Efficient full-wave electromagnetic analysis via model-order reduction of fast integral transforms

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Abstract—
An efficient full-wave electromagnetic analysis tool would be useful in many aspects of engineering design. Development of integral-equation based tools has been hampered by the high computational complexity of dense matrix representations and difficulty in obtaining and utilizing the frequency-domain response. In this paper we demonstrate that an algorithm based on application of a novel model-order reduction scheme directly to the sparse model generated by a fast integral transform has significant advantages for frequency- and time-domain simulation.

I. Introduction

Many aspects of engineering design, such as interconnect delay estimation, signal integrity analysis, and electromagnetic compatibility applications, require understanding the electrical properties of complex structures. However, because of the great computational cost, full-wave simulation of large, complex three-dimensional structures is rarely used in the engineering design and optimization process. At best, a range of representative structures is simulated, and/or a variety of engineering approximations are made to derive either analytical models, less computationally demanding numerical models, or sets of rule-of-thumb design guidelines. While these approaches are simple and intuitive, as interconnect technologies become more complex and signal frequencies rise, the task of obtaining simple yet accurate models of geometrically complex structures will become more difficult, and time spent deriving and applying simple models may become burdensome.

A principle difficulty in using standard integral-equation based electromagnetic solvers is the formidable computational complexity of dense matrix manipulations. A possible means of reducing this burden is the use of iterative Krylov-subspace linear system solution algorithms in combination with fast multilevel integral transform methods, such as the fast multipole method[5], [11]. Robust quasistatic electromagnetic analysis codes based on such methods have been developed which require orders of magnitude less storage and computation than algorithms based on direct matrix representations[7].

Integral-equation based solvers usually operate in the frequency domain. The simplest method of obtaining the frequency response is to sample the complex Laplace-domain response at discrete points along the imaginary axis. The frequency range of interest may span several decades, however, and the magnitude of the response may also vary over a similar range. Poles close to the imaginary axis can result in very sharp spectral features. Thus, the frequency response may be difficult to resolve by discrete sampling. An alternative approach is to exploit the analytic behavior of the electromagnetic model to construct a rational approximation to the frequency response. Rational approximation can also be used to derive a reduced-order model for use in time-domain coupled nonlinear circuit simulation, if the approximation is carefully constructed.

Methods based on rational approximation, such as asymptotic waveform evaluation (AWE)[10], have been popular for constructing low-order models of circuit interconnect. Algorithms such as AWE which are based on moments of the frequency response have certain numerical stability problems, but recently the connection between Padé approximation and the Lanczos algorithm has been exploited to obtain orthogonalized Krylov-subspace algorithms which can stably form high-order rational approximants to the frequency response of lumped linear systems[3], [4]. However, one advantage of moment based approaches such as AWE is that they can construct approximations to systems with *irrational* system response (e.g., a system with delay elements such as transmission lines or the retardation factors of a full-wave electromagnetic model) as easily as for a rational response[14], [2], whereas Krylov-subspace model-reduction algorithms for systems with irrational response have yet to be demonstrated.

In this paper, we introduce a hybrid algorithm which incorporates features of orthogonalized Krylov methods[13] and the series-expansion based methods to construct a multipoint rational approximant, for a system with distributed elements, in a manner similar to the "complex frequency hopping" (CFH) multipoint algorithm[2]. The resulting series-Krylov (SKCFH) algorithm in combination with a multilevel transform representation yields an efficient solution of the electromagnetic problem.

II. The rPEEC formulation

In this section we review the retarded partial-element equivalent circuit formulation(rPEEC)[6] used for full-wave electromagnetic analysis in this paper. We emphasize, however, that our numerical methods are not tied to this formulation.

