Singularity-treated quadrature-evaluated method of moments solver for 3-D capacitance extraction

Jinsong Zhao
Cadence Design Systems
2670 Seely Ave, MS11B2
San Jose, CA 95134
zhaojs@cadence.com

ABSTRACT

While research work on fast integral equation solver has resulted in several algorithms of similar linear equation solving performance, it has been well observed that the convergence of capacitance versus discretization is rather slow due to the most commonly used first-order collocation or Galerkin methods. This paper reports a new high-order scheme, Quadrature-evaluated Method of Moments Solver (QMMS), that uses high-order weighting and Gaussian quadrature to optimally handle the singularities at the edges and corners. For practical interconnect extraction problems, singularities at edges are analytically known and the corresponding Gaussian nodes allocation affords a near optimal discretization scheme. The new formulation avoids the special position-dependent quadrature rules, and surprisingly, provides a well-behaved matrix that converges rapidly without any pre-conditioning. Combining the high-order scheme with a kernel-independent fast solver yields an efficient algorithm for 3-D capacitance extraction.

1. INTRODUCTION

The strong demand in physical verification to extract parasitic capacitances within the deep submicron integrated circuits has resulted in many efficient algorithms and commercial tools. While these tools can be used to characterize a relatively simple and small structure, they are still deemed too slow for interactive circuit design and verification. Hence, most of the Poisson's equation-based solvers are used as a calibration tool to generate empirical formula for typical interconnect structures. Designers and tool users, however, face a difficult decision as to which tool to use and what algorithms to rely on. It is understood that while real circuits may be quite different from the extraction problem fed into the extraction tools, reliable algorithms and tools should produce a highly confident output for a well-defined structure and its boundary conditions. Benchmarks are needed for such comparisons. Unfortunately, benchmarks are hard to produce due to the low order approximation methods most commonly used. It was observed that achieving results from different tools within 1% is extremely difficult.

Research work in the past decade on the capacitance extraction mostly focuses on boundary equation method and its fast solving. Finite difference method, as a relatively mature method for Poisson's equation, has also been accelerated such as by the MEI method[5]. Fast boundary equation solver techniques (see [6] for a good many references it cites), such as multi-level multipole, pre-corrected FFT technique, hierarchical SVD technique, clustering monopole technique and the multi-scale wavelet method[6], exploit the fact that far fields are small and smooth and thus the low-rank block-to-block interactions can be efficiently compressed. In order to address the low convergence experienced in those developments, recently a Nystrom scheme has been developed[4]. In the proposed Nystrom method, quadrature rules are developed for the integral operator and thus equivalently the solution is projected onto a space spanned by a set of high-order basis functions. Compared to low-order schemes, the Nystrom method achieves a substantial accuracy improvement at a negligible additional computing cost. Further performance, however, is still severely limited by the singularities in the solution space. Approximation of singular functions by smooth basis functions (in the cited paper, polynomials were used) still requires a dense discretization to achieve desired accuracy. Non-uniform meshing may help to increase the efficiency, yet meshing according to the singularities is much desired.

This paper reports a new high-order formulation: Quadrature-evaluated Method of Moments Solver (QMMS). Method of moments was formalized in 1960s as a unified approach for the numerical solution of electromagnetic field problems, mostly formulated in integral equation forms[1]. Method of moments, or called Ritz-Galerkin in mathematical literature, uses two integrals to discretize the integral kernel: the solution expansion by basis functions and the residual expansion by weighting functions. Different from the Nystrom method, this paper uses high-order functions as the weighting functions; the solution expansion is then replaced by a quadrature formula specialized for the "pre-conditioning" function. The resulting high-order scheme handles the solution singularity and kernel singularity simultaneously and yields a well-behaved linear matrix.

DAC 2000, Los Angeles, California

The resulting linear matrix still preserves the local low-rank properties and thus can be efficiently compressed via the SVD technique[3]. Enjoying the high-accuracy approximation and high-speed solving, QMMS can be used either as a calibration tool for computing the benchmarks or as a practical capacitance extractor with a small system matrix and fast speed.

2. PROBLEM FORMULATION

The underlying formulation of capacitance extraction is the Poisson's equation

$$\nabla^2 \phi = \sigma \tag{1}$$

with proper boundary conditions for ϕ, the electric potential and σ, the charge distribution. By applying Green's theorem, Equation 1 can be reduced to the first-kind integral equation

$$\phi(r) = \int_R G(r, r')\sigma(r')dR, \tag{2}$$

where $G(r, r')$ is the Green's function that represents the potential at r excited by a unit charge at r'. In free space, the Green's function is $1/4\pi\epsilon r$; special Green's function and its efficient computation exist for multilayered media[7].

