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APPLICATION OF QUASI MONTE CARLO INTEGRATION TECHNIQUE IN EFFICIENT CAPACITANCE COMPUTATION

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Abstract—A new integration technique based on use of Quasi Monte Carlo Integration (QMCI) technique is proposed for Method of Moments (MoM) solution of Integral equation for capacitance computation. The integral equation for unknown charge distribution over the capacitors is formulated. The solutions are obtained by MoM using the QMCI technique. It is observed that the proposed method is not only capable of dealing with the problem of singularity encountered in the Integral Equation efficiently but also provides accurate computation of the capacitances of parallel plate, cylindrical and spherical capacitors.

1. INTRODUCTION

The Method of Moments (MoM) [1–4] is one of the widely used numerical techniques employed for the solution of variety of problems formulated in the form of integral equations [5–10]. The MoM is based upon the transformation of an integral equation, into a matrix equation by employing expansion of the unknown in terms of known basis functions with unknown coefficients to be determined.

One of the aspects of the MoM formulation is to deal with the problem of the singularity of the function that has to be integrated to obtain the matrix elements. It is in fact well known that MoM integrals posses a singular behavior inherent in their kernels and the point matching technique commonly employed in MoM solution usually makes the diagonal terms singular. The inclusion of singular Green's function as the kernel of the integral equation introduce singularities of

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order $1/R$ and $1/R^2$ as $R \to 0$, where $R = |\mathbf{r} - \mathbf{r}'|$ denotes the distance between the source and observation points. As such, traditional integration schemes based on Gaussian quadrature are ineffective and lead to inaccurate results. Various analytical and numerical techniques have been adopted to deal with such integrals. The Monte Carlo Integration (MCI) technique was suggested in [11, 12] for electromagnetic scattering problems which takes care of the problem of singularity by avoiding a small region around the location of singularity. A similar approach is used in Boundary Element Method (BEM) [13] where the singular point is surrounded by a small circle of radius ε and then the solution is examined as $\varepsilon \to 0$ However, the present paper proposes the Quasi Monte Carlo Integration (QMCI) technique [14–17] which takes care of the singularity problem inherently by judiciously choosing such methods for generation of quasi Monte Carlo points over the domain of integration, that the need for function evaluation at the singular point does not arise, thus proving to be a better option than MCI. Various methods have been used for extraction of capacitances of several capacitors [18, 19]. In this paper, the QMCI technique in MoM solution of integral equation for determining the unknown charge distribution and then the evaluation of capacitances of parallel plate, cylindrical and spherical capacitors has been implemented.

2. QUASI MONTE CARLO INTEGRATION TECHNIQUE

The Monte Carlo Integration (MCI) technique provides approximate solutions to a variety of mathematical problems by performing statistical sampling simulations on a computer. General idea of MCI technique is to change an integration problem into an average calculation. It makes use of random numbers to perform the calculation. This method is easy to implement. There are only minimal requirements that make the method applicable to very difficult integration problems. The evaluation requires only the ability to sample random points x and evaluate $f(x)$ for these points. Because of its intuitive sense and simplicity of implementation Monte Carlo methods are used in a wide range of applications. Their efficiencies relative to other numerical methods increase when the dimension of the problem increases e.g., Quadrature formula becomes very complex while MCI technique remains almost unchanged in more than one dimension. In addition to this, the convergence of the MCI is independent of dimensonality regardless of the smoothness of the integrand. However, the MCI technique suffers from the problem of generation of independent uniform random variables and the problem

of obtaining an absolute upper bound for the error due to probabilistic nature of the error which is overcome in QMCI technique. In numerical analysis, a Quasi Monte Carlo Integration (QMCI) method is a method for the computation of an integral that is based on low-discrepancy sequences. This is in contrast to a regular Monte Carlo method, which is based on sequences of pseudorandom numbers. The QMCI methods use points that are evenly distributed; the points are spread over the domain in such a way that there are no clusters. The classical QMCI method replaces the independent random points used in MCI by a deterministic set of distinct points that cover the region of integration more uniformly. The use of quasi random sequences in place of the usual pseudorandom numbers often improves the convergence of the numerical integration and it is also possible to compute an absolute bound for the error [20].

