

## MARKOV CHAIN MONTE CARLO SOLUTION OF POISSON'S EQUATION

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**Abstract :** - The classical Monte Carlo methods (fixed random walk, floating random walk, Exodus method) are useful in calculation potentials one point at a time. The Markov chain Monte Carlo method (MCMCM) overcomes this limitation by calculating the potential at all grid points simultaneously. This method has been used for whole field computation for problems involving Laplace's equation. This paper extends the application of MCMCM to problems involving Poisson's equations. The two illustrative examples are provided with hand calculation.

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### 1. INTRODUCTION

Monte Carlo methods (MCMs) have found many areas of applications in electromagnetics, especially potential theory [1-5]. The connection between potential theory and Brownian motion (or random walk) was first shown in 1944 by Kakutani [6]. An underlying concept of the probabilistic or Monte Carlo solution of differential equations is the random walk. Different types of random walk lead to different Monte Carlo methods. The most popular types are the fixed random walk, floating random walk, Exodus method, and Markov chain.

Our main interest in this paper is on Markov chain Monte Carlo method (MCMCM). This method has been used for whole field computation for problems involving Laplace's equations [7-9]. This paper extends the application of MCMCM to problems involving Poisson's equation. It provides a simple introduction on the apply MCMCM to Poisson's equation that undergraduate or graduates student can understand. Since the random walk provides a background for Markov chains, we will consider it first.

### 2. FIXED RANDOM WALK

Suppose the fixed random MCM is to be applied in solving Poisson's equation

$$\nabla^2 V = -g(x, y) = -\frac{\rho_s}{\epsilon} \quad \text{in region R} \quad (1)$$

subject to Dirichlet boundary condition

$$V = V_p \quad \text{on boundary B} \quad (2)$$

We begin by dividing the solution region R into a mesh and derive the finite difference equivalent of eq. (1). For  $V = V(x, y)$ , the problem is reduced to a two-dimensional one and (1) becomes

$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} = -g(x, y) \quad (3)$$

We first obtain the finite difference representation for a square grid as

$$-g = [V(x + \Delta, y) + V(x - \Delta, y) + V(x, y + \Delta) + V(x, y - \Delta) - 4V(x, y)] / \Delta^2$$

or

$$V(x, y) = p_{x+}V(x + \Delta, y) + p_{x-}V(x - \Delta, y) + p_{y+}V(x, y + \Delta) + p_{y-}V(x, y - \Delta) + \frac{\Delta^2 g}{4} \quad (4)$$

where the transient probabilities are given by

$$p_{x+} = p_{x-} = p_{y+} = p_{y-} = \frac{1}{4} \quad (5)$$

The term  $\Delta^2 g / 4$  in eq. (4) must be recorded at every step of the random walk. If  $m_i$  steps are required for the  $i$ th random walk originating at  $(x, y)$  to reach the boundary, then one records

$$V_p(i) + \frac{\Delta^2}{4} \sum_{j=1}^{m_i-1} g(x_j, y_j) \quad (6)$$

at the end of that walk. Thus the Monte Carlo estimate for  $V(x_o, y_o)$  after  $N$  walks is

$$V(x_o, y_o) = \frac{1}{N} \sum_{i=1}^N V_p(i) + \frac{\Delta^2}{4N} \sum_{i=1}^N \left[ \sum_{j=1}^{m_i-1} g(x_j, y_j) \right] \quad (7)$$

The inherent limitation of the fixed random Monte Carlo procedure is that it calculates the potential at one point at a time.

### 3. MARKOV CHAIN MONTE CARLO

Markov chains are named after Andrey Markov (1856-1922), the Russian mathematician who invented them. 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 [10-13]. 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

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

$\mathbf{P}$  is a stochastic matrix, meaning that the sum of the elements in each row is unity, i.e.

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

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.1 for a three-state Markov chain.

In our case, the Markov chain is the random walk and the states are the grid nodes. If we assume that there are  $n_f$  free (or nonabsorbing) nodes and  $n_p$  fixed (prescribed or absorbing) nodes, the size of the transition matrix  $\mathbf{P}$  is  $n$ , where

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

If the absorbing nodes are numbered first and the nonabsorbing states are numbered last, the  $n \times n$  transition matrix becomes

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

where the  $n_f \times n_p$  matrix  $R$  represents the probabilities of moving from nonabsorbing nodes to absorbing ones; the  $n_f \times n_f$  matrix  $Q$  represents the probabilities of moving from one nonabsorbing node to another;  $I$  is the identity matrix representing transitions between the absorbing nodes ( $P_{ii} = I$  and  $P_{ij} = 0$ ); and  $0$  is the null matrix showing that there are no transitions from absorbing to nonabsorbing nodes. For the solution of Poisson's equation in eq. (1), we obtain the elements of  $Q$  from eqs. (4) and (5). The same applies to  $R_{ij}$  except that  $j$  is an absorbing node.