2.1 Method of moments

In the method of moments formulation, we project σ onto the space spanned by the basis functions $\{f_1, f_2, \ldots, f_n\}$. We then project the residual of the approximation onto the space spanned by the weighting functions (or sometimes called testing functions) $\{t_1, t_2, \ldots, t_n\}$. We get

$$[< t_j, Lf_i >] \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix} = \begin{bmatrix} < t_1, \phi > \\ < t_2, \phi > \\ \vdots \\ < t_n, \phi > \end{bmatrix} \tag{3}$$

where c_i are the coefficients to be determined; $< \cdot, \cdot >$ denotes the inner product in the entire defining domain. $L(\cdot)$ is the integral operator defined as:

$$L(\cdot) = \int_R G(r, r') \cdot dR. \tag{4}$$

When f_i is chosen to be a piecewise constant function and t_j the δ function, method of moments formulation becomes the commonly used first-order collocation scheme or so called *point matching method*[1]. Choosing $t_i = f_i$ yields the *Galerkin method*. The piecewise constant functions as the basis functions to approximate the solution heavily rely on increasing the discretization to reduce the approximation error. In fact, the first order scheme results in a $O(h)$ rate of reduction of error for a uniform discretization, where $h = \theta(1/\sqrt{n})$ and n is the number of uniform panels.

2.2 Quadrature-evaluated Method of Moments

The new formulation, rather than explicitly using basis functions to approximate the solution, modifies the integral evaluation in the system matrix by a quadrature. Further, we introduce a preconditioning function $p(r')$

$$\sigma(r') = f(r')p(r') \tag{5}$$

where $p(r')$ contains all the singularities and $f(r')$ is the remaining piece-wise smooth part of the charge distribution. For each weighting function t_j, we have

$$< t_j, \phi > = < t_j, L(fp) > = < Lt_j, fp > . \tag{6}$$

The above equation holds because L is, in this particular case, a self-adjoining operator. $< Lt_j, fp >$ now can be approximated by a quadrature at nodes r'_i with to-be-determined solution points $f_i = f(r'_i)$, $i = 1, 2, \ldots, n$:

$$< Lt_j, fp > \approx \sum_i Lt_j(r'_i) w_i f_i. \tag{7}$$

In this formula, the singularity in the L operator at $r = r'$ is removed or, more precisely, significantly weakened by the weighting process. The vast advantage of the new formulation over the Nystrom method lies in the fact that the weights are *position-independent* (hence the lack of subscript j), i.e., construction of weights has nothing to do with r, rather, it is only directly related to the singularity structures in the solution space. Fortunately, we can in most cases analytically derive the singularities based on the geometric structures. For example, as explained in detail later, the singularities at the edges are *analytically known*, and thus the quadrature nodes and weights are *a priori* known before the system matrix setup and solving. The final system matrix equations become

$$[Lt_j(r_i)] \begin{bmatrix} w_1 f_1 \\ w_2 f_2 \\ \vdots \\ w_n f_n \end{bmatrix} = [< t_j(r_i), \phi >]. \tag{8}$$

Amazingly, we don't even need to know the exact weights to find the capacitance. Capacitance is the accumulation of total charges on each conductor when the potential on one conductor is enforced to be 1 volt and the rest to be 0. Thus, the capacitance (c_l) between the aggressive conductor and the reactive conductor (denoted as C_l) is:

$$c_l = \int_{C_l} \sigma(r')dR \approx \sum_{r_i \in C_l} w_i f_i. \tag{9}$$

Consequently, to compute the capacitance, all we need to do is to find the product of w_i and f_i. Yet placing nodes according to the preconditioning function p enjoys much higher order of accuracy than other schemes of node allocations.

3. GAUSSIAN QUADRATURE

The quadrature rules depend only on the precondition function p, which ideally leaves the remaining part f smooth (hence the high-accuracy of the quadrature). Our strategy is to first find the singularity structure of charge distributions and then devise the appropriate quadrature rules.

3.1 Singularity structure

We consider the edge formed by two conductor surfaces. The angle between these two surfaces are θ. The behavior of the charge distribution approaching $(0, 0)$ can be derived by separation of variables[2] or conformal mapping technique.

Table 1 shows the typical edge structures and charge distribution behaviors at the edge. For the two singular cases, the singularities are integrable.