In the Laplace domain, the electric field $\boldsymbol{E}$ is expressed in terms of the vector potential $\boldsymbol{A}$ and the scalar potential ϕ as

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33rd Design Automation Conference ®

DAC 96 - 06/96 Las Vegas, NV, USA

$\boldsymbol{E} = -s\boldsymbol{A} - \nabla\phi$. In the Lorentz gauge, the potentials are related to the currents $\boldsymbol{J}$ and charges q by:

$$\boldsymbol{A}(x,s) = \frac{\mu}{4\pi}\int d^3x'\boldsymbol{J}(x',s)\frac{e^{-s|x-x'|/c}}{|x-x'|} \quad (1)$$

$$\phi(x,t) = \frac{1}{4\pi\epsilon_0}\int d^3x' q(x',s)\frac{e^{-s|x-x'|/c}}{|x-x'|} \quad (2)$$

The exponential factor in the integrals of Eq. 1, 2 represents a delay (retardation) in the time-domain which is due to the finite propagation speed of light.

Assuming a set of conductors in a uniform medium, in every conductor, Ohm's law $\boldsymbol{E} = \boldsymbol{J}/\sigma$, with σ the conductivity, allows us to write

$$\frac{\boldsymbol{J}(x,t)}{\sigma(x)} + s\boldsymbol{A}(x,t) + \nabla\phi = 0 \ . \quad (3)$$

Adding the continuity equation, $\nabla\cdot\boldsymbol{J}(x,t) + sq(x,t) = 0$, to Eq. 3 produces a system of equations which, given appropriate boundary conditions, can be solved for the charges q on conductor surfaces and the currents $\boldsymbol{J}$ flowing in the conductors.

To discretize the system, rectangular elements of constant current are used to represent $\boldsymbol{J}$, and the charges are assumed to be piecewise-constant over rectangles which tile the conductor surfaces. After discretization, the charges are eliminated as variables, leading to the single equation for the vector of discretized currents $j(s)$

$$\left[T^T P(s)T + sR + s^2 L(s)\right] j(s) = su \quad (4)$$

with T the incidence matrix for the equivalent circuit. In Eq. 4, $P(s)$ is a dense matrix coupling all the capacitive cells (it represents the scalar potential, or "capacitive" interactions). Its elements are

$$p_{ij}(s) = \frac{1}{4\pi\epsilon_0}\int_{x'\in S_i}\int_{x\in S_j} d^2x'd^2x\frac{e^{-s|x-x'|/c}}{|x-x'|} \quad (5)$$

where S_i, S_j represent the i,jth rectangular charge basis function respectively. R is a diagonal matrix representing restistances. $L(s)$ represents the inductive interactions, and its matrix elements are similar to those of $P(s)$. Eq. 4 can be written in terms of a single frequency dependent matrix $A(s)$ (not to be confused with $\boldsymbol{A}$)

$$A(s)j(s) = su \quad (6)$$

Given a vector u of voltage source excitations of the equivalent circuit, Eq. 6 can be solved for the discrete currents $j(s_n)$ at a particular complex frequency s_n.

III. Grid-based matrix sparsification

The difficulty with the rPEEC formulation, as in all integral-equation based electromagnetic solvers, is that it contains frequency-dependent dense matrices. That is, the matrices $P(s)$ and $L(s)$ have $O(n^2)$ non-zero entries, where n is the number of degrees of freedom in the discretized system. Most full-wave integral-equation based solvers use Gaussian elimination to perform an LU-decomposition of the matrix $A(s)$. Storing the matrix requires $O(n^2)$ memory, and $O(n^3)$ floating-point operations are needed for the factorization.

A more effective approach is to construct a sparse representation $\hat{A}(s)$ of the system description $A(s)$, such that multiplication of a vector y by $\hat{A}(s)$ can be performed in close to $O(n)$ operations and storage, and such that the difference $||\hat{A}(s)y - A(s)y||$, where $||\quad||$ denotes vector norm, is small for an arbitrary vector y. To obtain the system response $j(s)$, a Krylov-subspace iterative matrix solver such as GMRES[12] is used. Given a complex frequency s_0, such algorithms can compute the solution $j(s_0)$ to the linear system of equations $\hat{A}(s_0)j(s_0) = b$, for given b by performing only matrix-vector product operations with the matrix $\hat{A}(s_0)$. If the number of iterations needed for convergence is bounded, the resulting algorithm will need close to $O(n)$ time and storage to compute a solution at a single frequency point.

