

Regional Monte Carlo Potential Calculation Using Markov Chains*

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A major objection to the idea of incorporating Monte Carlo methods along with other numerical methods such as finite difference and finite element into undergraduate classes such as heat transfer and electromagnetics is that they are only capable of calculating the potential at a single point at a time unlike other methods which provide simultaneously the solution at all the grid nodes. This paper shows how this major limitation is overcome using absorbing Markov chains to obtain the transition probability. Illustrative examples are provided to show that not only is this approach capable of providing the solution at all the grid nodes at once, the solution is more accurate than the fixed random walk and is not subject to randomness.

SUMMARY OF EDUCATIONAL ASPECTS OF THIS PAPER

1. The paper discusses materials/software for a course in Electromagnetics.
2. The course is for year 2 or junior students in Electrical Engineering or any engineering course involving partial differential equations.
3. The mode of presentation is classroom teaching and is offered as a regular course.
4. The hours required to cover the material is one hour; one homework project on Monte Carlo method (MCM) may be helpful.
5. A novel aspect presented in this paper is the ability to use MCM to generate potential at all nodes at once.
6. The standard text recommended in the course, in addition to author's notes is, for undergraduates, M. N. O. Sadiku, *Elements of Electromagnetics*, 3rd ed., Oxford University Press, or, for graduates, M. N. O. Sadiku, *Numerical Techniques in Electromagnetics*, 2nd ed., CRC Press. The material is not covered in the text.

INTRODUCTION

NUMERICAL TECHNIQUES have become well-established tools for solving engineering problems. The need for including numerical methods in undergraduate classes such as heat transfer and electromagnetics has been expressed

again and again [1–7]. There are several reasons for this. First, numerical solutions provide a significant aid in the teaching-learning process by helping to bridge the gap between the theoretical formulations and the real world in which the students live. Second, there is an increasing availability of computers in educational institutions and computer methods are revolutionizing the engineering profession. Third, problems that can be solved analytically have been solved already and students need to learn numerical tools for solving complex problems.

Although the pedagogical value of introducing numerical methods such as the finite element methods, finite difference methods, and moment method in an introductory electromagnetic course has been recognized, similar attempts to introduce Monte Carlo Method (MCM) has not been well received based on the fact that the classical MCM [8–14] calculates the potential one point at a time. To overcome this limitation, several techniques have been proposed. These include the shrinking boundary method [15], inscribed figure method [16], and the surface density method [17], but each of these techniques is complicated and hard to program. This paper proposes a simple technique for whole field calculations. The technique basically calculates the transition probabilities using absorbing Markov chains. It places MCM at the same footing as other numerical methods and encourages its incorporation in undergraduate classes.

