be given by equation (23):

$$
\begin{bmatrix}
A(\omega) & B(\omega) \\
C(\omega) & D(\omega)
\end{bmatrix}
\begin{bmatrix}
X \\
Y
\end{bmatrix}
=
\begin{bmatrix}
F \\
G
\end{bmatrix}.
$$

(23)

In here, the vector $X$ corresponds to the usual set of technology computer-aided design (TCAD) variables and the vector $Y$ corresponds to the electromagnetic (EM) extension to incorporate high-frequency effects, i.e.

$$
X = \begin{bmatrix}
\phi_p \\
\phi_n
\end{bmatrix}, \quad Y = \begin{bmatrix}
A \\
X
\end{bmatrix}.
$$

(24)

In particular the structure of the matrix becomes

$$
\begin{bmatrix}
A_0 + \omega A_1 \\
C_0 + \omega C_1
\end{bmatrix}
\begin{bmatrix}
\omega B \\
D_0 + \omega D_1 + \omega^2 D_2
\end{bmatrix}.
$$

(25)

Starting from the formulation given above, a new simulation tool has been constructed that allows a detailed computation of the electromagnetic behavior of on-chip structures, taking into account the presence of the semiconducting substrates and the junctions therein. As can be observed from (25), we see that at low frequencies a decoupling occurs. The $B$-matrix gets small and it suffices to compute the solution $X$ that can be inserted in the second equation for $Y$. The feedback of $Y$ on the solution for $X$ is negligible. In Fig. 2, the convergence behavior is illustrated that is typically observed by iteratively solving the TCAD and the EM problem.

Gauges and Ghosts: The History in a Nutshell

The history of gauge theories is a long and fascinating story. It is likely that the story has not reached its end. Reflecting back on electromagnetism, the first scientific formulation was done in terms of forces. The Coulomb law, experimentally verified by Cavendish, gives the forces acting between charges. Similarly, the law of Biot-Savart that lies at the heart of describing magnetic interactions is also expressed in terms of forces. A major breakthrough and change in perception was introduced by Faraday, who puts emphasis on the fields. In other words: whereas for forces it is always needed to have at least two particle participating in the description of electromagnetic interactions, the fields are modifications of the surrounding space of a single particle. The reality of such vacuum modifications have become even more acceptable after the discovery that light consists of electromagnetic waves. In order to compute the properties of electromagnetic fields it turned out to be quite convenient to introduce the scalar and vector potentials $V$ and $A$. Note that this incorporates a next level of abstraction: the potentials are not uniquely defined.
and equivalent descriptions exist by making the following substitutions or performing a gauge transformation:

\[ V(x, t) \rightarrow V'(x, t) = V(x, t) + \frac{\partial A(x, t)}{\partial t} \]

\[ A(x, t) \rightarrow A'(x, t) = A(x, t) + \nabla A(x, t) \quad (26) \]

It was Hermann Weyl [Weyl (1918)] great contribution to observe that this non-uniqueness can be related to a symmetry principle: In each space-time point the local frame that determines the real and imaginary part of a quantum-mechanical wave function, may be arbitrary chosen. This means that the wave function can be multiplied with an arbitrary phase factor \( g((x, t) = \exp{iA(x, t)} \) This is an element of the unitary group \( U(1) \). Weyl named this non-uniqueness "Maaßstab" (gauge) invariance. In 1954, C.N. Yang and R. Mills proposed a model that generalizes the group \( U(1) \) to a non-abelian group \( SU(2) \) The Weinberg-Salam model for weak interactions is (1967) is the first successful application of this idea. Soon the next success was recorded by applying the Yang-Mills concepts to the strong interactions that resulted into the theory of quantum-chromodynamics. Here the symmetry group is \( SU(3) \). Nowadays, so-called gauge theories are the basis for our understanding of fundamental interactions.

The use of gauge theories was very much enforced by the aim to understand the elementary particles at the quantum level. However, the quantization of
gauge theories was hampered precisely because of the underlying gauge invariance. A major achievement was realized by Fadeev and Popov Feynman and 't Hooft who were able to respect unitary principles by introducing a fictitious particle, a ghost particle that is only present inside closed loops of the scattering Feynman diagrams. The ghost particle paved the road towards a consistent quantization of gauge theories.

