Markov Chain Monte Carlo Solution of Poisson's Equation in Axisymmetric Regions

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Abstract

The advent of the Monte Carlo methods to the field of EM have seen floating random walk, fixed random walk and Exodus methods deployed to solve Poisson's equation in rectangular coordinate and axisymmetric solution regions. However, when considering large EM domains, classical Monte Carlo methods could be time-consuming because they calculate potential one point at a time. Thus, Markov Chain Monte Carlo (MCMC) is generally preferred to other Monte Carlo methods when considering whole-field computation. In this paper, MCMC has been applied to solve Poisson's equation in homogeneous and inhomogeneous axisymmetric regions. The MCMC results are compared with the analytical and finite difference solutions.

Index Terms – Poisson's equations, axisymmetric problem, inhomogeneous media, homogeneous medium, Markov Chain Monte Carlo (MCMC)

I. Introduction

Poisson's equation is an elliptic partial differential equation that frequently appears in many scientific problems such as electrostatics, surface reconstruction, gravitational problems, and semiconductors [1]-[2]. Due to its convenience, Poisson's equation in rectangular coordinate has been extensively studied using different numerical methods [3]-[5].

Stochastic methods such as the Monte Carlo techniques are nondeterministic numerical methods unlike the deterministic numerical methods such as finite difference, finite elements and moment methods used in solving mathematical and physical problems [6]. So Monte Carlo methods such as Floating random walk, Fixed random walk and Exodus methods have been used for solution of Poisson's equation in rectangular and axisymmetric regions [7]-[12]. With advancement in memory technology, MCMC method can handle EM problems in large solution domains within shortest possible time while serving as a viable alternative to other numerical methods.

In this paper, the solutions of axisymmetric Poisson's equations with the Markov Chain Monte Carlo are presented. Cases of homogeneous and inhomogeneous axisymmetric Poisson's equations are discussed. Simulation results are reported and they are compared with the finite difference method and analytical solutions. The solutions are found to be in close agreement.

II. Poisson's Equation

The Poisson's equation in solution region R subject to Dirichlet boundary condition is given as

$$\nabla^2 V = -g(\rho, z) = -\frac{\rho_S}{\varepsilon} \tag{1}$$

where ρ_S is the surface charge; $\varepsilon =$ absolute permittivity and $V = V_p$ on Boundary B.

Assuming a square grid, the step size is given as $\Delta\rho = \Delta z = \Delta$. Thus the finite difference equivalent of equation (1) is given as [13]

$$V(\rho, z) = p_{\rho+}V(\rho+\Delta, z) + p_{\rho-}V(\rho-\Delta, z) + p_{z+}V(\rho, z+\Delta) + p_{z-}V(\rho, z-\Delta) + \frac{\Delta^2 g}{4} \tag{2}$$

If $\rho = i\Delta$ and $z = j\Delta$, the transition probabilities, p_{z+}, p_{z-}, $p_{\rho+}$ and $p_{\rho-}$, for axisymmetric homogeneous domains are given as [14]

$$p_{z+} = p_{z-} = \frac{1}{4},\ p_{\rho+} = \frac{1}{4} + \frac{1}{8i},\ p_{\rho-} = \frac{1}{4} - \frac{1}{8i} \tag{3}$$

The term $\frac{\Delta^2 g}{4}$ is the source term that must be recorded at each step of the random walk.

The system is stochastic, thus

$$p_{z+} + p_{z-} + p_{\rho+} + p_{\rho-} = 1 \tag{4}$$

At $\rho = 0$, the finite difference equivalence of equation (2) becomes [14]

$$V(0, z) = p_{\rho+}V(\Delta, z) + p_{z+}V(0, z+\Delta) + p_{z-}V(0, z-\Delta) \tag{5}$$

where $p_{\rho+} = \frac{4}{6}$, $p_{\rho-} = 0$, $p_{z+} = p_{z-} = \frac{1}{6}$

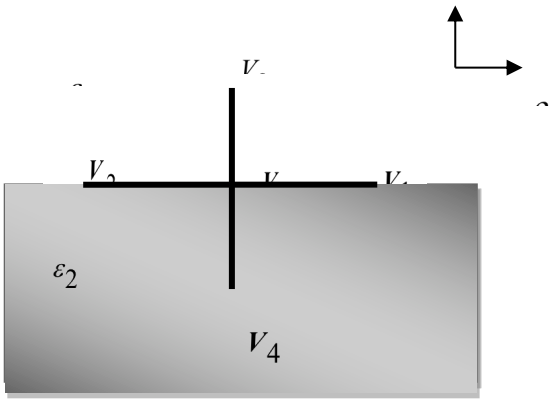

Figure 1. Interface between media of dielectric permittivity ε_1 and ε_2 [7].