In [8], [9] a multigrid-like[1] "precorrected-FFT" algorithm was presented which for not-too-inhomogeneous geometries significantly reduces the $O(n^2)$ time and memory needed to compute a matrix-vector product. This algorithm is of particular interest in the context of model reduction, as a single algorithm can be used to span the entire range of frequencies, including zero frequency.

To derive the algorithm, first consider the evaluation of the sum

$$y(x_j) = \sum_i g(|x_i - x_j|, s)q(x_i) \quad i,j = 1\ldots N \quad (7)$$

for some set of N discrete "charges" q at points x_i, and evaluating the "potential" y, as given by the Green function $g(|x_i - x_j|, s)$, at all the other charge positions x_j. This sum may be approximated in a four step process (Algorithm 1). A uniform grid is introduced which covers the problem domain (note that the grid is not in any way linked to the underlying problem discretization). The first step is to represent the charge q on the grid. By this we mean that for each charge, a small set of point charges that lie on the grid and surround the charge being "projected" is used to approximate the long-range potential of the charge. Second, the potential of all the grid charges is computed at the grid points. This operation can be accomplished in several ways, the simplest of which is by use of the FFT. Third, the potential on the grid is interpolated onto the evaluation points. Finally, since the grid representation will only be accurate far away from the charge being approximated [1], [9], the potential of nearby charges must be computed exactly.

Algorithm 1 (Precorrected-FFT)

1. Project "charge" q onto grid : $q_g = Wq$
2. Compute grid-charge potentials ϕ_g (FFT) : $\phi_g = U(s)q_g$
3. Interpolate grid potentials : $y_g = W^T\phi_g$
4. Add local interactions : $y = y_g + D(s)q$

Thus the precorrected FFT algorithm replaces the relation

$$y = G(s)q \tag{8}$$

with dense matrix $G(s)$ by an approximate representation

$$\hat{y} = \left[D(s) + W^T U(s) W\right] q \tag{9}$$

where $D(s)$ is a sparse matrix which represents interactions between nearby charge elements and $U(s)$ is a Toeplitz matrix which corresponds to convolution of the Green function with the grid charges to give grid potentials, and W is a sparse interpolation operator. Due to the use of the FFT $U(s)$ possesses a sparse representation. For the purposes of model reduction it is convenient to choose the interpolation and projection operators W to be frequency-independent. The simplest such choice corresponds to polynomial interpolation [1], [9].

It can be shown that Algorithm 1, resulting in the factorization of Eq. 9 calculates a product operation, including the effects of all long-range interactions, to engineering accuracy when even fairly low-order interpolation operators are used[1], [9].

IV. Model Reduction

In this section, we introduce a new method to obtain a high-order rational approximation (or reduced-order model) of the sparse representation (Eq. 9) in a numerically stable manner.† The high order is necessary in order to represent the fine spectral features and retardation in the frequency response of typical electromagnetic models. Explicit moment-matching techniques such as AWE are not numerically stable and will not be sufficient for this problem. Orthogonalized Krylov subspace methods, such as the nonsymmetric Lanczos algorithm or the Arnoldi method [4], [3], [13], while useful for stably constructing arbitrarily high order approximants of lumped systems, are not directly applicable to distributed (delay) systems such as transmission lines or rPEEC. We extend the techniques aforementioned to created a series-Krylov CFH (SKCFH) algorithm which is efficient (requires few expansion points), numerically stable, and applicable to model reduction of distributed and delay systems.

†Note that the use of the word "stable" in this section refers to numerical stability of the model reduction algorithm, not time-stability of the reduced-order model, which is an important but separate issue.