With the advent of computers, the ghost particle also can play an important role. This ghost field differs essentially from the quantum ghost field. Whereas the latter carries energy, albeit only inside virtual processes, i.e. inside quantum loops, the 'computational' ghost field is a zero-energy field. The field exists, i.e. is different from zero, while the computation is still iterating towards its solution. When arriving at the solution the computational ghost field fades out.

Ghost fields may appear a nuisance in modern physics. However, if one classifies ghost fields as indispensable computational but unphysical dynamical variables or degrees of freedom, they have been used for many years. An example is provided by the electromagnetic fields in the Lorentz gauge in free space. The Green function of this field is:

\[
G(k, \omega) = \frac{\delta^{\mu, \nu}}{|k|^2 - \omega^2 + i\varepsilon},
\]

where \(\delta^{\mu, \nu}\) with \((\mu, \nu = 0, 1, 2, 3)\) is the Minkowski metric of space and time.

\[
\delta^{\mu, \nu} = \begin{bmatrix}
-1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{bmatrix}
\]

Let the electromagnetic wave propagate in the z-direction. There are two transversal components, \(A_x\) and \(A_y\). Actually the time component, that corresponds to the \(\delta^{00} = -1\) weight of the Green function, is unphysical. This part cancels the longitudinal component, i.e. \(\delta^{33} = 1\), that is also unphysical, such that only the two physical transversal components remain. One can fairly say that the fields \(V\) and \(A_z\) are ghost fields for the description of electromagnetic waves in free space. An application of these ideas in computational electromagnetism is provided by a transformation of the variables \((V, A, \chi)\) to the variables \((V, E)\), by using \(A = \frac{1}{\varepsilon}(E + \nabla V)\). In this formulation, \(V\) can also be viewed as a ghost field. Note that a ghost field is still needed to regulate the singular operation \(\nabla \times \nabla \times E\).

4 Applications

In the section, we will present a number of applications. The examples illustrate how high-frequency effects are manifest in on-chip structures and how
the environment consisting of the substrate and dielectric material will impact the results. The first example shows that substrate currents are induced by high-frequency signals in the runners above the substrate. The second example discusses a metal-insulator-metal capacitor. It is shown that the lumped element parameter, i.e. the capacitance, varies as a function of the frequency. The third example shows how co-planar strip lines can be characterized starting from the Maxwell equations and the constitutive equations and deriving the lumped-element parameters. In the fourth example, a full analysis is done of a spiral inductor above a conductive substrate.

Substrate Currents.

A U-shaped conductor is positioned above a conductive substrate as is illustrated in Fig. 3. The conductor is biased with a high-frequency AC signal. An alternating magnetic induction is injected in the substrate and Faraday's law implies that circular electric fields are generated in the substrate. Since the substrate is conductive, eddy currents will flow. Naively, one might expect to interrupt the flow of the eddy currents by putting insulating trenches in the substrate. In Fig. 3, a "+"-shaped trench is etched in the substrate. This will indeed have some effect, however as can be seen in the Fig. 3, the eddy currents are still present. This is because displacement currents will be induced in the trenches. This example illustrates that in order to characterize structures that are composed of dielectrics and conductive materials at high-frequencies, all terms in the Maxwell equations are needed for capturing the full physical picture.

Fig. 3. Lay-out of a U-turn structure above a conductive substrate (left). The induced substrate current is shown in the right figure.
Metal-Insulator-Metal Capacitor

In Fig. 4, the lay-out of the MIM capacitor is show. Above a substrate, a metallic layer is deposited. Next a thin layer or dielectric is deposited and next a second metallic plate is deposited. Above this plate a 'thick' layer of dielectric material is deposited and the contact pad is attached. The contact pad is attached to the second metallic plate of the condenser by a grid of vias that are etched in the top dielectric layer. The vias are seen in Fig. 4.

Fig. 4. Lay out of the Metal-Insulator-Metal (MIM) capacitor.

