On the Inclusion of Floating Domains in Electromagnetic Field Solvers

Wim Schoenmaker
and Peter Meuris
MAGWEL NV
Leuven, Belgium
Email: wim@magwel.com, peter@magwel.com

***Abstract*— Floating regions in general-purpose electromagnetic field solvers are included by equation expansion, thereby converting a singular matrix into a regular square matrix.**

I. Introduction

Floating regions in device simulation are a potential source of convergence problems due to the singular character of the matrices that need to be inverted during the iteration towards the solution in the Newton-Raphson method. Floating regions typically occur if there exist domains where charge can get trapped. Such domains can be n-type regions surrounded by p-type domains, p-type regions surrounded by n-type domains, n- or p-type regions surrounded by insulators and variations thereof. Physically, the origin of the singular nature of the Newton-Raphson matrix is quite obvious: if the value of the trapped charge is not taken into account, as is often the case, then the solution is not unique (a different value of the total trapped charge gives rise to a different potential level). The mathematical problem is ill-posed and the result is a numerical problem that gives rise to convergence problems such as norm oscillations [1]. Several work-around methods have been suggested in the past. One option is to exploit transient simulations, thereby carefully controlling the amount of trapped charge. Another solution has been to introduce an artificial contact to the floating region and together with the constraint that no current is flowing into this contact. Finally, one can exploit the recombination-generation term in the drift-diffusion equations and elevate the isolating status of the floating region. Whereas, the latter option is feasible for floating regions that are only shielded from the contacts by pn junctions, e.g. SOI devices, such a work-around is not possible if the floating region is truly insulated. This is the case if the region is fully surrounded by insulators. Furthermore, if the floating region is metal surrounded by insulating materials, e.g. floating gates or dummy structures in the interconnect layout, then such an approach is not possible and alternative solutions must be found. Here, we will present such an alternative method that explicitly takes into account the trapped charge in the floating domain. We will concentrate here on floating metallic regions.

Recently, we introduced a method for solving electromagnetic field problems by including an additional scalar ghost field that needs to be obtained as part of the solution method. The solution for this additional field does not carry energy and can be viewed as being a mathematical aid that allows for the construction of a gauge-fixed, regular matrix representation of the curl-curl operator acting on edge elements [2], [3], [4], [5].

Instead of the curl-curl operator combined with the gauge condition

$$\mathcal{M}_{\rm old} = \left[\begin{array}{c} \nabla \times \nabla \times \\ \nabla \cdot \end{array} \right] , \quad (1)$$

leading to a sparse, well-posed, but non-square matrix $\mathcal{M}_{\rm old}$ that acts only on the vector field $\mathbf{A}$, the operator

$$\mathcal{M}_{\rm new} = \left[\begin{array}{cc} \nabla \times \nabla \times & \gamma \nabla \\ \nabla \cdot & \nabla^2 \end{array} \right] , \quad (2)$$

is considered that acts on the pair of variables $\mathbf{A}$ and a ghost field χ, according to

$$\mathcal{M}_{\rm new} \star \left[\begin{array}{c} \mathbf{A} \\ \chi \end{array} \right] = \mu \left[\begin{array}{c} \mathbf{J} - \epsilon \frac{\partial}{\partial t} \mathbf{E} \\ 0 \end{array} \right] . \quad (3)$$

This operator leads to matrices $\mathcal{M}_{\rm new}$ that are sparse, regular, square and semi-definite. Implicitly, we made an important conceptual step : by adding additional degrees of freedom, e.g. the ghost-field variables χ, we turned a numerically unattractive problem into an easy one: although the starting problem was well-defined it is problematic due to the fact that the matrices that need to be solved are not square. The extra degrees of freedom transformed the problem into one which generates well-defined and square matrices. Having noted this message, we will deal with the floating regions in a similar way : the inclusion of additional degrees of freedom will assist in turning an unsolvable (singular) problem into a solvable (regular) problem. In particular, we will address a long standing problem of dealing with floating domains in general-purpose electromagnetic field solvers.