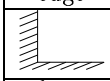
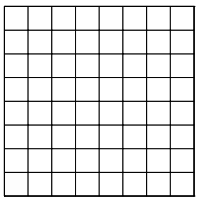
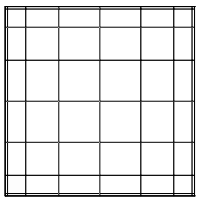
edge	θ	charge at edge	usage
	$\frac{\pi}{2}$	x	via structure
	$\frac{3\pi}{2}$	$x^{-\frac{1}{3}}$	conductor edges
———	2π	$x^{-\frac{1}{2}}$	2.5-D problems

Table 1: Typical applications of the edge structures



(a) Uniform discretization



(b) Gaussian discretization

Figure 1: Discretization

3.2 Gaussian Quadrature

Approximating a definite integral can be achieved through the *quadrature* formula:

$$\int_a^b w(x)f(x)dx \approx \sum_{i=1}^{n} A_i f(x_i), \tag{10}$$

where x_i are called nodes of the formula and the A_i are called weights. By properly positioning the nodes and calculating weights, the quadrature can achieve the highest degree of polynomial precision of $2n-1$. Such formulas are called Gaussian quadrature. The Gaussian quadratures for a class of weighting functions for a definite integral in $(-1,1)$:

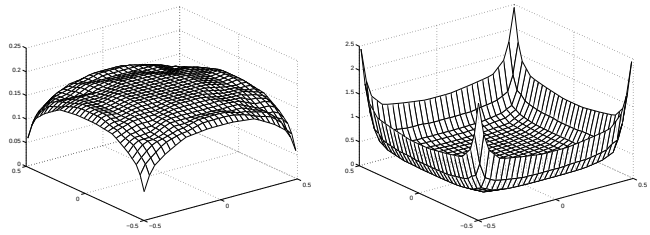
$$w(x) = (1-x)^{\alpha}(1+x)^{\beta}, \tag{11}$$

called Jacobi polynomials, are particularly useful in our capacitance extraction applications. We can choose appropriate α and β to form the preconditioning functions for conductor surface based on the edge properties that determine the singularity structures. Figure 1 shows two types of discretization. Since Gaussian nodes tend to be denser at edges, it naturally captures the singularity property and allocates resource more efficiently. Note that for high-order scheme, more than one node are placed in the non-uniform panels, and further, those nodes are again Gaussian nodes within each panel.

3.3 Accelerating the matrix solving

Quadrature-evaluated method of moments produces a system matrix that still preserves the low-rank properties for far fields. High-order method tends to spread the near field matrix entries, but for far field, not only the entry evaluation can be approximated rapidly, block-to-block interactions can be compressed with controlled accuracy via the SVD technique[3], which does not rely on the analytical form of the integral kernel.

In GMRES solving, a preconditioner can be used to reduce the number of iterations. The simplest preconditioner is to do column and/or row scaling either to remove the effects of different-scale quantities in the unknowns or to reorganize the weighting of each row. QMMS seems to have such preconditioners built in. Even without any preconditioner, the convergence is very rapid; system matrix of higher order only slightly degrades the convergence performance.



(a) Smooth part (b) with singularity

Y axis in the unit of $\frac{1}{4\pi\epsilon_0 a}$, a is the side length.

Figure 2: Charge distribution on a unit plate in free space

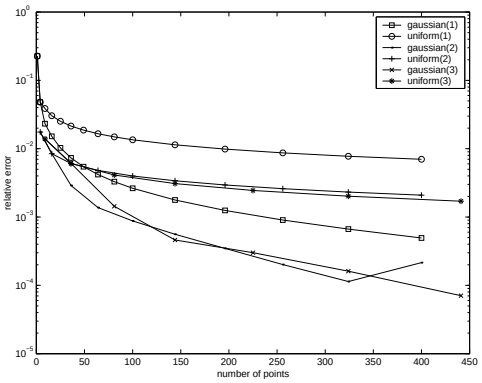


Figure 3: Comparison of various discretization and order schemes

4. NUMERICAL EXPERIMENTS

The first example extracts the capacitance of a plate of unit length (1 meter) in free space. In practical problems, charges on the edge of a thin plate demonstrates the strongest singularity ($1/\sqrt{r}$). Figure 2 is obtained via a tenth order extraction. Figure 2(a) shows the "smooth" part in the charge distribution (with singularities staying in the preconditioning function). Figure 2(b) gives the total charge distribution on the plate. It can be seen that singularities in the charge distribution are very strong, especially at the corners where the singularities of two edges merge together. Figure 3 depicts the convergence performance of various discretization and order schemes. Note that x axis corresponds to the total number of equations, thus the comparisons are fair for different schemes. Compared to the Gaussian discretization, the uniform discretization clearly loses ground. With a small number of points, resources are most efficiently used by high order methods and their results tend to jump right to the precision. In order to achieve within 1% of accuracy, only 16 points (and thus 16 equations) are needed.

