The stabilising effect of ghost field gauging on numerical simulations of Maxwell's equations

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ABSTRACT

Recently an approach was presented to model the electromagnetic environment of passive on-chip structures. This method was developed to describe high-frequency effects such as skin effect, proximity effect, current redistribution etc. As it uses a potential description of Maxwell's equations, an appropriate choice of the gauge condition is necessary for the uniqueness of the solution. The standard way to introduce this gauge condition is the construction of a 'gauge tree'. This is a highly non-local procedure to eliminate the independent variables and to end up with a uniquely defined potential. We propose a new way of gauge fixing by introducing an extra set of independent variables, a ghost field. This technique called 'ghost field gauging' is beneficial because it results into a local assembling method. In this paper we will show that ghost field gauging is numerically stable, and with the appropriate choice of a parameter, the tuning factor that can be chosen at wish, it is shown that the condition number of the resulting matrix can be reduced by some order of magnitudes. This is extremely beneficial for the iterative methods that we use to solve large and sparse systems of linear systems that arise in solving electromagnetic field problems.

INTRODUCTION

A new approach was presented [1-5] to model the electromagnetic environment of passive on-chip structures. This method was developed to describe high-frequency effects such as skin effect, proximity effect, current redistribution etc. The description includes also a detailed semiconductor behavior. The solver is three dimensional on a Cartesian grid, and the description is carried out in frequency domain.
The electromagnetic environment is characterized by a scalar electric potential V and a magnetic vector potential A.

$$-\nabla\cdot\left(\varepsilon\nabla V + \mathrm{j}\omega\varepsilon\,\mathbf{A}\right)=\rho \qquad (1)$$

$$\nabla\times\left(\nabla\times\mathbf{A}\right)=\mu_0\mathbf{j}-\mathrm{j}\omega\,\mu_0\,\varepsilon\left(\nabla V+\mathrm{j}\omega\mathbf{A}\right) \qquad (2)$$

Because the potentials are not uniquely defined, we must add a gauge condition. The most commonly used gauge condition is the Coulomb gauge

$$\nabla\cdot\mathbf{A}=0 \qquad (3)$$

because this reduces the first equation to the electrostatic approach. However, the system (1-3) is not easy to solve in a discretized version. Equation (1) becomes a simple Poisson equation for which solution methods exist. Solving (2-3) is more cumbersome. Assigning the vector potential **A** to the links, leaves us with a singular system [7,9] that makes it difficult to solve with standard iterative techniques [10]. In order to obtain a consistent and stable discretization scheme, a ghost field χ is introduced [1]. The Maxwell equations and the gauge condition, are described as follows ($\mu=\mu_0$):

$$-\nabla\cdot\left(\varepsilon\nabla V + \mathrm{j}\omega\varepsilon\,\mathbf{A}+\mathrm{j}\omega\varepsilon\,\nabla\chi\right)=\rho \qquad (4)$$

$$\nabla\times\left(\nabla\times\mathbf{A}\right)-\gamma\nabla\chi=\mu_0\mathbf{j}-\mathrm{j}\omega\,\mu_0\,\varepsilon\left(\nabla V+\mathrm{j}\omega\mathbf{A}+\mathrm{j}\omega\nabla\chi\right) \qquad (5)$$

$$\nabla\cdot\mathbf{A}+\nabla^2\chi=0 \qquad (6)$$

In here ρ and J stand for the free charge and current density. The constant γ (tuning factor) guarantees matching of dimensions and can take any real value, except zero. The expression $\nabla\chi$ vanishes for all physical solutions, and hence no spurious currents are introduced by the ghost field.
Besides Maxwell equations, appropriate constitutive laws must be considered. For dielectrics, no additional relations are needed. For conductors, the current continuity equation is solved together with Ohm's law.

$$J = \sigma E \qquad (7)$$

$$\nabla . J + j\,\omega\,\rho = 0 \qquad (8)$$

Both equations are then expressed in the independent potential variables (V, A and χ). The standard drift-diffusion equations are solved in the semi-conductor regions.