II. Problem Description

In general-purpose electromagnetic field solvers the constitutive laws for the current densities are used in such a way that they reflect the material properties of the underlying domain. In particular, for metals Ohm's law is used in the form

$$\mathbf{J} = \sigma \mathbf{E} = -\sigma \nabla V , \quad (4)$$

 0-7803-7826-1/03/$17.00

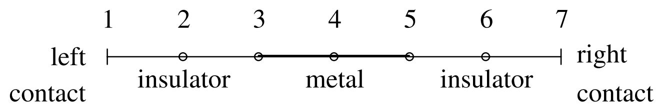

Fig. 1. Grid of a one-dimensional structure of a metallic region squeezed between two insulating regions.

together with the continuity equation :

$$\nabla \cdot \mathbf{J} = 0\ . \tag{5}$$

In insulating regions the Poisson equation

$$-\nabla(\epsilon \nabla V) = \rho \tag{6}$$

is solved. Continuity at the interfaces between metallic and insulating regions should be guaranteed. A finite-element implementation of both equations for the several domains automatically takes the continuity into account, but ignores the fact that *no* currents flow in the floating regions, since the finite-element method as well as the box-integration method refer to the *balance* of the current flow in the metallic nodes. Since the metal-insulator nodes do participate in the current balance, the latter ones are dealt with according to their metallic nature. All this works fine as long as the metal is not floating. However, for floating regions, this implementation leads to solutions that describe constant currents in the metallic regions, thereby respecting the balance in the metal nodes but at the same time putting arbitrary values of the potential on the interface nodes.

In order to illustrate above remarks we consider a simple one-dimensional static problem that is described with a grid of seven nodes. However, the idea can be equally applied to bigger problems at higher frequencies. A metallic domain is squeezed between two insulating regions as is illustrated in Fig. 1. There are five variables $(V_2, V_3, V_4, V_5, V_6)$ for which the finite-element equations read :

$$\begin{bmatrix} -2\epsilon & \epsilon & 0 & 0 & 0 \\ 0 & \sigma & -\sigma & 0 & 0 \\ 0 & -\sigma & 2\sigma & -\sigma & 0 \\ 0 & 0 & \sigma & -\sigma & 0 \\ 0 & 0 & 0 & \epsilon & -2\epsilon \end{bmatrix} \star \begin{bmatrix} V_2 \\ V_3 \\ V_4 \\ V_5 \\ V_6 \end{bmatrix} = \begin{bmatrix} -\epsilon V_1 \\ 0 \\ 0 \\ 0 \\ -\epsilon V_7 \end{bmatrix} \tag{7}$$

It can be easily checked that the determinant of the matrix in (7) is zero. A basis for the null space is given by the vector $\mathbf{v}_0 = (1/2, 1, 1, 1, 1/2)$. Therefore, any vector that obeys equation (7) can be displaced by an arbitrary amount proportional to $\mathbf{v}_0$. For such a small system one can easily recognize the singularity of the matrix, however this is not longer the case for real world problems. For such problems, the matrix is huge and also the linear system can be solved to get *a solution*. With this treatment of the floating areas their potential value is undefined, and can become whatever value due to the ill-posedness of the problem and the singularity of the corresponding matrix.

Thus we find that the cause of the arbitrariness is the ill-posed formulation of above assignment of the various equations for the Poisson potential. For the potentials at the nodes, the discretized problem reads

$$\mathcal{M}_{\text{float}} \star [\mathbf{V}] = [\mathbf{b}]\ , \tag{8}$$

where $\mathbf{V}$ is the column vector of the Poisson potential at the internal nodes and $\mathbf{b}$ describes the coupling to the contacts. $\mathcal{M}_{\text{float}}$ is a singular matrix.
In the spirit of the ghosts, we will now transform this problem into a regular one by extending the size. In other words, we will construct a *regular* matrix and a larger vector for the unknown variables such that the floating region problem is described by the following equation :

$$\begin{bmatrix} \mathcal{M} & \mathcal{P} \\ \mathcal{Q} & \mathcal{N} \end{bmatrix} \star \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{0} \end{bmatrix}\ , \tag{9}$$

where $\mathcal{P}, \mathcal{Q}$ and $\mathcal{N}$ are extra entries for making the complete matrix non-singular and keeping it square at the same instant.