III. Inhomogeneous Media

Inhomogeneous media occur when two or more media have variations in dielectric permittivity. The Figure 1 shows transition probabilities at a node at the interface between two dielectric permittivity ε_1 and ε_2.

For the $z = constant$ interface, $\varepsilon_1 \frac{\partial V_1}{\partial z} = \varepsilon_2 \frac{\partial V_2}{\partial z}$, and the transition probabilities at the interface are determined as [14]:

$$p_{z+} = \frac{\varepsilon_1}{2(\varepsilon_1 + \varepsilon_2)} \tag{6a}$$

$$p_{z-} = \frac{\varepsilon_2}{2(\varepsilon_1 + \varepsilon_2)} \tag{6b}$$

$$p_{\rho+} = \frac{1}{4} + \frac{1}{8i}; \; p_{\rho-} = \frac{1}{4} - \frac{1}{8i} \tag{6c}$$

Similarly, for $\rho = constant$ interface, $\frac{\varepsilon_1}{\rho}\frac{\partial V_1}{\partial \rho} = \frac{\varepsilon_2}{\rho}\frac{\partial V_2}{\partial \rho}$, and the transition probabilities are given as [15]:

$$p_{\rho+} = \frac{\varepsilon_1}{2(\varepsilon_1 + \varepsilon_2)}\left(1 + \frac{\Delta}{2\rho}\right) \tag{7a}$$

$$p_{\rho-} = \frac{\varepsilon_2}{2(\varepsilon_1 + \varepsilon_2)}\left(1 - \frac{\Delta}{2\rho}\right) \tag{7b}$$

$$p_{z+} = p_{z-} = \frac{1}{4}. \tag{7c}$$

In this paper, $z = constant$ interface is used for the inhomogeneous problem discussed in the section V.

IV. Markov Chain Monte Carlo

Given a sequence of random variables $X^{(0)}, X^{(1)}, \ldots, X^{(n)}$ with probability distribution of $X^{(n)}$ determined by the probability distribution of $X^{(n-1)}$ [16]-[22]. The sequence is referred to as a Markov Chain with time-invariant conditional probability distributions. Markov chains are mathematical models that remember only the most recent past. In this paper, the Markov chain is the random walk while the discrete states are the grid nodes. The transition probability P_{ij} is defined as the probability that a randomly walking particle at node i will move to node j and it is expressed as,

$$P_{ij} = P(x_{n+1} = j \mid x_0, x_1, \ldots, x_n) = P(x_{n+1} = j \mid x_n), \; j \in X, n = 0, 1, 2, \ldots \tag{8}$$

The transition probabilities are derived from the finite difference equivalence equation and they correspond to the random walks that form the background to the MCMC method.

The transition probability **P** is defined as

$$\mathrm{P} = \begin{bmatrix} \mathrm{P}_{00} & \mathrm{P}_{01} & \mathrm{P}_{02} & \cdots \\ \mathrm{P}_{10} & \mathrm{P}_{11} & \mathrm{P}_{12} & \cdots \\ \mathrm{P}_{20} & \mathrm{P}_{21} & \mathrm{P}_{22} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix} \tag{9}$$

P is stochastic and it is given by,

$$\sum_{j \in X} P_{ij} = 1, \quad i \in X \tag{10}$$

If n_f are free (non-absorbing) nodes and n_p are fixed (absorbing) nodes, the size of **P** is $n \times n$ given as

$$n = n_f + n_p \tag{11}$$

Also, n_p are numbered first and n_f are numbered last, then $n \times n$ transition matrix, **P** becomes

$$\mathbf{P} = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{R} & \mathbf{Q} \end{bmatrix} \tag{12}$$

where

$n_f \times n_p$ **R** matrix is the probabilities of moving from non-absorbing nodes to absorbing ones;

$n_f \times n_f$ **Q** matrix is the probabilities of moving from one non-absorbing node to another;

$n_f \times n_f$ $\boldsymbol{I}$ matrix is the identity matrix representing transitions between the absorbing nodes $(P_{ii} = 1 \; and \; P_{ij} = 0)$.