$$\nabla \cdot \mathbf{j}_n - j\omega q\, n = U(n,p) \quad (9)$$

$$\nabla \cdot \mathbf{j}_p + j\omega q\, p = -U(n,p) \quad (10)$$

In here, the charge and current densities are:

$$\rho = q(p - n + N_D - N_A) \quad (11)$$

$$\mathbf{j}_n = q\mu_n n\mathbf{E} + kT\mu_n \nabla n \quad (12)$$

$$\mathbf{j}_p = q\mu_p p\mathbf{E} - kT\mu_p \nabla p \quad (13)$$

$$\mathbf{j} = \mathbf{j}_n + \mathbf{j}_p \quad (14)$$

and U(n,p) is the generation/recombination of charge carriers. This results in two extra independent variables (n and p), i.e. the semiconductor carrier densities.

STATIC APPROACH

Although the method also works for high frequency effects, such as skin effect, current crowding and substrate currents [8], we will restrict the remainder of this paper to the static-stationary system. In this approach we get the following version of the Maxwell equations by setting ω to zero in (4-6):

$$-\nabla \cdot (\varepsilon \nabla V) = \rho \quad (15)$$

$$\nabla \times (\nabla \times \mathbf{A}) - \gamma \nabla \chi = \mu_0 \mathbf{j} \quad (16)$$

$$\nabla \cdot \mathbf{A} + \nabla^2 \chi = 0 \quad (17)$$

In order to solve these equations, we use the discretization assignments as depicted in Fig. 1. The electric potential V, the ghost field χ, n and p are associated with the nodes of a Cartesian gridding. For a correct evaluation the vector potential needs to be associated with the links [6, 14].

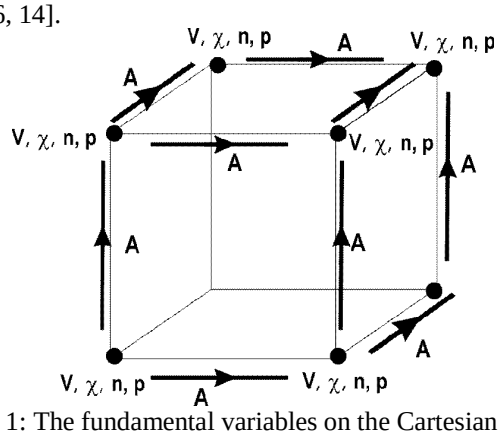
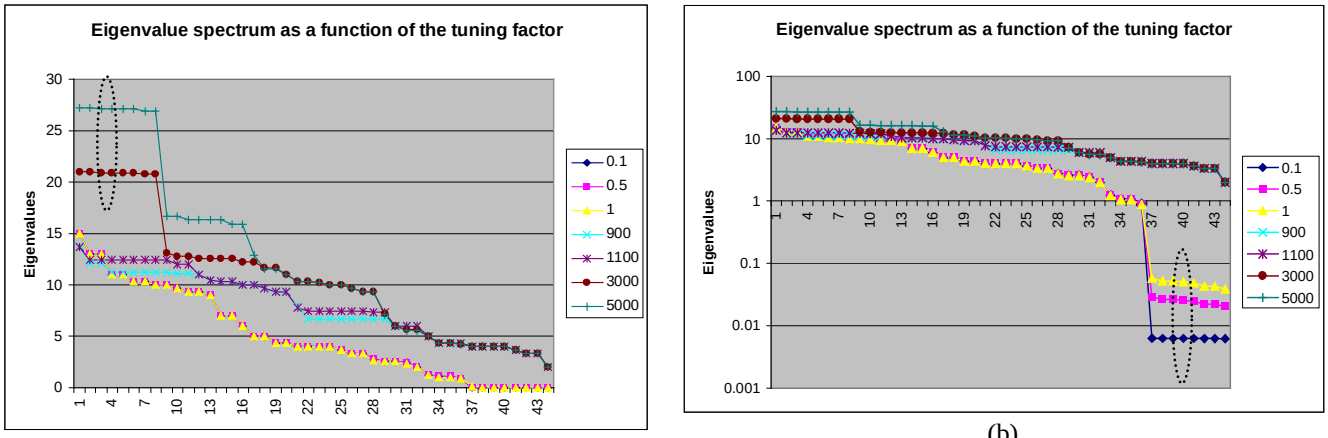