A. Rational approximation via orthogonalized Krylov methods

Consider the Laplace domain system description of a linear lumped network,

$$sAx = x + b \tag{10}$$

$$y = c^T x \tag{11}$$

where A is the matrix desciption of the system that relates the entries of the input vector b to the set of unknown system variables in the vector x, and y is the vector of outputs obtained from the internal system variables via a mapping vector c^T. It is clear that the solution of such a system will be $y(s) = c^T(I - sA)^{-1}b$. Moment matching methods use the sequence of moments $c^T b, c^T Ab, c^T A^2 b \ldots c^T A^k b$ to obtain a Padé approximation to $y(s)$. In finite arithmetic, at some k (which could be small!) the vectors $A^k b$ and $A^{k-1}b$ will no longer be linearly independent and the process breaks down.

In order to obtain a more stable algorithm, we consider algorithms that operate explicitly in the Krylov subspace

$$\mathcal{K}\{A, b\} \equiv \{b, Ab, A^2 b, \cdots\} \tag{12}$$

of the matrix-vector pair $\{A, b\}$. In orthogonalized Krylov-subspace approaches to model reduction, a reduced order matrix model is constructed based on a set of vectors that span the Krylov subspace $\mathcal{K}\{A, b\}$ (and possibly $\mathcal{K}\{A^T, c\}$). By retaining an orthogonality relation among the vectors, linear independence can be maintained, and so high order rational approximants can be constructed. Our approach to distributed systems is easiest to describe and implement using the Arnoldi approach to model-order reduction. Additionally, with the Arnoldi method a rational approximant for all the variables in the system is directly and naturally generated, which is useful in, for example, electromagnetic compatibility analysis.

The Arnoldi algorithm applied to the matrix pair A, b for q steps generates $q + 1$ orthonormal vectors spanning the subspace $\mathcal{K}\{A, b\}$ as the q columns of the matrix V_q and the vector v_{q+1}. As a product of the orthogonalization procedure, the method produces a $q \times q$ upper Hessenberg matrix H_q. It can be shown that the matrix rational function $G_q^A(s) = \|b\|_2 c^T V_q (I - sH_q)^{-1} e_1$ is a reduced order model of the original $y(s)$, which matches its first $q - 2$ moments[13]. Generally an accurate model can be obtained with q much smaller than the system dimension. The only operations with the matrix A which are needed are matrix-vector product operations, making the method attractive for sparse systems. The difficulty with applying these algorithms to distributed systems such as those described by rPEEC is that distributed systems have a frequency-dependent A matrix, $A(s)$. In order to be able to apply the Arnoldi method to distributed systems such as networks with transmission lines, or rPEEC models, we must construct a first-order lumped system description.

B. Reduction of distributed systems

Consider the Laplace domain representation of a distributed system

$$A(s)x = b \tag{13}$$

$$y = c^T x \tag{14}$$

In general, Eq. 13 may describe an infinite-order linear system. That is, the Taylor expansion of the matrix operator $A(s)$ may contain infinitely many non-zero terms. We must convert this infinite-order, finite-dimensional system into a first-order, infinite dimensional system before proceeding with model reduction.

One way to obtain a first-order representation of Eq. 13 is to expand $A(s)$ in a Taylor series

$$A(s) = A_0 + sA_1 + \frac{s^2}{2!}A_2 + \frac{s^3}{3!}A_2 + \dots \tag{15}$$

The equivalence above is satisfied for all values of s if the matrix $A(s)$ is entire in the complex plane; that is, if it contains no entries with finite singularities. This is true for rPEEC circuits and transmission line networks.

Substituting Eq. 15 into Eq. 13 and multiplying by A_0^{-1}, the system becomes

$$\left[I + s\tilde{A}_1 + \frac{s^2}{2!}\tilde{A}_2 + +\frac{s^3}{3!}\tilde{A}_3 + \dots\right] x = A_0^{-1}b \tag{16}$$

where $\tilde{A}_k = A_0^{-1}A_k$ and I is the unity matrix. We recursively define new variable vectors as follows,

$$x_0 \equiv x, \quad x_1 = \frac{s}{2}x_0, \quad x_2 = \frac{s}{3}x_1, \quad \cdots, \quad x_k = \frac{s}{k+1}x_k, \quad \cdots$$