For any absorbing Markov chain,  $I - Q$  has an inverse. This is usually referred as the fundamental matrix

$$N = (I - Q)^{-1} \tag{13}$$

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  $B$  is

$$B = N R \tag{14}$$

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  $j$ .  $B$  is an  $n_f \times n_p$  matrix and is stochastic like the transition probability matrix, i.e.

$$\sum_{j=1}^{n_p} B_{ij} = 1, \quad i = 1, 2, \dots, n_f \tag{15}$$

If  $V_f$  and  $V_p$  contain potentials at the free and fixed nodes respectively, then

$$V_f = B V_p + N G_f \tag{16}$$

where  $G_f$  is the evaluation of the term  $\frac{\Delta^2}{4} g(x, y)$ . Unlike the classical random walk technique, eq. (16) provides the solution at all the free nodes at once.

#### 4. ILLUSTRATIVE EXAMPLES

Two simple examples will be used to illustrate the solution to Poisson's equation in eq. (16). The examples are done with hand calculation so that no computer programming is needed.

*Example 1:*

Consider an infinitely long conducting trough with square cross-section with the sides grounded, as shown in Figure 2. Let  $\rho_s = x(y-1) \text{ nC/m}^2$  and  $\epsilon = \epsilon_o$ . Then,

$$g(x, y) = \frac{\rho_s}{\epsilon} = \frac{x(y-1) \times 10^{-9}}{10^{-9} / 36\pi} = 36\pi x(y-1) \tag{17}$$

In this case [9],

$$Q = 0, \quad N = (I - Q)^{-1} = I \tag{18}$$

Since  $V_p = \mathbf{0}$ , and there is only one free node (node 5) eq. (16) becomes

$$V_f = \mathbf{N}G_f \tag{19}$$

$$N=1, G_f = G_5 = \frac{\Delta^2}{4} g(x, y) \tag{20}$$

But  $\Delta = \frac{1}{2}, x = \frac{1}{2}, y = \frac{1}{2},$

$$G_5 = \frac{(1/2)^2}{4} 36\pi(1/2)(-1/2) = -\frac{9\pi}{16} = -1.7671$$

$$V_5 = G_f = -1.7671 \tag{21}$$

We can compare this with the finite difference solution. From eq. (4),

$$V_5 = \frac{1}{4}(0) + \frac{\Delta^2 g(x, y)}{4} = \frac{(1/2)^2}{4} 36\pi \left(\frac{1}{2}\right) \left(-\frac{1}{2}\right) = -\frac{9\pi}{16} = -1.7671 \tag{22}$$

The exact solution, based on series expansion [14], is -2.086. The error is due to the fact that the step size  $\Delta$  is large in this example.

*Example 2:*

This is the same problem as in Example 1 except that we now select  $\Delta = \frac{1}{3}$ . We have four free nodes as shown in Figure 3. The fundamental matrix is obtained as [9]

$$N = \frac{1}{6} \begin{bmatrix} 7 & 2 & 2 & 1 \\ 2 & 7 & 1 & 2 \\ 2 & 1 & 7 & 2 \\ 1 & 2 & 2 & 7 \end{bmatrix} \tag{23}$$

$$G_f = \frac{(1/3)^2}{4} \begin{bmatrix} g(x_9, y_9) \\ g(x_{10}, y_{10}) \\ g(x_{11}, y_{11}) \\ g(x_{12}, y_{12}) \end{bmatrix} = \frac{1}{36} (36\pi) \begin{bmatrix} \frac{1}{3} \left(-\frac{1}{3}\right) \\ \frac{2}{3} \left(-\frac{1}{3}\right) \\ \frac{1}{3} \left(-\frac{2}{3}\right) \\ \frac{2}{3} \left(-\frac{2}{3}\right) \end{bmatrix} = -\frac{\pi}{9} \begin{bmatrix} 1 \\ 2 \\ 2 \\ 4 \end{bmatrix} \tag{24}$$