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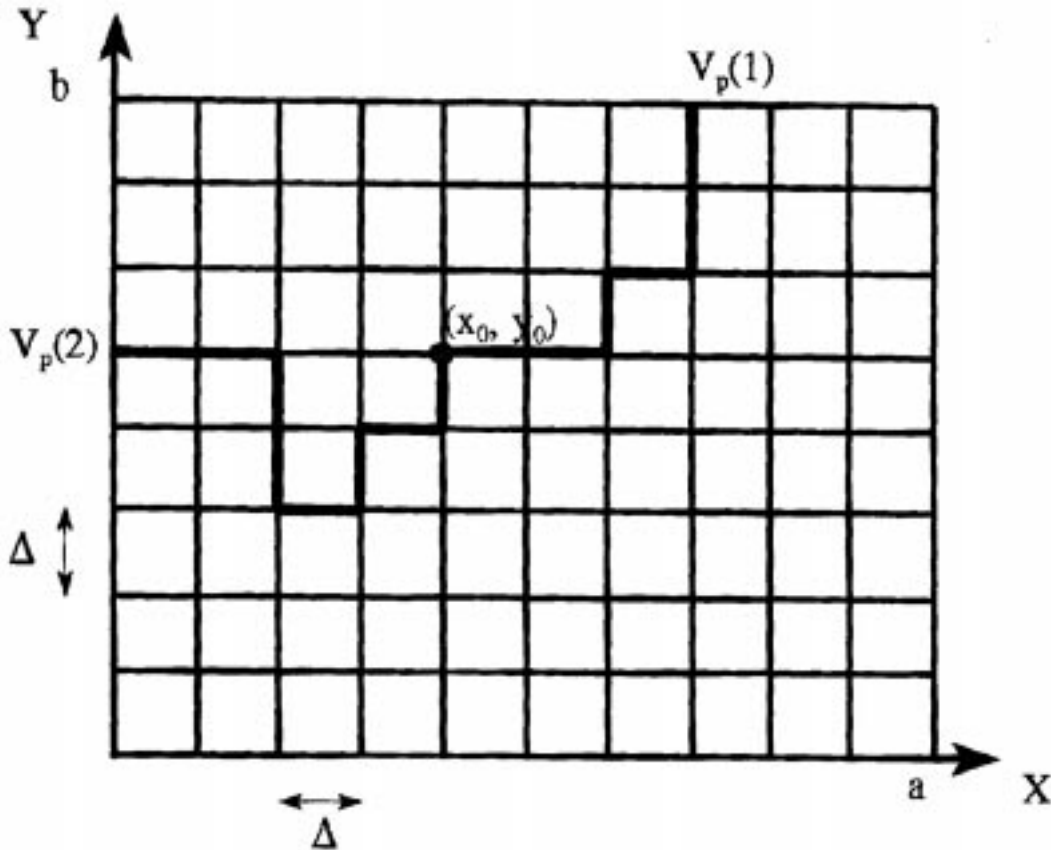


Fig. 1. Fixed random walk from point (x_0, y_0) where the potential is to be determined.

REGULAR MONTE CARLO METHOD

The most popular Monte Carlo method is the fixed random walk. Suppose that this method is to be applied in solving Laplace’s equation:

$$\nabla^2 V = 0 \text{ in region R} \tag{1}$$

subject to Dirichlet boundary condition:

$$V = V_P \text{ on boundary B} \tag{2}$$

The region R is divided into a mesh (as in finite difference), as typically shown in Fig. 1. Equation (1) is replaced by its finite difference equivalent as [18]:

$$V(x, y) = p_{x+} V(x + \Delta, y) + p_{x-} V(x - \Delta, y) + p_{y+} V(x, y + \Delta) + p_{y-} V(x, y - \Delta) \tag{3}$$

where

$$p_{x+} = p_{x-} = p_{y+} = p_{y-} = \frac{1}{4} \tag{4}$$

A probabilistic interpretation of equation (3) is that if a walking particle is momentarily at point (x, y) , the probability of moving to $(x + \Delta, y)$, $(x - \Delta, y)$, $(x, y + \Delta)$, or $(x, y - \Delta)$, is p_+ , p_{x-} , p_{y+} , or p_{y-} respectively.

To find the potential at a free point (x_0, y_0)

(where the potential is unknown), a random-walking particle is asked to begin its walk at that point. It wanders through the mesh according to the probabilities in equation (4) until it reaches the boundary where it is absorbed and the prescribed potential $V_p(1)$ is recorded. By sending out N particles from (x_0, y_0) and recording the potential at the end of each walk, we obtain:

$$V(x_0, y_0) = \frac{1}{N} \sum_{i=1}^N V_p(i) \tag{5}$$

If there are n_p fixed nodes on B with prescribed potential V_1, V_2, \dots, V_{n_p} , equation (5) becomes:

$$V(x_0, y_0) = \frac{N_1}{N} V_1 + \frac{N_2}{N} V_2 + \dots + \frac{N_{n_p}}{N} V_{n_p} \tag{6}$$

where N_k is the number of random walks ending at fixed node k and $N_1 + N_2 + \dots + N_{n_p} = N$. Thus:

$$V(x_0, y_0) = \sum_{k=1}^{n_p} p_k V_k \tag{7}$$

where $p_k = N_k/N$ is the probability that a random walk starting at free node (x_0, y_0) ends at fixed node k . Calculating p_k is the major goal of this paper.