III. Proposed Solution

In order to construct the extended matrix system we will use the fact that the total charge on each floating region is fixed. Moreover, since no current can flow in the floating regions, each region has a fixed value of the potential, V_{fl}. These two facts suffice to perform the construction. From Gauss' law we find that for the k-th floating region, we must add to the evaluation of the Poisson equation at the insulator side of the interface, a charge term

$$\rho_i = \sum \epsilon \Delta A_i \left(V_{\text{fl}}^k - V_i \right)\ , \tag{10}$$

where the sum runs over all nodes in the insulating region that couple to the k-th floating region and ΔA_i is the interface area assigned to the i-th node. The variable V_{fl}^k can be added to the vector $\mathbf{y}$, thereby extending the set of unknowns. At the same time we obtain the entries for the matrix part $\mathcal{P}$, since they follow from the Newton-Raphson derivatives $\partial\rho/\partial V_{\text{fl}}^k$. The additional equations follow from setting the total charge that is trapped on each floating region : all that needs to be done is to sum the charge density that is stored at each node of the surface of the k-th floating region. Therefore, each floating region generates one additional equation. The sums determine the matrix parts $\mathcal{Q}$ and $\mathcal{N}$. Finally, we note that the node equations for the Poisson potentials at the interfaces are simply

$$V_{\text{int},i} - V_{\text{fl}}^k = 0\ . \tag{11}$$

Using the simple example of Fig. 1, we arrive at the following non-singular matrix problem :

$$\begin{bmatrix} -2\epsilon & \epsilon & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & -1 \\ 0 & -\sigma & 2\sigma & -\sigma & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & \epsilon & -2\epsilon & 0 \\ -1 & 0 & 0 & 0 & -1 & 2 \end{bmatrix} \star \begin{bmatrix} V_2 \\ V_3 \\ V_4 \\ V_5 \\ V_6 \\ V_{\text{fl}}^1 \end{bmatrix} = \begin{bmatrix} -\epsilon V_1 \\ 0 \\ 0 \\ 0 \\ -\epsilon V_7 \\ Q^1/\epsilon \end{bmatrix} \tag{12}$$

IV. Example

A. Example 1

We have inserted above ideas in a general-purpose electromagnetic field solver. In Fig. 2, a structure is depicted with two floating metallic regions and an applied bias of two Volts from the bottom contact to the top contact. In Fig. 3, the potential along a cut line from the bottom contact to the top contact is shown that is obtained by solving the problem according to above described method. Note that the potential in the metal regions is flat (equipotential) and that the level is between the values of the applied biases (no charge was put on the floating regions).

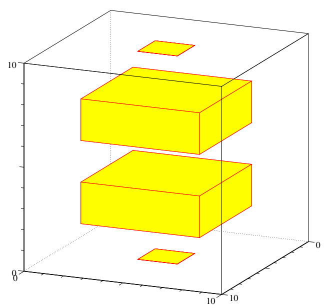

Fig. 2. Two floating metallic regions embedded into an insulating volume and two contacts.

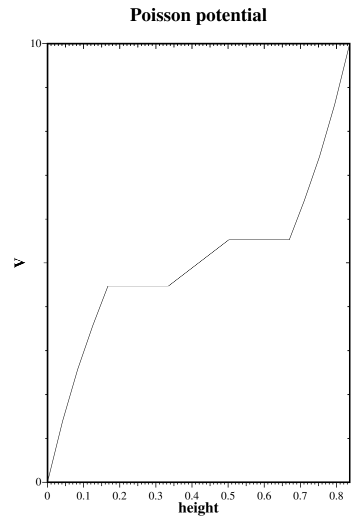

Fig. 3. The Poisson potential along a line from the bottom to the top contact.