There are several well-known constructions for Quasi Random Number (QRN) sequences. In the one dimensional case, it is achieved, for example, by the Van der Corput sequence using a given prime base [14]. obtained by reversing the digits in the representation of some sequence of integers in a given base. To obtain a QRN sequence in several dimensions, we use a different sequence in each dimension. The classic example of this construction is the Halton sequence [15]. The first dimension of the Halton sequence is the van der Corput sequence base 2 and the second dimension is the van der Corput sequence using base 3 as shown in Table 1. Dimension s of the Halton sequence is the van der Corput sequence using the s-th prime number as the base. In one dimension for a prime base p, the nth number in the sequence $\{H_n\}$ is obtained by the following steps.

For each n:

1. Write n as a number in base p. For example, suppose $p = 3$ and $n = 22$, then we can write 22 in base 3 as $22 = 2*3^2+1*3^1+1*3^0 = 211$.
2. Reverse the digits and put a radix point (i.e., a decimal point base p) in front of the sequence (in the example, we get 0.112 base 3).
3. The result is the H_n.

In s-dimension problem, each component a Halton sequence are made with a different prime base p. First n primes can be used such as *Base 2*, *Base 3* and *Base 5* for first three dimensions. Every time the number of digits in n increases by one place, n's digit-reserved fraction becomes a factor of p finer-meshed. So, at each step as n increases points of Halton sequence are better and better filling Cartesian grids. In addition to this, the terms H_n of the Halton sequence can be computed only once, because they do not depend on the geometry of the problem.

Table 1. Halton sequences for first 3 dimensions.

Dim	***Dim = 1 (Base 2)***	***Dim = 2 (Base 3)***	***Dim = 3 (Base 5)***
n = 1	1/2	1/3	1/5
n = 2	1/4	2/3	2/5
n = 3	3/4	1/9	3/5
n = 4	1/8	4/9	4/5
n = 5	5/8	7/9	1/25
n = 6	3/8	2/9	6/25
n = 7	7/8	5/9	11/25
n = 8	1/16	8/9	16/25

3. FORMULATION OF THE PROBLEM AND MOM SOLUTION

The problem under investigation is that of finding the unknown charge density over a metallic plate maintained at constant potential. We know that the potential $V(\mathbf{r})$ due to a charge distribution characterized by density $\rho(\mathbf{r}')$ over a region R is given by:

$$V(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0} \int_R \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' \tag{1}$$

Where $\mathbf{r}'$ and $\mathbf{r}$ are the source and observation points respectively. If this equation is applied to the metal surface where the potential $V(\mathbf{r})$ is known, then this becomes an integral equation for the unknown charge density $\rho(\mathbf{r}')$.

For MoM solution of the integral equation, taking some known basis function $f_n(r')$, the unknown charge on the conducting surface is expanded as $\rho(\mathbf{r}') = \sum_{n=1}^{M} a_n f_n(\mathbf{r}')$ with unknown coefficient a_n to be determined. Then on the surface we have

$$4\pi\varepsilon_0 V(\mathbf{r}) = a_1 \int_R \frac{f_1}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' + \ldots + a_M \int_R \frac{f_M}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' \tag{2}$$

Applying the above equation on M observation points

$\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_M$, on the surface, we get a matrix equation

$$\begin{bmatrix} 4\pi\varepsilon_0 V(\mathbf{r}_1) \\ \vdots \\ 4\pi\varepsilon_0 V(\mathbf{r}_M) \end{bmatrix} = [A_{mn}] \begin{bmatrix} a_1 \\ \vdots \\ a_M \end{bmatrix} \tag{3}$$

where

$$A_{mn} = \int_R \frac{f_n}{|\mathbf{r}_m - \mathbf{r}'|} d\mathbf{r}' \tag{4}$$

The unknown vector a_n can be obtained by matrix inversion and an approximate solution can be obtained for the entire surface.

