AN ITERATION-FREE FAST MULTILEVEL SOLVER FOR DENSE METHOD OF MOMENT SYSTEMS

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Abstract

A fast multilevel direct solver for the Method of Moments applied to electrically small structures is presented. The approach is based on a combination of low-rank decompositions and fill-in control. It is particularly advantageous for multiple right-hand-side problems such as those encountered in digital circuit and IC analyses, as is demonstrated by numerical simulation results presented here.

I. Introduction

Quasi-static parasitic extraction is an important problem in digital circuits and in mixed signal IC analysis. While several fast integral equation-based techniques have been proposed and developed to address this problem, practically all these methods, including Fast Multipole, FFT, and QR-based methods, rely on fast algorithms to accelerate the iterative solution of the Method of Moments (MoM) system. These approaches primarily solve one right hand side (RHS) at a time, and therefore become considerably slower when a problem involves a large number of RHS vectors such as substrate coupling, or parasitic extraction for a large number of nets. Moreover, in certain formulations, such as the Partial Equivalent Electric Circuit (PEEC) method, or in coupled electromagnetic circuit simulation, it is advantageous to rapidly obtain the explicit inverse or LU factors of the MoM system.

While fast iterative solvers reduce the cost of \( N \times N \) MoM matrix-vector products to \( O(N) \) or \( O(N \log N) \) from \( O(N^2) \), the overall solution cost is also proportional to the number of RHSs and the number of iterations per RHS. The overall cost for large RHS problems can be very large depending on the number of iterations or the conditioning of the system. A regular direct solver such as LU decomposition, on the other hand, has no iterative steps, and the single initial \( O(N^3) \) decomposition step is performed only once. Subsequent solutions are obtained through an \( O(N^2) \) forward and backward substitution. While the relative advantage of the LU method for small problems increases with the number of RHSs, and more so if the problem is inherently poorly conditioned, the large costs of the initial step and subsequent solution steps relative to fast iterative methods is a large bottleneck. Moreover, regular direct solvers consume \( O(N^2) \) memory for matrix storage compared to the \( O(N) \) or \( O(N \log N) \) memory requirements of fast iterative solvers.

The multilevel schemes developed for fast matrix-vector products do not inherently lend themselves to obtain fast methods for direct decomposition or inversion. To accomplish fast direct solution Canning and Rogovin [1] suggested sparse-LU and Sherman-Morrison-Woodbury schemes based on a multilevel sparse representation of the full-wave MoM matrix. In this work, the QR-based low-rank representation and the sparse-LU computation are integrated in order to alleviate the computational overhead associated with fill-ins for an arbitrary block structure and thus make feasible the fast analysis of general 3D structures. No a priori block structures are assumed in the MoM matrix, unlike in [1]. A fast iteration-free scheme to rapidly compute the sparse LU factorization of the dense MoM matrix is proposed, and the factorization can be applied rapidly to each RHS vector. This approach thus bypasses the need for an iterative solver, associated pre-conditioning and the convergence uncertainty and iteration time in an iterative scheme. The method is general enough to be relevant to both quasi-static and full-wave analyses of electrically small structures, in free-space and in multi-layered media.

II. Approach
Capacitance problems formulated using the MoM are solved by transforming the electrostatic equation \( V^2 \phi(r) = -\rho(r)/\varepsilon \) relating potential \( \phi \) and charge-density \( \rho \) to the corresponding integral equation.

The discretization of the integral equation results in a matrix system of the form \( \bar{Z} \mathbf{I} = \mathbf{V} \) where the \( N \times N \) MoM matrix \( \bar{Z} \) is a dense Green’s function matrix, \( \mathbf{I} \) represent the unknown coefficients of known basis functions for charge density, and \( \mathbf{V} \) represents the known potential excitation. Each element of the MoM matrix denotes the interaction between a testing and a basis function and is written as follows:

\[
\bar{Z}_{(j,i)} = \int_{S_j} ds t_j(r) \int_{S_i} ds' g(r,r') f_i(r')
\]

where \( t_j \) is the testing function defined over \( S_j \), \( f_i \) is the basis function defined over \( S_i \) and \( g(r,r') \) is the relevant Green’s function. In the electrostatic case for \( P \) disconnected conductors, each column of the required \( P \times P \) capacitance matrix is obtained by enforcing a voltage of 1V on the excited conductor, 0V on all other conductors, solving the above system, and integrating the charge density over each conductor. The \( N \times N \) system of equations is therefore solved \( P \) times to obtain the capacitance matrix.