$n_p \times n_f$ $\mathbf{0}$ matrix is the null matrix indicating no transitions from absorbing to non-absorbing nodes.

From equation 3, the elements of matrix **Q** at nodes in the $\rho \neq 0$ region are obtained summarily as

$$Q_{ij} = \begin{cases} \frac{1}{4}, & if\ i\ is\ directly\ connected\ to\ j \\ \left(\frac{2i+1}{8i}\right), & if\ i\ is\ directly\ connected\ to\ i+1 \\ \left(\frac{2i-1}{8i}\right), & if\ i\ is\ directly\ connected\ to\ i-1 \\ 0, & if\ i = j\ or\ i\ is\ not\ directly\ connected\ to\ j \end{cases} \tag{13}$$

Similarly, from equation 5, the elements of matrix **Q** for nodes at the line of Symmetry, $\rho = 0$, are obtained as

$$Q_{ij} = \begin{cases} \frac{1}{6}, & if\ i = 0\ and\ is\ directly\ connected \\ & to\ j\ and\ j-1 \\ \frac{4}{6}, & if\ i = 0\ and\ is\ directly\ connected \\ & to\ i+1 \\ 0, & if\ i = j\ or\ i\ is\ not\ directly\ connected \\ & to\ j \end{cases} \tag{14}$$

The elements of matrix R_{ij} are obtained in the same manner from equations (13) and (14) except that j is an absorbing node.

The fundamental matrix, **N** for any absorbing Markov chain is given as,

$$\mathbf{N} = (\mathbf{I} - \mathbf{Q})^{-1} \tag{15}$$

where N_{ij} is the average number of times that the randomly walking particle starting at node i will pass through node j before being absorbed.

The absorption probability matrix ***B*** is thus

$$\mathbf{B} = \mathbf{N}\,\mathbf{R} \tag{16}$$

where $n_f \times n_p$ B_{ij} matrix is the probability of moving from non-absorbing node i to absorbing node j. The **B** matrix is stochastic and it is given as

$$\sum_{j=1}^{n_p} B_{ij} = 1, \quad i = 1, 2, ..., n_f \tag{17}$$

Thus,

$$\mathbf{V_f} = \mathbf{B}\mathbf{V_p} + \boldsymbol{NG}_f \tag{18}$$

where $\mathbf{V}_f$ and $\mathbf{V}_p$ are the free and fixed nodes potentials respectively.

The term $G_f = \frac{\Delta^2}{4} g(\rho, z)$ is the vector of interior point contributions to be recorded at every step of the random walk [13]. The first term in RHS of equation (18), $\mathbf{BV}_\mathrm{p}$ is used to evaluate the Laplace's equation. The second term, $\mathbf{NG}_\mathrm{f}$ in equation (18) is used for the analysis of Poisson's equation provided that $\mathbf{V_p} = 0$. Otherwise, the equation (18) is used for analysis of Poisson's equation for prescribed potential, $\mathbf{V_p} \neq 0$.

In terms of the prescribed potentials $\boldsymbol{V}_1, \boldsymbol{V}_2, ..., \boldsymbol{V_{np}}$, the first term in the RHS of equation (18), $\mathrm{V_f} = \mathbf{BV_p}$ becomes

$$V_i = \sum_{j=1}^{n_p} B_{ij} V_j, \; i = 1, 2, ..., n_f \tag{19}$$

where $\boldsymbol{V_i}$ is the potential at any free node i. The Equation (19) provides solution at all the free nodes at once.