Fig. 5. Comparison of the measured and simulated capacitor of the MIM structure as a function of the frequency.
A coplanar line for which the lay-out is shown in Fig. 6 was simulated in a frequency range from 1GHz to 30GHz. At these frequencies, the skin effect and current crowding are present in the structure. Both effects are clearly shown in Fig. 7. The simulation shows that, when using all terms in the Maxwell equations, it is possible to capture the full physical picture and determine the line parameters. In Fig. 8, Fig. 9 and Fig. 10, a comparison is shown between the simulated line parameters and the measured line parameters. Even at high frequencies, there is a very good match between simulation and experiment.
Fig. 8. The resistance of the coplanar line.

Fig. 9. The inductance of the coplanar line.

Fig. 10. The capacitance of the coplanar line.

**Spiral inductor**

One of the standard examples of on-chip passives is the design of a spiral conductor. The structure under study is depicted in Fig. 11. This design is car-
ried out by austriamicrosystems in the framework of the CODESTAR project. The Q-factor has been measured and simulated and the results are shown in

**Fig. 11.** The geometry of the spiral inductor under study.

**Fig. 12.** The Q-factor as a function of frequency. The measurements are indicated by solid line, while the simulation result is shown as a dashed line.
Fig. 12. The simulation is carried out using a mesh of 44550 nodes, in a simulation domain of 1000 \( \mu m \times 1000 \mu m \times 307.56 \mu m \), for 24 frequency points in a frequency range from DC to 23 GHz.

The simulation predicts the location of the resonance frequency. At this frequency the electric energy equals the magnetic energy and the structure's behavior changes from inductive to capacitive and the resulting quality factor vanishes.

5 Conclusions

This paper presented an approach to handle on-chip electromagnetic effects. The underlying idea is that at high frequencies, the inductive parts of the electric fields are a substantial fraction of the total electric field. This is clearly illustrated for the skin effect: at the inner part of the runner where the skin effect is manifest, the inductive part of the electric field will compensate the external electric field with the result that the total electric field vanishes. As a consequence, no current is present. In general, at high frequencies the inductive effects will be present ubiquitously. The computation of these fields requires that the environment is faithfully included in the set up of the computation. In particular, the simulation of part of the integrated circuits puts severe demands on the structure editor. Whereas "toy" problems can still be edited using rather elementary building blocks, the industrial problems need much more powerful tools to prepare the simulation. Within the EUI project CODESTAR, a structure editor is developed that is capable of reading GDS files. The latter contain the mask information that is needed to print the on-chip structures. The geometrical data is very fine-detailed, since processing constraints are also taken into consideration. For example, the vias that connect the metal layers in Fig. 4, are drilled in a 0.35 micron technology. This via structure introduces about 10,000 additional nodes in the grid. Keeping in mind a rule of thumb that every node introduces 10 fundamental unknowns, the computational burden that induced by the vias is tremendous. For that reason mesh cleaning is a necessity and tools for that purpose have been developed. Once that an appropriate mesh has been found, the computation of the fields should be done. Now the boundary conditions come into the picture. For TCAD-alike problems, the boundary conditions for the vector potential can be chosen of the Dirichlet type. In the simulations that have been discussed in this paper, the boundary conditions for the vector potential was chosen to be \( A_{ij} = 0 \) for the link \( ij \) being at the surface of the simulation domain and \( \chi_i = 0 \) for node \( i \) being at the surface of the simulation domain. Such an approach requires a sufficient amount of space around the structures of interest in order to capture the electromagnetic energy. This free-field space adds additional grid nodes to the computational problem and hands-on experience has to be gathered to find sensible trade-off between accuracy and speed. Our method to discretize the vector potential by taking into account
its geometrical meaning, i.e. by respecting the fact that it is a vector field, contrary to a scalar field, turns out to be beneficial in the sense that even rather crude meshes are able to grab the behavior of these fields under high-frequency biases. There is a lesson to be learned from this observation: The discretization of physical fields should be guided by the geometrical character of the field under consideration. Many software tools implicitly take this aspect already into account. However, there are also numerous tools that ignore the geometrical connection and assign vectors (one-forms) and surfaces (two-forms) to the nodes of the computational grid. Our observations discourage such implementations.

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