The system of Eq. 13 becomes

$$\left\{ I - (s) \begin{bmatrix} -\tilde{A}_1 & -\tilde{A}_2 & -\tilde{A}_3 & \dots \\ I/2 & & & \\ & I/3 & & \\ & & \ddots & \end{bmatrix} \right\} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \end{bmatrix} = \begin{bmatrix} A_0^{-1}b \\ 0 \\ 0 \\ \vdots \end{bmatrix} \tag{17}$$

$$y(s) = \begin{bmatrix} c^T & 0 & 0 & \dots \end{bmatrix} \begin{bmatrix} x_1(s) \\ x_2(s) \\ x_3(s) \\ \vdots \end{bmatrix} \tag{18}$$

or

$$(I - s'\overline{A})\overline{x} = \overline{b} \tag{19}$$

$$y(s) = \overline{c}^T\overline{x}(s) \tag{20}$$

This is a first order system which allows us to apply a Krylov-subspace based model-reduction algorithm. More importantly, for finite order models, the model-reduction algorithm can be executed in a finite number of steps since the starting vector, $\overline{b}$, is bottom sparse (only the first n entries are non-zero). When an Arnoldi process is used to generate a upper-Hessenberg representation of the matrix $\overline{A}$, from the structure of $\overline{A}$, each Arnoldi vector v_k will have kn non-zero entries in it. So, at order k, the number of original n-size matrix products required to obtain the next Arnoldi vector v_{k+1} will be k. Thus total storage and computational costs will be $O(q^2n)$ for an order-q model.

Now we apply this algorithm to the sparse rPEEC factorization (Eq. 9). Assuming a Taylor expansion about a complex frequency s_0, the matrices in the Taylor expansion of the system description are

$$A_k = D_k(s_0) + W^T U_k(s_0) W \tag{21}$$

where D_k and U_k are the Taylor-expansion matrices of $D(s)$ and $U(s)$. To implement the model reduction algorithm, it is necessary to compute matrix-vector products with the matrices $A_k, k > 0$, and solve linear systems of the form $A_0 x = b$ for arbitrary b. Step k of the Arnoldi model-order reduction algorithm requires k products with $A_1, \dots, A_k$ and one linear system solution with A_0. The A_k products are straightforward. Since it is possible to compute matrix-vector products with A_0, the linear systems can be solved using a Krylov-subspace iterative algorithm.

C. Multipoint rational approximants

Our approach is based on a Taylor series expansion of the exponential function, and for large arguments, corresponding to frequencies far from the expansion point, it is not possible to accurately sum an arbitrary number of terms in this series. Thus, unlike Krylov methods for lumped systems, we cannot obtain accurate models of *arbitrarily* high order from a single expansion point. This is not a concern, however, as it is more efficient to obtain the rational approximant from moderate-order expansions about multiple expansion points, rather than a single high order expansion, particularly since the cost of the model generation grows as q^2. Several options exist to utilize the information from multiple expansion points. A CFH[2] style algorithm can be used to construct a single reduced-order model by extracting the poles and residues at each expansion point and rejecting inaccurate ones. Pole convergence may be determined by identifying common poles in neighboring expansions, as in CFH, or by using estimates based on residuals of Ritz pairs, which are available directly from the Arnoldi process[3], [13]. Alternatively, the two expansion points can be deemed to be accurate in the range between them when their frequency response matches at some intermediate point, and the full frequency response obtained via piecewise-rational function interpolation using the frequency responses from the various expansion points as interpolation functions.

V. Computational Results

We now consider two examples which illustrate various aspects of the model-order-reduction algorithm as applied to the sparse rPEEC representation.