In the past, p_k was calculated directly or indirectly for just one point (x_0, y_0) at a time

using fixed random walk [14, 19], floating random walk [1, 20], or the exodus method [21, 22]. In this paper, we want to employ Markov chains to calculate p_k for all the free nodes in the entire solution region at once.

ABSORBING MARKOV CHAINS

A Markov chain is a sequence of random variables $X^{(0)}, X^{(1)}, \dots$, where the probability distribution of $X^{(n)}$ is determined by the probability distribution $X^{(n-1)}$. A Markov process is a type of random process that is characterized by the memoryless property [23–27]. It is a process evolving in time that remembers only the most recent past and whose conditional probability distributions are time invariant. Markov chains are mathematical models of this kind of process. The Markov chains of interest to us are *discrete-state, discrete-time* Markov chains. In our case, the Markov chain is the random walk and the states are the grid nodes. The transition probability P_{ij} is the probability that a random-walking particle at node i moves to node j . It is expressed by the Markov property:

$$P_{ij} = \mathbf{P}(x_{n+1} = j | x_0, x_1, \dots, x_n) = \mathbf{P}(x_{n+1} = j | x_n), j \in X, n = 0, 1, 2, \dots \quad (8)$$

The Markov chain is characterized by its transition probability matrix \mathbf{P} , defined by:

$$\mathbf{P} = \begin{bmatrix} P_{00} & P_{01} & P_{02} & \cdots \\ P_{10} & P_{11} & P_{12} & \cdots \\ P_{20} & P_{21} & P_{22} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix} \quad (9)$$

\mathbf{P} is a stochastic matrix, meaning that the sum of

the elements in each row is unity, i.e.

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

We may also use the state transition diagram as a way of representing the evolution of a Markov chain. An example is shown in Fig. 2 for a three-state Markov chain.

If we assume that there are n_f free (or non-absorbing) nodes and n_p fixed (prescribed or absorbing) nodes, the size of the transition matrix \mathbf{P} is n , where:

$$n = n_f + n_p \quad (11)$$

(An absorbing node is one in which a random-walking particle reaches and is absorbed.) If the absorbing nodes are numbered first and the non-absorbing states are numbered last, the $n \times n$ transition matrix becomes:

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

where the $n_f \times n_p$ matrix \mathbf{R} represents the probabilities of moving from non-absorbing nodes to absorbing ones; the $n_f \times n_f$ matrix \mathbf{Q} represents the probabilities of moving from one non-absorbing node to another; \mathbf{I} is the $n_p \times n_p$ identity matrix representing transitions between the absorbing nodes ($P_{ii} = 1$ and $P_{ij} = 0$); and $\mathbf{0}$ is the null matrix showing that there are no transitions from absorbing to non-absorbing nodes. For the solution of Laplace’s equation in (1), we obtain the elements of \mathbf{Q} from (4) as:

$$Q_{ij} = \begin{cases} \frac{1}{4}, & \text{if } i \text{ is directly connected to } j \\ 0, & \text{if } i = j \text{ or } i \text{ is not directly} \\ & \text{connected to } j \end{cases} \quad (13)$$