The IES\(^3 \) fast iterative solver [2], based on the QR method reduces the cost of performing the matrix vector product \( \bar{Z} \mathbf{I} \) to \( O(N \log N) \) from quadratic time. It exploits smoothness of the Green’s function to decompose the numerically rank-deficient far-field sub-matrices of the MoM using QR decomposition; a sub-matrix \( \bar{A} \) of the MoM matrix \( \bar{Z} \) can be decomposed as \( \bar{A}_{mn} = \bar{Q}_{mx} \bar{R}_{xn} \) where \( \bar{R} \) is upper triangular and \( \bar{Q} \) is orthogonal i.e. \( \bar{Q}^T \bar{Q} = \mathbf{I} \) . However, as with any fast iterative solver, the cost of this scheme is proportional to the number of iterations and the number of RHS vectors and therefore can prove to be expensive for large number of RHS vectors, as is the case of IC parasitic analysis and substrate coupling.

The proposed method presented herein relies on a combination of QR-based compression for reduced representation of far-field sub-matrices the MoM matrix using the Modified Gram-Schmidt (MGS) method [3], followed by a fast method to obtain the LU-decomposition of the compressed matrix. The crucial component of the algorithm is the manipulation of the QR step in order to reduce fill-ins generated in the sparse LU process.

To illustrate the QR-based sparse LU paradigm, consider the low ranked sub matrix \( \bar{A} \) in Fig. 1. For ease of illustration assume \( \bar{A} \) has rank 1 i.e. \( \bar{A}_{mn} = \bar{Q}_{m1} \bar{R}_{1n} \) . While performing the LU transformation on this block, the first row will remain unchanged. Notice that all the elements of the second row are transformed by changing the second element of \( \bar{Q} \) as follows \( \bar{Q}^lu(2) = \bar{Q}(2) - \bar{Q}(1)L(1) \) where \( L(1) \) is the appropriate coefficient from the lower triangular part. Thus the sparse LU transform of block A is \( \bar{Q}^lu \bar{A} \). For block B, in addition to modifying \( \bar{Q} \), contributions from block A in the form of fill-ins are also necessitated. The sparse LU representation for block B will thus be of the form of \( \bar{Q}^lu \bar{A} - \bar{F} \bar{B} \bar{A} \) where \( \bar{F} \bar{B} \) is the fill in contribution to block B from block A.

In a similar manner, the sparse representation of block C is of the form \( \bar{Q}^lu \bar{A} - \bar{F} \bar{C} \bar{B} \bar{A} - \bar{F} \bar{C} \bar{B} \bar{A} \). When the blocks A,B, and C have arbitrary rank, then the relevant LU transforms for each block are of the form \( \bar{Q}^lu \bar{A} \bar{m} \times \bar{A} \bar{n} \times \bar{A} \), \( \bar{Q}^lu \bar{B} \bar{m} \times \bar{B} \bar{n} \times \bar{B} \), \( \bar{Q}^lu \bar{C} \bar{m} \times \bar{C} \bar{n} \times \bar{C} \), \( \bar{F} \bar{A} \bar{m} \times \bar{A} \bar{n} \times \bar{B} \), \( \bar{F} \bar{B} \bar{m} \times \bar{B} \bar{n} \times \bar{B} \), \( \bar{F} \bar{C} \bar{m} \times \bar{C} \bar{n} \times \bar{B} \), where \( \bar{F} \bar{A} \bar{m} \times \bar{B} \bar{n} \times \bar{B} \bar{n} \times \bar{A} \) and \( \bar{F} \bar{B} \bar{m} \times \bar{B} \bar{n} \times \bar{A} \bar{m} \times \bar{A} \bar{n} \times \bar{A} \) are fill-in contributions to block A from block B. The situation is reversed for lower triangular blocks, where \( \bar{Q} \) factors are unaltered and fill-in factors act as substitutes for \( \bar{R} \) instead of for \( \bar{Q} \).
In general, both the computational cost and memory are strongly influenced by the fill-in factors, depending on the specific QR structure. The presented work aims at minimizing the overall cost and memory, including the effect of fill-ins, by controlling the QR block distribution. In other words the QR block formation and sparse LU are treated as a combined operation.