In this paper, Poisson's equation in homogeneous and inhomogeneous axisymmetric domains is presented where the boundary (prescribed) potentials are zeros, that is, $\mathbf{V_p} = 0$. So the equation (18) reduces to

$$\mathbf{V_f} = \boldsymbol{NG}_f \tag{20}$$

where $\mathbf{V}_f$ are the free nodes potentials;

$\boldsymbol{N}$ is the fundamental matrix;

$\mathbf{G_f}$ is the vector of the contributions of interior points.

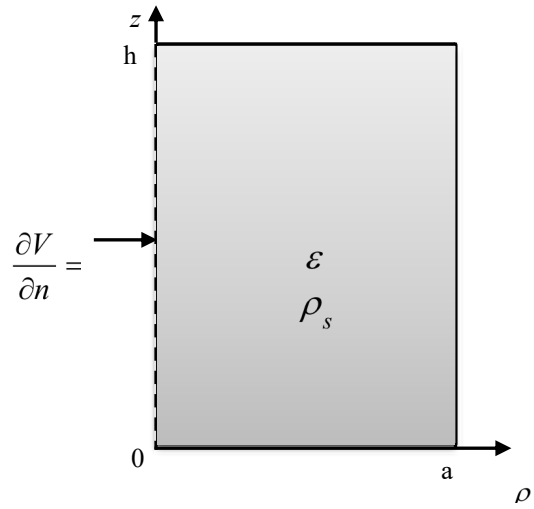

Figure 2. Axisymmetric Homogeneous Domain Approximation of a cylindrical tank of radius *a* and height *h*.

V. Simulation Results

A. Simulation Results for Axisymmetric Homogeneous Poisson's Equation

Poisson's equation in axisymmetric homogeneous domain is given as:

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial V}{\partial\rho}\right)+\frac{\partial^2 V}{\partial z^2}=-\frac{\rho_s}{\varepsilon} \tag{22}$$

Subject to boundary conditions:

$V(a,z)=0;\ V(a,h)=0;\ V(a,0)=0$ and
$\frac{\partial V}{\partial n}=0$ at $\rho=0$.

Suppose the axisymmetric domain of an earthed metal cylindrical tank of radius ***a*** and height ***h*** shown in the Figure 2 is completely filled with a charged liquid such as hydrocarbon. The Neumann boundary condition is imposed at the line of symmetry while the Dirichlet boundary conditions are imposed on the remaining three boundaries with zero potential. The analytical solution to the problem is presented in [8] as:

$$V(\rho,z)=\frac{2\rho_S}{\varepsilon_0\varepsilon_r a}\sum_{n=1}^{\infty}\frac{J_0(\lambda_n\rho)}{\lambda^3 J_1(\lambda_n a)}\left(\begin{array}{l}1-\cosh(\lambda_n z)\\ +\dfrac{\sinh(\lambda_n z)}{\sinh(\lambda_n h)}\left[\cosh(\lambda_n h)-1\right]\end{array}\right) \tag{23}$$

Table 1. Parameters for Poisson's Equation in Axisymmetric Homogeneous Domain.

Parameter	Value
ρ_s	$10^{-5}C/m^2$
a	1m
h	2m
ε	$2.0\varepsilon_0$

where λ_n are the roots of $J_0(\lambda_n a)=0$.

J_0 and J_1 are Bessel functions of first kind, order zero and one respectively.

With the background theory of the MCMC method discussed in the preceding section, all the simulations in this paper are carried out. Using the parameters in the Table 1, the results for the potential distributions along $\rho=0.5m,\ 0\le z\le 2m,\ \rho=0,\ 0\le z\le 2m$ (line of symmetry) and that along $\rho=0.9m,\ 0\le z\le 2m,$ are reported in the Figures 3(a)–(c). Similarly, the potential distribution along $z=1,\ 0\le\rho\le 1m$, the surface plot and contour plot for all the grid nodes are presented in the Figure 3(d)–(f).

In the Table 2, the MCMC results for some randomly selected grid points are compared with the finite difference solution and analytical solution. The MCMC solution is, as evident, more accurate than the finite difference solution even after the step size is reduced from *0.05m* to *0.025m* as shown in the Table 2.