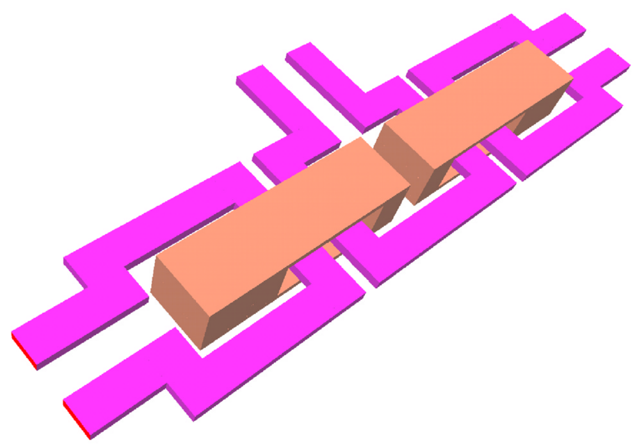

Fig. 4. A 3D view of the geometry of a ring transformer used to show the validity of the method.

B. Example 2: A transformer system

To show that the method also works on a more complex application, we examined the system shown in Figure 4.

A three-ring transformer system has been analyzed. Three metal rings in the horizontal plane, containing each two ports (or contacts) are connected by two metal floating regions (rings in the vertical plane). Although we restrict the analysis to the static case, also the high-frequent analysis can be carried out with the same method as will be shown later. The transformer is embedded in a dielectric.

All the ports of the rings have zero-voltage boundary conditions for the electric potential, except for one of port of one ring (Figure 5). The rings with zero-voltage boundary conditions are equipotential volumes at zero Volt as expected. The floating areas in between are also equipotential volumes. Their potential value is fixed by the extra condition (10).

One of the advantages of this technique is the treatment of trapped charges. Indeed in equation (12), the variable Q^i pops up. This charge stands for the trapped charge on the floating region i. The influence of the trapped charge on the solution of the Poisson problem, can be studied very easily using this technique. Additional positive (negative) charge will increase (decrease) the floating potentials.

V. Initial Guess

In realistic simulations the additional equation for each floating region involves the nodes of surface of the floating domain. Although this number of nodes is an order of magnitude less than the total number of nodes, it represents still a considerable amount of non-local coupling. As a consequence the matrix inversion (in practice: the iterative solving procedure) is hampered by such a degree of non-locality.

Moreover, the new matrix (12) is not symmetric and the

 0-7803-7826-1/03/$17.00

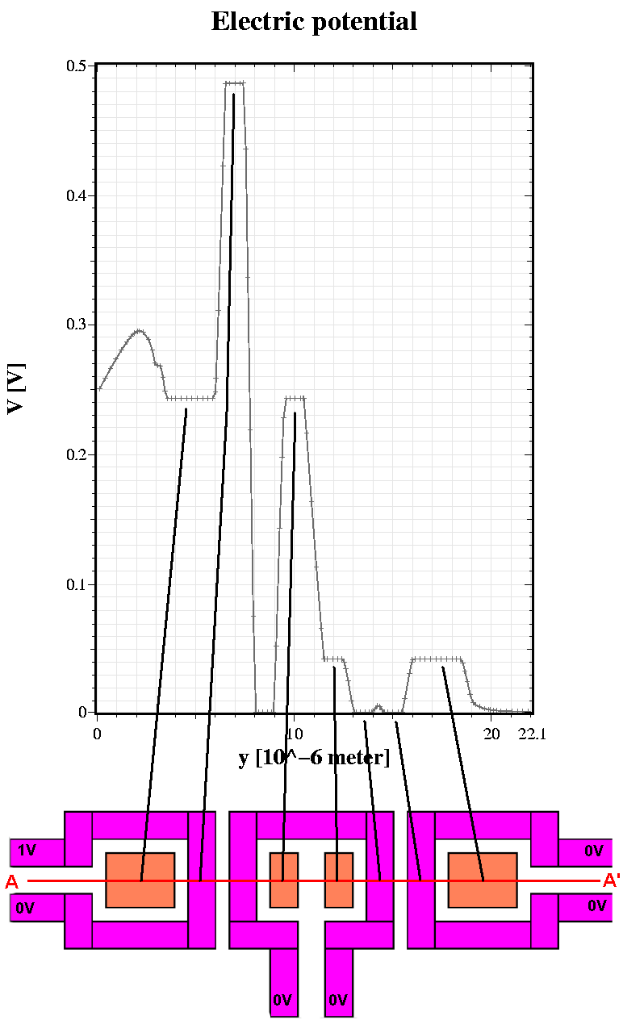

Fig. 5. The electric potential along the line AA' in the cross-section. The applied potentials on the ports are also shown.

conjugate gradient method for symmetric systems, that exist for solving this kind of systems fails.