The basic QR building blocks are splits and merges. A given low-rank sub-block of the MoM matrix, is split into four low-rank sub-blocks if the computed costs (QR and fill-in costs) are lower due to this split. Similarly, four low-rank sub-blocks are merged into a single low-rank block if the computed costs are lower due to the merge. In the case when the sub-block is dense, the potential split involves two low-rank off-diagonal sub-blocks and two dense sub-blocks. Any off-diagonal block is represented by its QR form.

III. Simulation Results

Timing and memory results for a variety of complex 3D problems, including bus crossover, comb drive, multi-pin package, and multiple contact points on a substrate are presented. The relatively lower time and memory costs of the proposed method compared to regular LU, even for small-size problems, are demonstrated in Fig. 2. Figure 3 shows the accuracy of solution for the first column of a 14×14 capacitance matrix for a multi-pin package. The corresponding low-rank matrix structure obtained by the SLU method is shown in Fig. 4, where each QR block is shown by different colors.

<table>
<thead>
<tr>
<th>Row</th>
<th>Number</th>
<th>Log (Capacitance in F)</th>
</tr>
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<tbody>
<tr>
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<td>2</td>
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<tr>
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<td>8</td>
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</tr>
<tr>
<td>10</td>
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<td>-12.5</td>
</tr>
<tr>
<td>12</td>
<td>14</td>
<td>-12</td>
</tr>
</tbody>
</table>

Table 1 demonstrates the reduced complexity of the SLU method. The LU setup cost is reduced from $N^3$ to exponents as low as 2.31 for a true 3D problem. Solution costs and memory are also reduced considerably from the $N^2$ requirements of the LU method. Figure 7 shows the applicability of SLU to non-free-space problems. In particular the situation addressed is a substrate-coupling example where capacitance between multiple contacts on top of a conductor-backed dielectric is computed. Furthermore, the advantage of SLU compared to a fast iterative solver for multiple RHS vectors is evident from Fig. 8 where the larger setup cost for SLU is offset by the rapid solution time per RHS.
Table 1: Exponents $\gamma$ for order of computations $N^\gamma$ with SLU

<table>
<thead>
<tr>
<th>Structure</th>
<th>Max. $N$</th>
<th>Setup ($\gamma = 3$ for LU)</th>
<th>Solution per RHS ($\gamma = 2$ for LU)</th>
<th>Memory ($\gamma = 2$ for LU)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thin strip</td>
<td>3500</td>
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<td>1.29</td>
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<td>Plate</td>
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<td>Bus crossing</td>
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<td>Comb drive</td>
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<tr>
<td>Multi-pin package</td>
<td>3158</td>
<td>2.51</td>
<td>1.667</td>
<td>1.61</td>
</tr>
</tbody>
</table>

Figure 7: Solve time with conductor-backed substrate

Figure 8: Total solution time for multiple contacts on a conductor-backed substrate

IV. Conclusions

The presented SLU method exploits the QR structure with no a priori assumptions in order to obtain a fast sparse LU representation of dense MoM matrices for arbitrary 3D electrically small structures, in contrast to previous approaches that relied on specific QR block structures. In particular the algorithm controls fill-in by tuning the QR block structures to minimize overall LU formation costs. It has been shown that this fast direct solver is particularly suitable for multiple right hand side problems and that it can be used without modification for multi-layered media Green’s functions. Future and continuing work will focus on full-wave applications for systems-on-chip, as well as for the efficient representation of coupled electromagnetic-circuit matrices.

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References