4. QUASI MONTE CARLO INTEGRATION IN MOM

It is evident from (4) that a typical element of the moment matrix is singular at $\mathbf{r}' = \mathbf{r}_m$. The integration of singular function cannot be evaluated exactly or by ordinary numerical quadrature methods. However, the specialized Gauss Quadrature rules are developed for integrating singular functions. One specific rule is the Lin-Log rule for integrating singular functions with known Log type singularity. However, it requires the calculation of appropriate weights for each type singularity problem such as point or line singularity separately. Thus it is necessary to adopt means that is universal for any type of singularity inside the integral and provides a good approximation of the actual result. The technique adopted here is the QMCI technique that gets rid of the singularity, making integration much simpler and justified specially, in case of two dimensional and three dimensional problems. As a matter of fact the technique does not even require any prior knowledge of the occurrence and location of the singularity in the integrand. It can be seen from Table 1 that the Halton points generated for $Dim = 2$ with the prime base 3 or $Dim = 3$ with prime base 5 are such that the point 0.5 is never generated. This means that for the regions which are being sampled by the Halton sequences with any prime base except 2 for integration of some function in that region, the midpoints are never sampled. This property can be used for the Monte Carlo integration of such functions which are singular only at the midpoints. Indeed in case of point matching technique of the MoM solution with pulse basis functions where the structure is divided into segments, the self term observation points $\mathbf{r}_m$ as given by (4) are the midpoints of the segments over which the integration is performed. Thus the proposed QMCI technique takes care of this point singularity by sampling the segments with Halton points. It is also seen that the

kernel of the integral equation has been retained in its exact form and no approximation has been made in order to deal with the singularity. Thus the QMCI technique does not require any analytical reduction of the kernel before going for the numerical integration.

5. NUMERICAL RESULTS

In this section, the results from computational evaluation of the capacitances are presented to demonstrate the efficiency and accuracy of the method described above. As the first example, a square metallic plate of dimension 1 m × 1 m is considered which is placed over the xy plane. It is maintained at a constant potential 1 V. The geometry is shown in Figure 1.

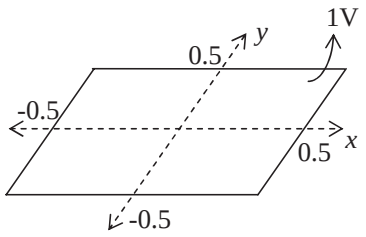

Figure 1. Square metallic plate at constant potential.

The problem is to find the unknown induced charged density distribution over the plate by method of moments. The basis function employed is the sub domain pulse i.e., piecewise (unit) constant over the segments, basis function after dividing the source region R, i.e., the plate, into M square segments of equal area. The observation points $(x_1, y_1), (x_2, y_2), \ldots, (x_M, y_M)$ are the mid points of the 1st, 2nd, ..., Mth segments respectively. Then (3) takes the form

$$\begin{bmatrix} 4\pi\varepsilon_0 \\ \vdots \\ 4\pi\varepsilon_0 \end{bmatrix} = [A_{mn}] \begin{bmatrix} a_1 \\ \vdots \\ a_M \end{bmatrix} \tag{5}$$

with

$$A_{mn} = \iint\limits_{S_n} \frac{1}{\sqrt{(x_m - x')^2 + (y_m - y')^2}} dx'dy' \tag{6}$$

The subscript of S_n denotes that the integration is done over the nth segment.

In evaluating the self term matrix element A_{nn} using point matching moment method [1], S_n is sampled with Halton points x' derived with base 3 in the x-direction, and the points y' with base 5 in the y-direction to deal with the singularity at the mid point (x_n, y_n). The result obtained for the charge distribution on the metallic plate obtained for $M = 100$ sub domains is presented in Figure 2, where the charge density is obtained at discrete points and the graph presents a linear interpolation between each computed point.

Next, a parallel plate capacitor with square plates of dimension $1\,\mathrm{m} \times 1\,\mathrm{m}$ is maintained at a potential difference $V_0 = 2\,\mathrm{V}$ is taken. Thus one of the plates is maintained at $+1\,\mathrm{V}$ while the other at $-1\,\mathrm{V}$ and are separated by a distance 1 m. Once the surface charge density $\rho(x, y)$ is determined by MoM on the plates, the total charge on each plate is found as:

$$Q = \iint\limits_{Plate} \rho(x, y)dxdy \tag{7}$$

and then the capacitance is $C = Q/V_0$.

In this work, the magnitude of the charge Q over either of the plates, and the capacitance C of the parallel plate capacitor is computed as a function of number of segments M employed in method of moments for a fixed number of Halton points $N = 100$. The results are tabulated in Table 2. As expected, the increase in number of segments facilitates the convergence of the capacitance.