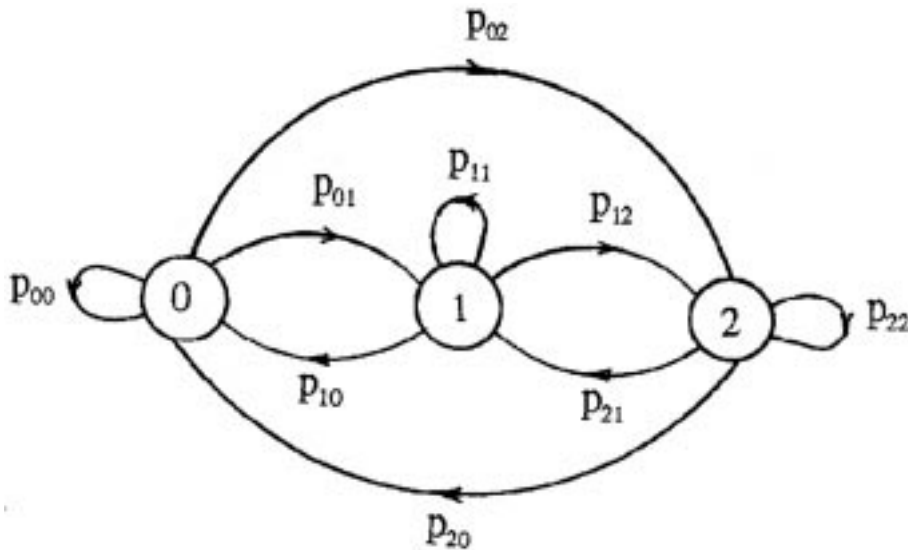


Fig. 2. State transition diagram for a three-state Markov chain.

The same applies to R_{ij} except that j is an absorbing node. For any absorbing Markov chain, $\mathbf{I} - \mathbf{Q}$ has an inverse. This is usually referred as the fundamental matrix

$$\mathbf{N} = (\mathbf{I} - \mathbf{Q})^{-1} \tag{14}$$

where N_{ij} is the average number of times the random walking particle starting from node i passes through node j before being absorbed. The absorption probability matrix \mathbf{B} is:

$$\mathbf{B} = \mathbf{NR} \tag{15}$$

where R_{ij} is the probability that a random-walking particle originating from a non-absorbing node i will end up at the absorbing node j . \mathbf{B} is an $n_f \times n_p$ matrix and is stochastic like the transition probability matrix, i.e.

$$\sum_{j=1}^{n_p} B_{ij} = 1, \quad i = 1, 2, \dots, n_f \tag{16}$$

If \mathbf{V}_f and \mathbf{V}_p contain potentials at the free and fixed nodes respectively, then

$$\mathbf{V}_f = \mathbf{BV}_p \tag{17}$$

In terms of the prescribed potentials V_1, V_2, \dots, V_{n_p} , used in equations (6) and (7), equation (17) becomes:

$$V_i = \sum_{j=1}^{n_p} B_{ij} V_j, \quad i = n_p + 1, \dots, n \tag{18}$$

where V_i is the potential at any free node i . Unlike equations (7), (17) or (18) provides the solution at all the free nodes at once.

An alternative way to obtain the solution in equation (17) is to exploit a property of the transition probability matrix \mathbf{P} . When \mathbf{P} is multiplied by itself repeatedly for a large number of times, we obtain [24, 25]:

$$\lim_{n \rightarrow \infty} \mathbf{P}^n = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{B} & \mathbf{0} \end{bmatrix} \tag{19}$$

Thus

$$\begin{bmatrix} \mathbf{V}_p \\ \mathbf{V}_f \end{bmatrix} = \mathbf{P}^n \begin{bmatrix} \mathbf{V}_p \\ \mathbf{V}_f \end{bmatrix} = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{B} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{V}_p \\ \mathbf{V}_f \end{bmatrix} \tag{20}$$

Either equation (17) or (20) can be used to find \mathbf{V}_f but it is evident that equation (17) will be more efficient and accurate. From equation (17) or (18), it should be noticed that if \mathbf{N} is calculated accurately, the solution is ‘exact’.

ILLUSTRATIVE EXAMPLES

Two simple examples will corroborate the claims above. Neither requires any computer programming.

Example 1

Consider an infinitely long conducting trough with square cross-section. A conducting lid is maintained at 100 V while the sides and bottom are grounded as shown in Fig. 3.