The second example is a unit cube in free space, the basic example for 3-D capacitance extraction. The free-space cube has a unit length. $1/r$ is used as the Green's function. Table 2 shows the computed results from various schemes. To

# points	Gaussian(1)	Gaussian(2)
4x6	6.482958e-01	6.564097e-01
324x6	6.606045e-01	6.606679e-01
3600x6	6.606478e-01	

Table 2: Capacitance for unit cube in free space

# points	Gaussian(1)			Gaussian(2)		
	1e-2	1e-3	1e-4	1e-2	1e-3	1e-4
600	2	3	7	3	11	28
2400	2	4	14	3	9	31
9600	2	4	12	3	7	33

Table 3: GMRES iteration numbers of QMMS on unit cube

achieve 4 digits accuracy, QMMS only needs less than 2000 points, a workload for which regular LU decomposition suffices. To achieve 1% accuracy, only 24 points are needed! This clearly demonstrates the superiority of Gaussian nodes allocations and high-order schemes. Another interesting benefit of QMMS is its "built-in preconditioner". Table 3 shows the GMRES iteration numbers for two schemes *without preconditioner* for different accuracy requirement and order schemes.

The third example is an interdigitated capacitor that seriously challenges any 3D field solver without high-order scheme. Capacitance can be realized using the interdigitated structure. These passive components are usually designed by summing up the capacitance of the fingers. The capacitance of those fingers can be approximated by the transmission line theory. The modeling of these structures poses a substantial modeling obstacle, due to the strong coupling nature. It has much more charge singularities than in interconnect structures. In this example, the Green's function for the multilayered structure is used[7]. Figure 4 shows the order 3 discretization: each original panel is split into 3 by 3 subpanels. For second order method, LU is used. When using a separate meshing code to generate the edge-adapted meshes and feeding the mesh data into a solver, results converge at 21908 panels. For the same accuracy, QMMS uses only 480 nodes. Figure 5 depicts the convergence rate of QMMS method for the interdigitated capacitor. This example shows the vast superiority of QMMS over conventional low order collocation methods.

5. CONCLUSION AND FUTURE WORK

This paper presents a new capacitance extraction algorithm, QMMS, that incorporates the singularity in solution space and uses Gaussian quadrature technique. Numerical results show that this technique substantially reduces the discretization cost. QMMS can further be combined with a kernel-independent fast solver to efficiently solve for complicated structures. It is recognized that QMMS largely removes the difficulty at interconnect edges and weakens that at corners. Further development will be focused on incrementally and adaptively refining discretization and order.

The author would like to thank Joel Phillips and Baolin Yang for interesting discussions. The author also thanks Sharad Kapur who helped gain insight into high order integration and integral equation solving.

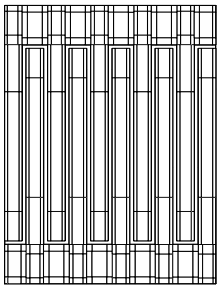


Figure 4: Discretization of an interdigitated capacitor

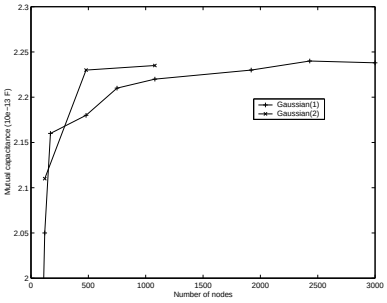


Figure 5: Convergence comparison for the interdigitated capacitor

6. REFERENCES

[1] R. F. Harrington. *Field computation by moment methods*. New York: Macmillan, 1968.

[2] J. D. Jackson. *Classical electrodynamics*. Wiley, New York, 3rd ed. edition, 1999.

[3] S. Kapur and D. Long. IES^3: A fast integral equation solver for efficient 3-dimensional extractions. In *37th International Conference on Computer Aided Design*, Nov 1997.

[4] S. Kapur and D. Long. High-order Nystrom schemes for efficient 3-d capacitance extraction. In *IEEE/ACM International Conference on Computer-Aided Design*, pages 178–85, San Jose, CA, Nov. 1998. New York, NY, USA: ACM.

[5] W. Sun, W. Wei-Ming Dai, and W. Hong. Fast parameter extraction of general interconnects using geometry independent measured equation of invariance. *IEEE Transactions on Microwave Theory and Techniques*, 45(5):827–36, May 1997.

[6] J. Tausch and J. White. A multiscale method for fast capacitance extraction. In *Design and Automation Conference*, pages 537–542, New Orleans, June 1999. New York, NY, USA: IEEE.

[7] J. Zhao, W. Dai, S. Kapur, and D. Long. Efficient three-dimensional extraction based on static and full-wave layered green's functions. In *Design and Automation Conference*, pages 224–9, San Francisco, June 1998. New York, NY, USA: IEEE.