However, the number of iterations for the finite difference method increased from *500* to *5000* with the step size reduction. For problems with larger domain size, this could increase the computation time and memory requirement significantly. The solution to the same problem using the floating random walk Monte Carlo method with different domain size is reported in [8].

Table 2. Comparison for Analytical, FDM and MCMC for Poisson's Equation in Axisymmetric Homogeneous Domain.

Coordinate (ρ, z)	Analytical (KV)	FDM (KV) $\Delta = 0.05$ Iteration=500	FDM (KV) $\Delta = 0.025$ Iteration=5000	MCMC (KV) $\Delta = 0.05$	MCMC (KV) $\Delta = 0.025$
(0.25, 0.5)	86.870	86.042	86.784	86.486	86.849
(0.5, 0.5)	71.730	71.212	71.715	71.409	71.743
(0.75, 0.5)	44.080	43.881	44.130	43.942	44.141
(0.5, 0.75)	83.662	83.019	83.643	83.030	83.677
(0.5, 0.25)	46.838	46.543	46.834	46.701	46.851

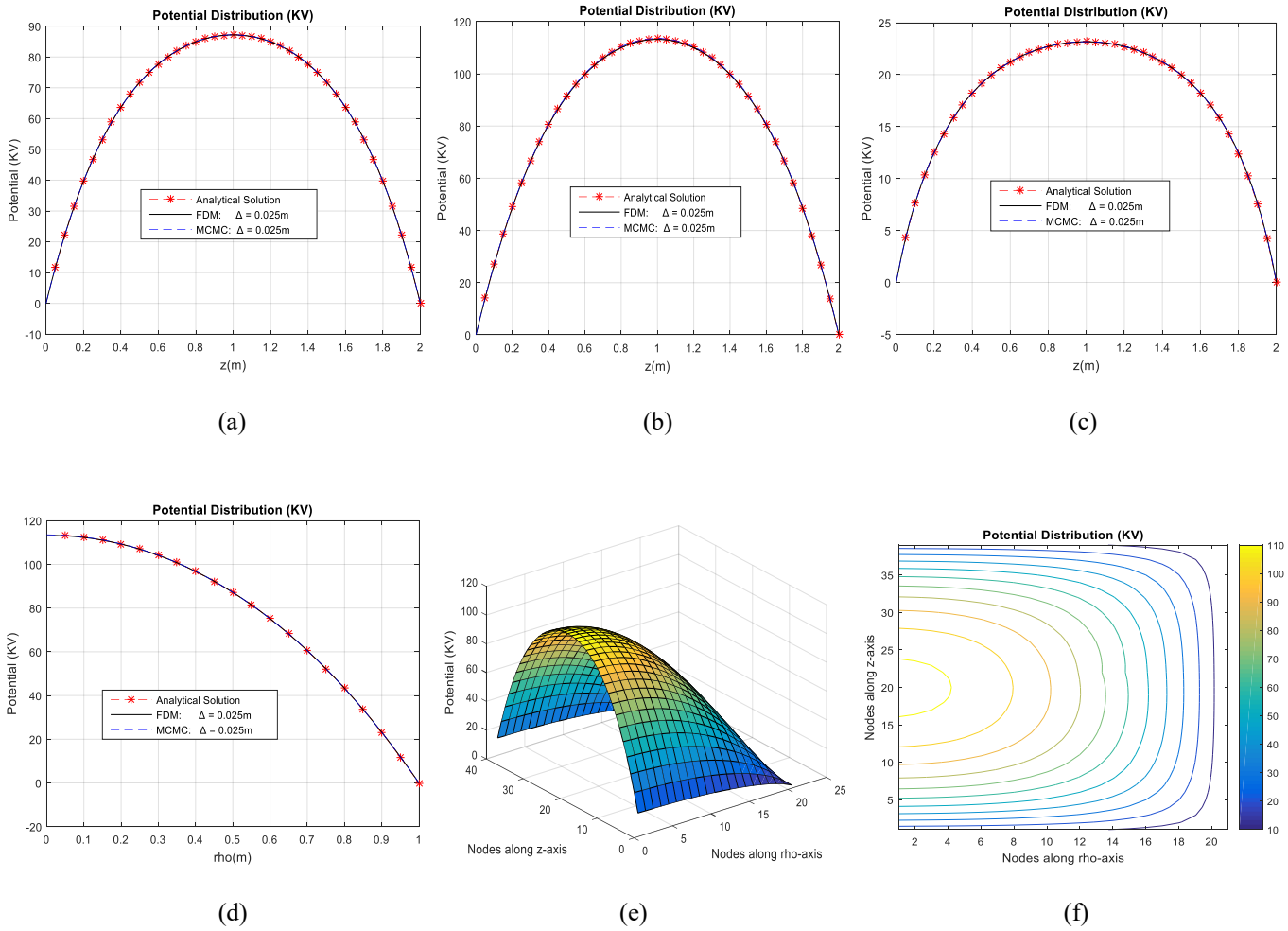

Figure 3. Potential Distribution along (a) $\rho = 0.5m,\ 0 \le z \le 2m$ (b) Line of symmetry, $\rho = 0, 0 \le z \le 2m$ (c) $\rho = 0.9m,\ 0 \le z \le 2m$ (d) $z = 1,\ 0 \le \rho \le 1m$ (e) Surface plot (f) Contour Plot for Poisson's equation in Homogeneous Axisymmetric Domain.

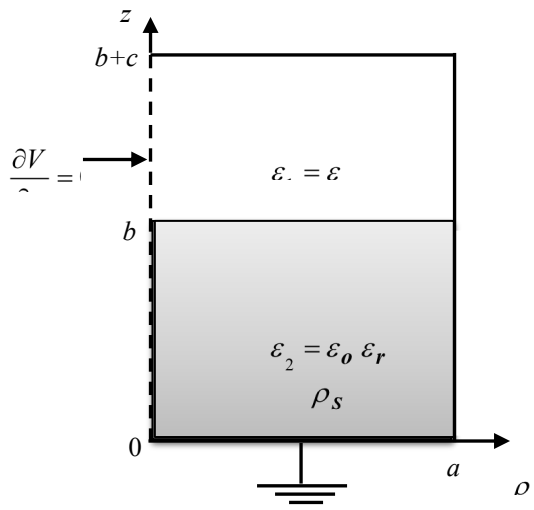

Figure 4. Inhomogeneous Axisymmetric Solution Region.

B. *Simulation Results for Axisymmetric Inhomogeneous Poisson's Equation*

Poisson's equation in axisymmetric inhomogeneous domain is given as [14], [23]-[24]:

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial V_l}{\partial\rho}\right)+\frac{\partial^2 V_l}{\partial z^2}=-\frac{\rho_s}{\varepsilon} \tag{24}$$

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial V_g}{\partial\rho}\right)+\frac{\partial^2 V_g}{\partial z^2}=0 \tag{25}$$

Subject to boundary conditions (B.C):

$V(a,z)=0; V_g(a,b+c)=0; V(a,0)=0; V_g=V_l, z=b;$

$\frac{\partial V_g}{\partial z}=\varepsilon_r\frac{\partial V_l}{\partial z}, z=b$ and $\frac{\partial V}{\partial n}=0$ at $\rho=0$.

Suppose an earthed metal cylindrical tank is partly filled with a charged liquid such as hydrocarbon as shown in the Figure 4. The problem is described mathematically in equations (24) – (25). From the Figure 4, region $z>b$ is filled with gas, posing Laplace's equation problem while $z<b$ region is filled with charged hydrocarbon, constituting Poisson's equation. The analytical solution for the problem is presented in [14], [23]-[24]:

$$V(\rho,z)=\begin{cases}\sum_{n=1}^{\infty}\frac{2\rho_s}{R_n K_n}J_0(\lambda_n\rho)\left[\cosh(\lambda_n b)-1\right]\sinh\left[\lambda_n(b+c-z)\right] & z\geq b\\ \sum_{n=1}^{\infty}\frac{2\rho_s}{R_n\varepsilon_r}J_0(\lambda_n\rho)\left(\begin{array}{l}\frac{\sinh(\lambda_n z)}{K_n}[\cosh(\lambda_n b)\cosh(\lambda_n c)\\ +\varepsilon_r\sinh(\lambda_n b)\sinh(\lambda_n c)\\ -\cosh(\lambda_n c)]-\cosh(\lambda_n z)+1\end{array}\right) & z\leq b\end{cases} \tag{26}$$

where $K_n=\sinh(\lambda_n b)\cosh(\lambda_n c)+\varepsilon_r\cosh(\lambda_n b)\sinh(\lambda_n c)$;

$R_n=\varepsilon_0 a\lambda_n^3 J_1(\lambda_n a)$; λ_n are the roots of $J_0(\lambda_n a)=0$.