We wish to determine the potential at the center. Mathematically, the problem is posed as:

$$\nabla^2 V = 0 \tag{21}$$

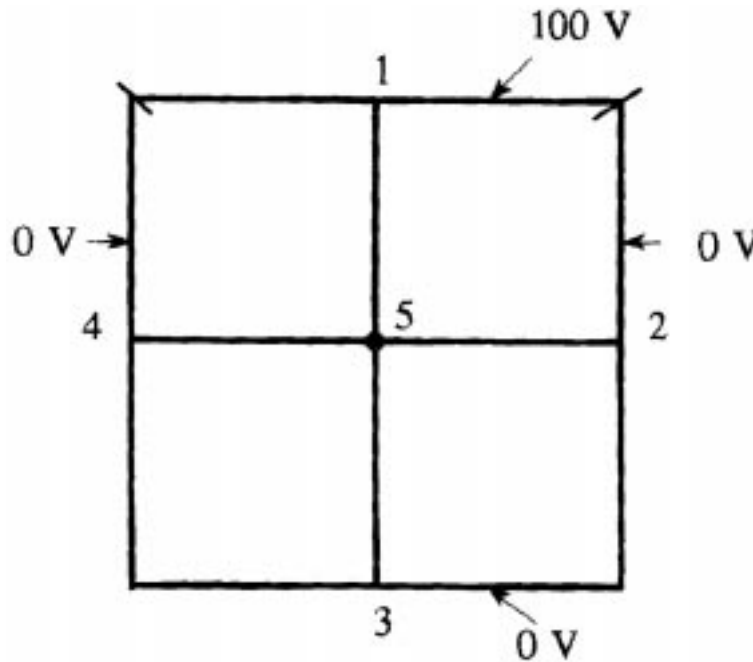


Fig. 3. For Example 1.

subject to:

$$V(0, y) = V(a, y) = V(x, 0), \quad V(x, a) = 100 \tag{22}$$

and we are to determine $V(a/2, a/2)$. Although one may assume that $a = 1$, that is not necessary.

The exact solution obtained by the separation of variables is [28]:

$$V(x, y) = \frac{400}{\pi} \sum_{k=1}^{\infty} \frac{\sin \frac{n\pi x}{a} \sinh \frac{n\pi y}{a}}{n \sinh n\pi}, \quad n = 2k - 1 \tag{23}$$

To apply Markov chain technique, we number the nodes as in Fig. 3. Node 5 is the only free node so that $n_f = 1, n_p = 4$. The transition probability matrix is given by:

$$\mathbf{P} = \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & 5 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{matrix} & \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & 0 \end{bmatrix} \end{matrix}$$

It is evident that:

$$\mathbf{Q} = \mathbf{0}, \mathbf{N} = (\mathbf{I} - \mathbf{Q})^{-1} = \mathbf{I}$$

and

$$\mathbf{R} = [\frac{1}{4} \quad \frac{1}{4} \quad \frac{1}{4} \quad \frac{1}{4}]$$

Thus:

$$\mathbf{B} = \mathbf{NR} = [\frac{1}{4} \quad \frac{1}{4} \quad \frac{1}{4} \quad \frac{1}{4}]$$

and

$$\mathbf{V}_f = \mathbf{BV}_p = [\frac{1}{4} \quad \frac{1}{4} \quad \frac{1}{4} \quad \frac{1}{4}] \begin{bmatrix} V_1 \\ V_2 \\ V_3 \\ V_4 \end{bmatrix}$$

or

$$V_5 = \frac{1}{4}(100 + 0 + 0 + 0) = 25.0$$

which agrees with the exact solution in equation (23). Although the method gives exact solution in this case, one cannot generalize from this simple example. If the regular fixed random walk method is used and we dispatch 1000 particles from point 5, we may get the numbers of particles absorbed of boundary points as $N_1 = 252, N_2 = 251, N_3 = 250, N_4 = 247$ so that:

$$V_5 = \frac{252}{1000} 100 + 0 = 25.2$$

which is less accurate than the solution from Markov chain and is subject to randomness.