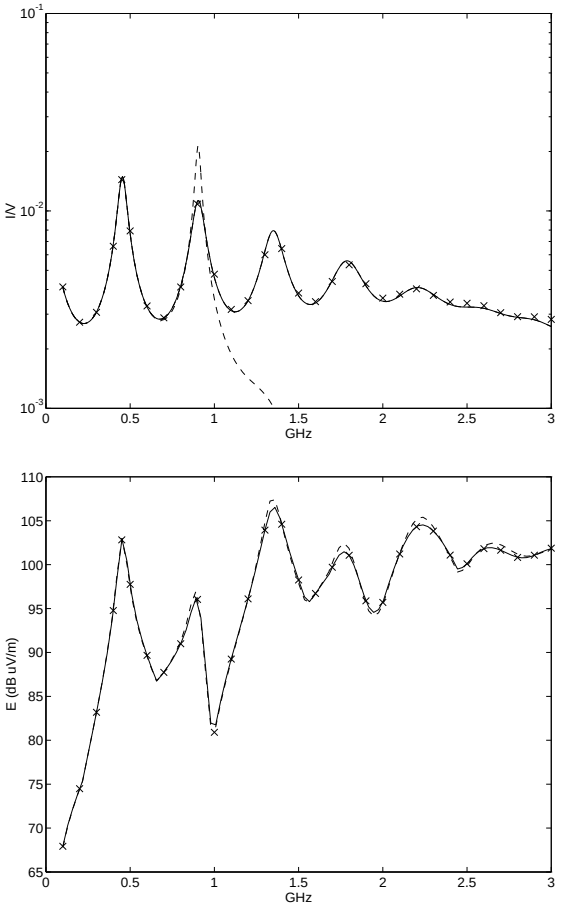

Fig. 1. Frequency response of the two-strip example. Top : Amplitude of driven current vs. excitation frequency, 100 MHz to 3 GHz. Solid lines show directly computed response and Arnoldi-based approximation of dense model. Dashed line shows AWE approximation of dense model. 'x' shows response at selected frequency points of sparse model, computed using the iterative algorithm GMRES. Bottom : maximum amplitude of electric field at 3 meters from structure. Solid line shows reduced-order model of dense system. Dashed line shows reduced-order model of approximate sparse system. 'x' shows full dense model.

The first example is a simple configuration intended to illustrate the capabilities of the new model-order reduction algorithm. Two parallel 30cm long strips, 5cm apart and 1cm wide, are driven at one end by a voltage source with 50 ohm internal impedance, and are terminated at the other end by a 10 ohm resistive load. Figure 1 shows the magnitude of the current driven through the load by a unit voltage source.

We have calculated the response using explicit single point moment-matching (AWE), by using the Arnoldi-based model-reduction algorithm applied to the dense rPEEC model, by solving iteratively for the frequency response using the sparse rPEEC model, and by performing matrix factorization of the the dense rPEEC model. The best AWE approximant it was possible to obtain used 20 moments. AWE can resolve the first resonance and detect the presence of the second, but cannot match the actual frequency response past about 0.8 GHz. The Arnoldi based approached was able to accurately match the frequency response over a 3GHz range using an 85th order model. We stress that this is an example where AWE performs well. Examples are easily constructed[4] for which a single point moment expansion breaks down after a few moments, in which case virtually no information about the frequency response can be obtained. CFH, using multiple expansions, will require too many expansions due to the limitation, once again, of a single-point explicit moment-matching.

Figure 1 (bottom) demonstrates that the proposed algorithm generates a rational approximant for all the currents that is sufficently accurate for radiated field calculations. The maximum amplitude of the radiated field was calculated at 3m from the parallel strips. The reduced-order model of the dense system achieves an excellent match to the actual field amplitude. The reduced-order model of the precorrected-FFT method is only slightly less accurate.

The second example is a multiconductor interconnect structure, which illustrates the capability of the combined multilevel/model-order-reduction algorithm to analyze large, complex problems. Several signal traces, 200 μm wide run 3mm over a 10cm wide ground plane, as shown in Figure 2. A narrow mesh of traces is located over the signal paths, 6mm above the ground plane.

An automatic discretization routine requires that the ground plane contain an "image" discretization of the narrow traces, resulting in a final discretization with a large number of unknowns. The full model contains 5270 capacitive nodes and 9161 inductor currents. The final matrix which must be factored has 9129 unknowns, containing 8.3×10^7 entries. The code using the dense model would need about 3 gigabytes of storage, with 1.3 gigabytes needed just to store and factor the matrix. On a machine capable of 100MFLOPS sustained, about 5.6 hours would be needed for an LU-factorization.