J_0 and J_1 are Bessel functions of first kind, order zero and one.

With the parameters in the Table 3, the MCMC in this section is essentially the same as in the previous section except that the transition probabilities at the media interface are described by the equations (6). The potential distributions along $\rho=0.5m, 0\leq z\leq 2m$, $\rho=0, 0\leq z\leq 2m$ (line of symmetry) and $\rho=0.9m, 0\leq z\leq 2m$, are reported in the Figures 5(a)–(c). Also, the potential distribution at the media interface, $z=1, 0\leq\rho\leq 1m$, surface and contour plots are presented in the Figure 5(d)–(f). The solution to the same problem using finite difference method and Exodus method are presented in [7] and [14].

The MCMC solutions for selected grid points are compared with the FDM and analytical solution as in the Table 4. With $\Delta=0.05m$, the MCMC solution is much more accurate than the FDM when compared with the analytical solution. Further reduction in Δ from *0.05m* to *0.005m* for the FDM with *100,000* iteration steps gives accurate solution that agrees with the MCMC and analytical solutions.

However, the computation time for the FDM increased from 0.0253seconds to 7mins and 30seconds compared to MCMC which is 0.06281seconds. The MCMC agrees perfectly with the analytical solution while the FDM requires further reduction in step size to converge to the analytical solution.

Table 3. Parameters for Inhomogeneous Poisson's Problem.

Parameter	Value
ρ_s	$10^{-5}C/m^2$
a	1m
$b=c$	1m
ε_1	ε_0
ε_2	$2.0\varepsilon_0$

Table 4. Comparison for Analytical, FDM and MCMC for Axisymmetric Inhomogeneous Problem.

Coordinate (ρ, z)	Analytical (KV)	FDM (KV) $\Delta = 0.05m$ Iteration=500	FDM (KV) $\Delta = 0.005m$ Iteration=100,000	MCMC (KV) $\Delta = 0.05m$
(0.25, 0.3)	57.8821	56.7096	57.8192	58.0019
(0.35, 1.5)	19.3922	17.7028	19.2520	19.7284
(0.5, 1.05)	51.4958	47.3810	51.1197	52.2268
(0.6, 1.6)	9.6358	8.7791	9.5643	9.8021
(0.8, 0.6)	34.8676	34.0749	34.8509	34.8935