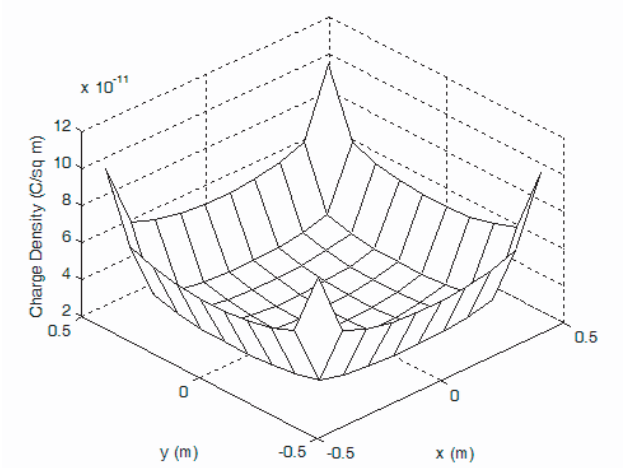

Figure 2. Charge density distribution over the plate with 100 sub domain pulse basis functions.

Finally, the capacitance values are computed as a function of variable number N of Halton points, for a fixed number of segments $M = 100$ as shown in Table 3.

Table 2.

Number of segments M	Magnitude of charge on either plates Q (coulomb)	Capacitance of the parallel plates C (farad)
100	5.6327e-011	2.8163e-011
225	5.7215e-011	2.8607e-011
400	5.7676e-011	2.8838e-011
625	5.7960e-011	2.8980e-011

Table 3.

Number of Halton points N	Magnitude of charge on either plates Q (coulomb)	Capacitance of parallel plates C (farad)
20	5.8844e-011	2.9422e-011
50	5.6888e-011	2.8444e-011
75	5.7190e-011	2.8595e-011
100	5.6327e-011	2.8163e-011

Next to examine the accuracy of the proposed technique; the result is validated for the problem of capacitance calculation of the unit cube. This problem has no analytic solution, and has long been regarded as a benchmark in the electrostatic theory. The result is obtained with total 96 segments (16 segments/face) i.e., 20 halton points only. The result is compared with the result obtained by the quadrature evaluated MoM solution for unit cube [21]. As evident from Table 4, the result is within 5% of error. The interesting part of the solution is that it does not require any analytical treatment for singularity removal or extraction.

As the third example, a cylindrical capacitor is considered as shown in Figure 3 with inner cylinder radius $a = 1\,\mathrm{m}$, outer radius $b = 2\,\mathrm{m}$ and length $L = 2\pi\,\mathrm{m}$. The self term matrix element as given

Table 4.

Capacitance of the Unit Cube [21] No. of Points 24	Capacitance of the Unit Cube Proposed Method	Relative Error (%)
0.6482958	0.6765784	4.36

by (4) for this problem in cylindrical (ρ, ϕ, z) coordinates is

$$A_{nn} = \iint_{S_n} \frac{1}{\sqrt{(\rho_n \cos\phi_n - \rho_n \cos\phi')^2 + (\rho_n \sin\phi_n - \rho_n \sin\phi')^2 + (z_n - z')^2}} {\rho_n}^2 d\phi' dz' \tag{8}$$

with ρ_n taking constant values a or b depending on the value of n. The segment S_n has the midpoints (ρ_n, ϕ_n, z_n) and is sampled by Halton points ϕ' and z' along the ϕ and z directions respectively with base 3. The capacitance values are computed for several cases such as with respect to variation in number of segments and variation in spacing between the cylindrical plates. The results are tabulated in Tables 5 and 6 respectively. The capacitance value is also compared with the value obtained from analytical formula for variation in number of segments and variation in spacing between the plates for fixed segment number of 100. As evident with the increase in number of segments, the results tend to converge and the deviation in analytical and numerical results reduces.

As the last example, a spherical capacitor is considered as shown in Figure 4 with radii of inner and outer spheres $a = 1\,\text{m}$ and $b = 2\,\text{m}$. The self term matrix element as given by (4) for this problem in spherical

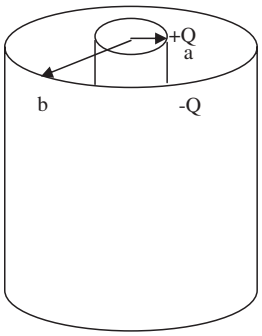

Figure 3. Cylindrical capacitor.