Fig. 1: The fundamental variables on the Cartesian grid

In order to solve (15-17), the differential operators are constructed, leading us to a Newton-Raphson matrix for the electric approach (15) giving rise to a Poisson operator. The electric potential in all nodes act as unknowns. With the knowledge of the electric potential, the current density and hence the RHS of (16) can be constructed. This makes it possible to construct the Newton-Raphson operator for (16-17), with **A** and χ as unknowns. However this matrix depends on the tuning factor γ. This parameter has the dimension (m^{-2}), and is introduced for dimensional reasons.

CONDITION NUMBER AS A FUNCTION OF THE TUNING FACTOR

The Newton-Raphson matrix is usually solved by iterative techniques. To mention some examples, it may be the preconditioned restarted generalized minimum residual method (RGMRES) [11], the preconditioned conjugate gradient squared method (CGS) [12] or the bi-conjugate gradient stabilized method (Bi-CGSTAB) [13].



(a) (b)

Fig. 2. The eigenvalue spectrum for different values of the tuning factor γ using a linear (a) and a logarithmic scale (b).

The condition number is defined as the ratio between the highest and the lowest eigenvalue of the system. When the condition number is high, there is strong correlation with slow convergence of most iterative systems. Therefore we consider the influence of the tuning factor on the condition number of the matrix generated by discretizing the system (16-17).

A system with 44 degrees of freedom is examined. This is a small system in order to keep the analysis tractable, but the same conclusions hold for larger systems. In Fig. 2, we see the eigenvalue spectrum for different values of the tuning factor using a linear and a logarithmic scale. For the limit of vanishing values of γ, the situation is reduced to the singular system (2-3). This is shown in Fig 2b: for low values of γ, we see that the smallest eigenvalues are nearly constant and get smaller for lower values of the tuning factor, resulting in a high condition number for the matrix. Figure 2a shows us that for high values of the tuning factor, the nearly constant eigenvalues pop up at the other end of the spectrum, resulting again in a high condition number. For intermediate values the lowest condition number can be found. Figure 3 shows the condition number as a function of this tuning factor and we see indeed that a good choice of this factor will result in lower condition numbers.

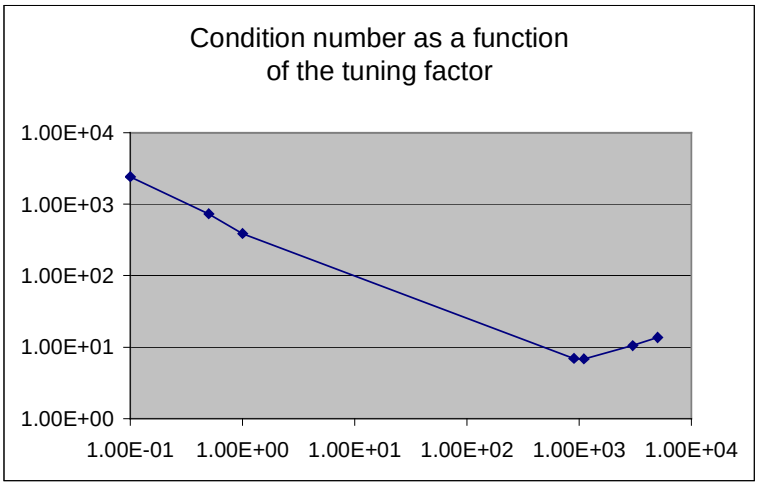


Fig. 3. The condition number of the matrix (16-17) as a function of the tuning factor γ.

CONCLUSIONS

Solving the curl-curl equation combined with the Coulomb gauge condition leaves us with a singular system, difficult to solve with standard iterative techniques due to a high condition number of the matrix. If we introduce a ghost field, the system gets bigger due to the ghost field unknowns. However, an improvement in the convergence behaviour is achieved by taking an adequate value of the tuning factor. This is extremely beneficial for the iterative methods that we use to solve large and sparse systems of linear systems that arise in solving electromagnetic field problems.

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