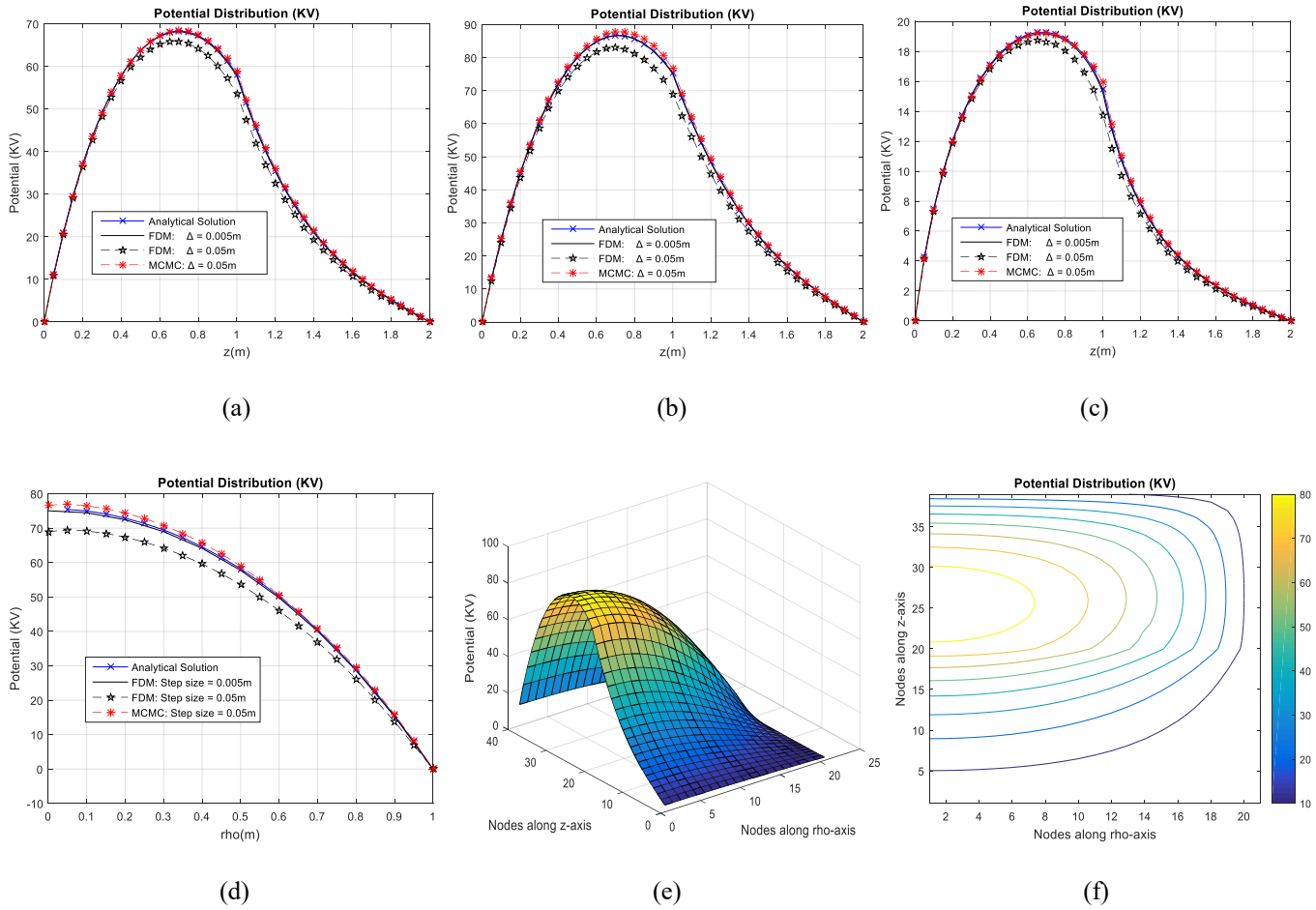

Figure 5. Potential Distribution along (a) $\rho = 0.5m,\ 0 \le z \le 2m$ (b) Line of symmetry, $\rho = 0, 0 \le z \le 2m$ (c) $\rho = 0.9m,\ 0 \le z \le 2m$ (d) Media interface, $z = 1,\ 0 \le \rho \le 1m$ (e) Surface plot (f) Contour Plot for Poisson's equation in Inhomogeneous Axisymmetric Domain.

VI. Conclusion

Poisson's equation has been extensively studied using different numerical methods and analytical method for few simple cases. Thus, for complex problems, there is a need for continuous development of simple and efficient numerical methods. Since the introduction of probabilistic method such as Monte Carlo method to the field of electromagnetics, several Monte Carlo methods developed such as floating random walk, fixed random walk and Exodus method have been used to solve Poisson's equation, notably in rectangular coordinate and axisymmetric solution regions. However, these methods calculate potentials one point at a time and are time-consuming when solving complex electromagnetic problems. In this paper, the MCMC method which is an improvement on the classical Monte Carlo method has been applied to solve Poisson's equations in axisymmetric region in homogeneous and inhomogeneous regions. The MCMC solutions reported in this paper are compared with analytical and finite difference method. In the case of homogeneous problem, the MCMC method agrees with the analytical and the finite difference method with difference in computation time being only a fraction of seconds. In the case of inhomogeneous problem, the MCMC method agrees perfectly with the analytical solution. However, further reduction in step size is required for the finite difference solution to converge to the analytical solution with attendant increase in iteration steps and computation time.

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