The sparse model generated by the precorrected-FFT algorithm has only about 6.2×10^6 non-zero entries, corresponding to a factor of 13 reduction in model size. The code requires 600 megabytes of storage (a considerable portion of which is for storage of vectors needed for the recycled Krylov-subspace iterative matrix solution technique), and executes on a machine with 512 megabytes of physical memory without swap activity in the main solution phase. Figure 2 shows the response of the computed reduced-order model. It was possible to compute the order 20 model, which nearly spans the entire frequency range, in about 12 hours on an IBM RS6000/560 architecture.

VI. Conclusions

In this paper we demonstrated that a relatively simple approach[8] to multilevel integral transforms, when combined with a numerically stable algorithm for model order reduction of systems with delay elements, can dramatically reduce the size of interconnect models generated by complicated three-dimensional interconnect structures. Compared to commonly-

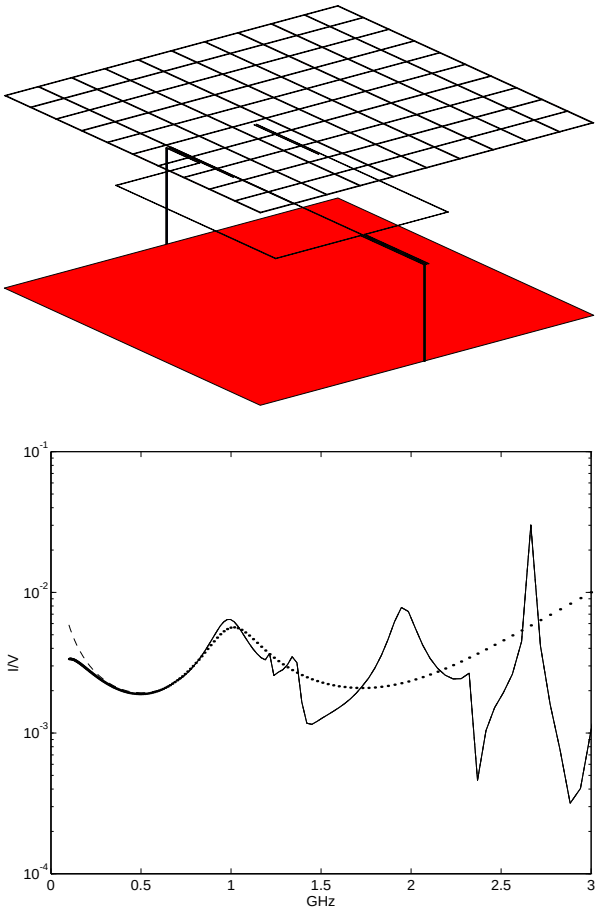

Fig. 2. Top : a large interconnect structure. Vertical axis is not to scale. Bottom: Current driven by voltage source through resistive termination to ground plane. Dotted line: order-20 Arnoldi model with $s_0/(2\pi) = 0.5+2i$ GHz. Dash line: order-15 Arnoldi model with $s_0/(2\pi) = 0.5$ GHz. Solid line: response obtained without model reduction, as well as the piecewise-rational approximation obtained from combining models at separate expansion points; the results overlap. Note that the expansion at $0.5 + 2i$ Ghz gives a very good approximation up to 3 GHz but is not good near $s = 0$ whereas the opposite is true of the expansion at 0.5 GHz.

used techniques, on a problem with 10,000 unknowns, the resulting algorithm has a fivefold storage advantage, and computes a complete, continuous, analytic frequency response in the same time as standard techniques require for solutions at a few discrete frequency points. More importantly, the size of the sparse model and cost of generating the system response should grow less rapidly with problem size than for standard techniques[9].

Acknowledgments

The authors wish to acknowledge helpful discussions with Prof. Jacob White of MIT and with Dr. Albert Ruehli. JRP wishes to thank the electrical simulation and modeling group of the IBM T. J. Watson Research Center for their hospitality while this work was being performed.

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