Example 2

This is the same problem as in Example 1 except that we are now to calculate the potential at points $(a/3, a/3), (a/3, 2a/3), (2a/3, a/3),$ and $(2a/3, 2a/3)$.

In this case, there are four free nodes ($n_f = 4$) and eight fixed nodes ($n_p = 8$) as shown in Fig. 4. The transition probability matrix is obtained by inspection as:

$$\mathbf{P} = \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \end{matrix} & \begin{bmatrix} 1 & & & & & & & & & & & & \\ & 1 & & & & & & & & & & & \\ & & 1 & & & & & & & & & & \\ & & & 1 & & & & & & & & & \\ & & & & 1 & & & & & & & & \\ & & & & & 1 & & & & & & & \\ & & & & & & 1 & & & & & & \\ & & & & & & & 1 & & & & & \\ \frac{1}{4} & & & & & & & & \frac{1}{4} & 0 & \frac{1}{4} & \frac{1}{4} & 0 \\ 0 & \frac{1}{4} & \frac{1}{4} & & & & & & & \frac{1}{4} & 0 & 0 & \frac{1}{4} \\ 0 & 0 & 0 & & & \frac{1}{4} & \frac{1}{4} & 0 & \frac{1}{4} & & & & \frac{1}{4} \\ 0 & & & \frac{1}{4} & \frac{1}{4} & 0 & 0 & 0 & \frac{1}{4} & \frac{1}{4} & 0 & & \end{bmatrix} \end{matrix}$$

Other entries in \mathbf{P} shown vacant are zeros. From \mathbf{P} , we obtain:

$$\mathbf{R} = \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \end{matrix} \\ \begin{matrix} 9 \\ 10 \\ 11 \\ 12 \end{matrix} & \begin{bmatrix} \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{4} \\ 0 & \frac{1}{4} & \frac{1}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{4} & \frac{1}{4} & 0 \\ 0 & 0 & 0 & \frac{1}{4} & \frac{1}{4} & 0 & 0 & 0 \end{bmatrix} \end{matrix}$$

$$\mathbf{Q} = \begin{matrix} & \begin{matrix} 9 & 10 & 11 & 12 \end{matrix} \\ \begin{matrix} 9 \\ 10 \\ 11 \\ 12 \end{matrix} & \begin{bmatrix} 0 & \frac{1}{4} & \frac{1}{4} & 0 \\ \frac{1}{4} & 0 & 0 & \frac{1}{4} \\ \frac{1}{4} & 0 & 0 & \frac{1}{4} \\ 0 & \frac{1}{4} & \frac{1}{4} & 0 \end{bmatrix} \end{matrix}$$

The fundamental matrix \mathbf{N} is obtained as:

$$\mathbf{N} = (\mathbf{I} - \mathbf{Q})^{-1} = \begin{bmatrix} 1 & -\frac{1}{4} & -\frac{1}{4} & 0 \\ -\frac{1}{4} & 1 & 0 & -\frac{1}{4} \\ -\frac{1}{4} & 0 & 1 & -\frac{1}{4} \\ 0 & -\frac{1}{4} & -\frac{1}{4} & 1 \end{bmatrix}^{-1}$$