In order to improve the iterative solution scheme, a good initial guess will usually substantially reduce the calculation time. For floating regions, one may obtain a good initial guess by realizing that the Poisson potential is constant in each floating domain. A neglegible gradient of the Poisson potential can also be obtained by treating the metal as a high-K dielectric material, since the large permittivity will force the electric field to become small. Therefore, as an initial guess this approach will lead to almost flat Poisson potentials in the floating domains. The cusp in the potential at the interface nodes is fully determined by the the ratios of the permittivities and therefore in general this initial guess work fine, if the total charge on the floating domain vanishes.

VI. High-frequency problems

The present method is robust and also gives a detailed insight in how to handle time-dependent problems. In the latter case, one finds that floating regions do carry currents due to inductance effects. These currents are fully displacement currents. It suffices to realize that the electric field is obtained as

$$\mathbf{E} = -\nabla V - \frac{\partial \mathbf{A}}{\partial t} \tag{13}$$

The first term corresponds to a conservative field and can therefore be dealt with as before in floating domains. In other words, we have that $\mathbf{E} = \mathbf{E}_{\mathrm{C}} + \mathbf{E}_{\mathrm{NC}}$, where the first term is the conservative contribution arising from the scalar potential and the second term is the electric field arising from inductive effects which is in general non-conservative. In floating regions we can put $\mathbf{E}_{\mathrm{C}} = 0$, therefore the electric field is *fully* inductive.

We can also argue that with the choice of the Coulomb gauge, the poisson eqation for the electric potential remains the same for the static and the dynamic treatment. This means that also Gauss' law must hold for the dynamic regime, and that we can write down (10) in the dynamic regime.

VII. Conclusions

We presented a new method for solving floating domain problems. The method is based on treating each floating region potential as an additional unknown variable that can be determined from demanding that the total charge on the floating region has a prescribed value.

The novelty of the method consists in the way of handling the metallic nodes inside the floating region: their degrees of freedom are not eliminated in favor of the floating potential. In stead, the degrees of freedom corresponding to the floating regions, are treated according to the local Ohm's law as is done for non-floating metallic domains.

Results on test problems correspond with the expected values. If trapped charge is introduced, the corresponding floating region potential is shifted.

Acknowledgements

This work was partly financially supported by the European Union, in the framework of the IST project CODESTAR. Wim Magnus is greatfully acknowledged for valuable comments and inspiring discussions. The authors thank Michael Verschaeve and Erik Janssens for additional help on the implementation of these ideas and for the testing. Also Chris Kerner is kindly acknowledged for his contribution to the ring system.

References

[1] S. P. Edwards K. J. Yallup and K. De Meyer, *Two-dimensional Numerical Analysis of the Floating Region in SOI MOSFET's*, IEEE Trans. on ED, **35**, 7, 1012–1020, July 1988

[2] P. Meuris, W. Schoenmaker and W. Magnus, *Strategy for electromagnetic interconnect modeling*, IEEE Trans. on CAD, **20** , 6, 753–762, June 2001

[3] W. Schoenmaker, P. Meuris, *Electromagnetic interconnects and passives Modeling : Software Implementation Issues*, IEEE Trans. on CAD , **21**, 5, 534–543, May 2002

[4] W. Schoenmaker, W. Magnus, P. Meuris, *Ghost fields in Classical Gauge Theories*, Phys. Rev. Lett., **88**, 18, May 2002

[5] W. Schoenmaker P. Meuris W. Magnus and B. Maleszka, *Simulation of Substrate Currents*, Proc. SISPAD 2002 Kobe, Japan.