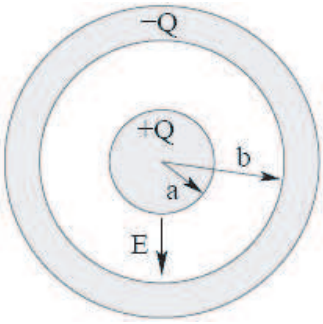

Figure 4. Spherical capacitor.

Table 5.

Number of segments M	Capacitance of the Cylindrical Capacitor C (farad) (Numerical Computation)	Capacitance of the Cylindrical Capacitor C (farad) (Analytical Formula) $C = 4\pi\varepsilon L/\ln(b/a)$	Relative Error (%)
64	5.2289e-010	5.037e-010	4.66
100	5.2828e-010		3.45
225	5.3599e-010		2.13
324	5.3710e-010		1.77
400	5.4010e-010		1.60
441	5.4070e-010		1.54

Table 6.

Spacing between the Plates (m)	Capacitance of the Cylindrical Capacitor C (farad) (Numerical Computation)	Capacitance of the Cylindrical Capacitor C (farad) (Analytical Formula)
1	5.2828e-010	5.0354e-010
2	3.4312e-010	3.1770e-010
4	2.4436e-010	2.1686e-010
5	2.2334e-010	1.9480e-010
10	1.7840e-010	1.4556e-010
20	1.5267e-010	1.1464e-010

polar (ρ, θ, ϕ) coordinates is

$$A_{nn} = \iint_{S_n} \frac{1}{\sqrt{(x_n - x')^2 + (y_n - y')^2 + (z_n - z')^2}} {\rho_n}^2 \sin\theta' d\theta' d\phi' \qquad (9)$$

where $x_n = \rho_n \sin\theta_n \cos\phi_n$, $x'_n = \rho_n \sin\theta' \cos\phi'$, $y_n = \rho_n \sin\theta_n \sin\phi_n$, $y' = \rho_n \sin\theta' \sin\phi'$, $z_n = \rho_n \cos\phi_n$ and $z' = \rho_n \cos\phi'$ with ρ_n taking constant values a or b depending on the value of n. The segment S_n has the singular midpoint $(\rho_n, \theta_n, \phi_n)$ and is sampled by Halton points θ' and φ' along the θ and ϕ directions respectively with base 3. Again, the capacitance values are computed for several cases such as with

Table 7.

Number of segments M	Capacitance of the Spherical Capacitor C (farad) (Numerical Computation)	Capacitance of the Spherical Capacitor C (farad) (Analytical Formula) $C = 4\pi\varepsilon/(1/b - 1/a)$	Relative Error (%)
15	2.2585e-010	2.2231e-010	1.59
25	2.4140e-010		8.59
36	2.2331e-010		0.45
64	2.2259e-010		0.13
100	2.2233e-010		0.008
121	2.2236e-010		0.008

Table 8.

Spacing between the Spheres (m)	Capacitance of the Spherical Capacitor C (farad) (Numerical Computation)	Capacitance of the Spherical Capacitor C (farad) (Analytical Formula)
1	2.2233e-010	2.2231e-010
2	1.6696e-010	1.6673e-010
5	1.3367e-010	1.3338e-010
10	1.2256e-010	1.2227e-010
20	1.1701e-010	1.1671e-010
100	1.1256e-010	1.1227e-010

respect to variation in number of segments and variation in spacing between the spherical shells. The results are tabulated in Tables 7 and 8 respectively. The capacitance value is also compared with the value obtained from analytical formula for variation in number of segments and variation in spacing between the spheres for fixed segment number of 100. As seen the increase in number of segments converges the results. A very good agreement between the numerical and analytical results is evident.

It should be noted that with the sub domain pulse basis function, the matrix elements have been obtained in this work by

actual integration of the functions without using any closed form or approximation for them.

6. CONCLUSION

The QMCI technique using Halton sequence is proposed in the MoM solution of the EFIE. This technique has been applied on problem for unknown charge distribution on surfaces of metallic structures and the capacitance computation of the parallel plate, cylindrical and spherical capacitors. The results demonstrate that the proposed QMCI technique produce results that are accurate. The higher accuracy is evident especially at the edges where charge concentration is very high. In addition to this, the QMCI is very effective in overcoming the problem of singularity arising in the MoM formulation without any need for analytical preprocessing and prior knowledge of occurrence and location of singularity. This characteristic of QMCI makes it more suitable for the problems in two and higher dimensions.

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