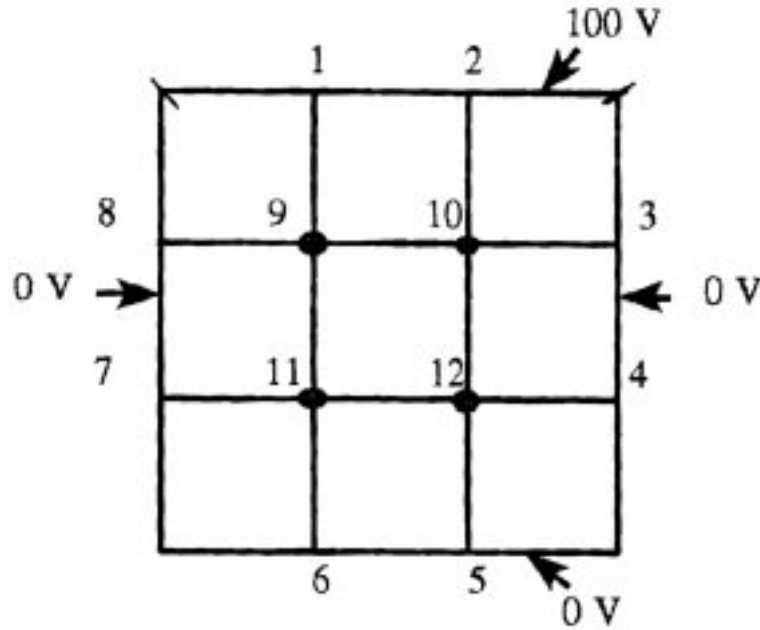


Fig. 4. For Example 2.

or

$$N = \frac{1}{6} \begin{bmatrix} 7 & 2 & 1 & 1 \\ 2 & 7 & 1 & 2 \\ 2 & 1 & 7 & 2 \\ 1 & 2 & 2 & 7 \end{bmatrix}$$

The absorption probability matrix **B** is obtained as:

$$B = NR = \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \end{matrix} \\ \begin{matrix} 9 \\ 12 \\ 10 \\ 11 \end{matrix} & \begin{bmatrix} \frac{7}{24} & \frac{1}{12} & \frac{1}{12} & \frac{1}{24} & \frac{1}{24} & \frac{1}{12} & \frac{1}{12} & \frac{7}{24} \\ \frac{1}{12} & \frac{7}{24} & \frac{7}{24} & \frac{1}{12} & \frac{1}{12} & \frac{1}{24} & \frac{1}{24} & \frac{1}{12} \\ \frac{1}{12} & \frac{1}{24} & \frac{1}{24} & \frac{1}{12} & \frac{1}{12} & \frac{7}{24} & \frac{7}{24} & \frac{1}{12} \\ \frac{1}{24} & \frac{1}{12} & \frac{1}{12} & \frac{7}{24} & \frac{7}{24} & \frac{1}{12} & \frac{1}{12} & \frac{1}{24} \end{bmatrix} \end{matrix}$$

Notice that equation (16) is satisfied. We now use equation (18) to obtain the potentials at the free nodes. For example:

$$V_9 = \frac{7}{24} V_1 + \frac{1}{12} V_2 + \frac{1}{12} V_3 + \frac{1}{24} V_4 + \frac{1}{24} V_5 + \frac{1}{12} V_6 + \frac{1}{12} V_7 + \frac{1}{24} V_8$$

Table 1

Node	Finite Difference Solution	Markov Chain Solution	Exact Solution
9	37.499	37.5	38.074
10	37.499	37.5	38.074
11	12.499	12.5	11.926
12	12.499	12.5	11.926

Since $V_1 = V_2 = 100$ while $V_3 = V_4 = \dots = V_8 = 0$,

$$V_9 = \left(\frac{7}{24} + \frac{1}{12}\right)100 = 37.5$$

By symmetry, $V_{10} = V_9 = 37.5$. Similarly,

$$V_{11} = V_{12} = \left(\frac{1}{24} + \frac{1}{12}\right)100 = 12.5$$

Table I compares these results with the finite difference solution (with 10 iterations) and the exact solution using equation (23). It is evident that the Markov chain solution compares well.

CONCLUSION

This paper has presented a means for using Monte Carlo method to solve Laplace's equation for the entire solution region at once as opposed to a single-point calculation. The approach uses Markov chains to calculate the transition probabilities. This approach is not subject to randomness because a random-number generator is not required. The approach also provides a pseudo-exact solution. The ideas presented in this paper can be extended to solution regions that are inhomogeneous or nonrectangular or both [29]. All it takes is calculating the transition probability **P**. The idea of Markov chain may also be used to solve Poisson's equation and wave equation. It is hoped that this paper will encourage the introduction of MCM in undergraduate courses.

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