Since  $V_p = \mathbf{0}$ ,

$$V_f = \mathbf{N}G_f = \frac{1}{6} \left(-\frac{\pi}{9}\right) \begin{bmatrix} 7 & 2 & 2 & 1 \\ 2 & 7 & 1 & 2 \\ 2 & 1 & 7 & 2 \\ 1 & 2 & 2 & 7 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 2 \\ 4 \end{bmatrix} = \begin{bmatrix} -1.1054 \\ -1.5126 \\ -1.5126 \\ -2.1526 \end{bmatrix} \tag{25}$$

We may compare this solution with the finite difference solution. Applying eq.(4) to node 9 in Figure 3, we obtain

$$V_9 = 0 + 0 + \frac{V_{10}}{4} + \frac{V_{11}}{4} + \frac{(1/3)^2}{4} 36\pi \left(\frac{1}{3}\right) \left(-\frac{1}{3}\right) \quad (26)$$

or

$$V_9 = 0.25V_{10} + 0.25V_{11} - \frac{\pi}{9} \quad (27)$$

Similarly, at node 10,

$$V_{10} = 0.25V_9 + 0.25V_{12} - \frac{2\pi}{9} \quad (28)$$

At node 11,

$$V_{11} = 0.25V_9 + 0.25V_{12} - \frac{2\pi}{9} \quad (29)$$

At node 12,

$$V_{12} = 0.25V_{10} + 0.25V_{11} - \frac{4\pi}{9} \quad (30)$$

Putting eqs. (27) to (30) in matrix form yields

$$\begin{bmatrix} -1 & 0.25 & 0.25 & 0 \\ 0.25 & -1 & 0 & 0.25 \\ 0.25 & 0 & -1 & 0.25 \\ 0 & 0.25 & 0.25 & -1 \end{bmatrix} \begin{bmatrix} V_9 \\ V_{10} \\ V_{11} \\ V_{12} \end{bmatrix} = \frac{\pi}{9} \begin{bmatrix} 1 \\ 2 \\ 2 \\ 4 \end{bmatrix} \quad (31)$$

Matrix A can easily be obtained by inspection using the band matrix method [15]. By inverting the matrix A, we obtain

$$\begin{bmatrix} V_9 \\ V_{10} \\ V_{11} \\ V_{12} \end{bmatrix} = \begin{bmatrix} -1.1054 \\ -1.5126 \\ -1.5126 \\ -2.1526 \end{bmatrix} \quad (32)$$

It is not surprising the finite difference solution is exactly the same as the Markov chain. It is easy to see that the inverse of matrix A in eq. (32) produces matrix N in eq. (23). The two solutions may be compared with the exact solution [14]:

$$\begin{bmatrix} V_9 \\ V_{10} \\ V_{11} \\ V_{12} \end{bmatrix} = \begin{bmatrix} -1.1924 \\ -1.6347 \\ -1.6347 \\ -2.373 \end{bmatrix} \quad (33)$$

The Markov chain solution agrees exactly with the finite difference solution. The two solutions differ slightly from the exact solution due to the large step size. By reducing the step size and using a computer, the Markov chain solution can be made accurate.

## 5. CONCLUSIONS

This paper has presented a brief introduction on how Markov chain Monte Carlo technique can be applied to solve Poisson's equation. The technique is illustrated with two simple examples. The Markov chain solutions compare well with the finite

difference solution and the exact solution. To increase the accuracy of Markov chain solution, we need to reduce the step size. This is best done by a computer programming.

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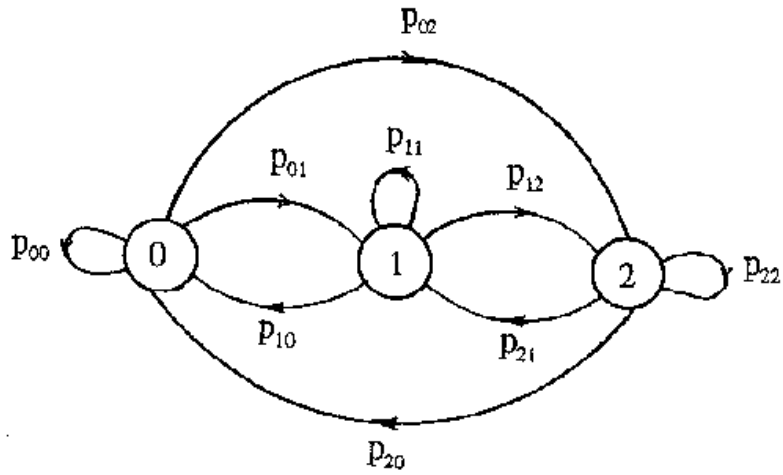


Fig. 1 State transition diagram for a three-state Markov Chain.

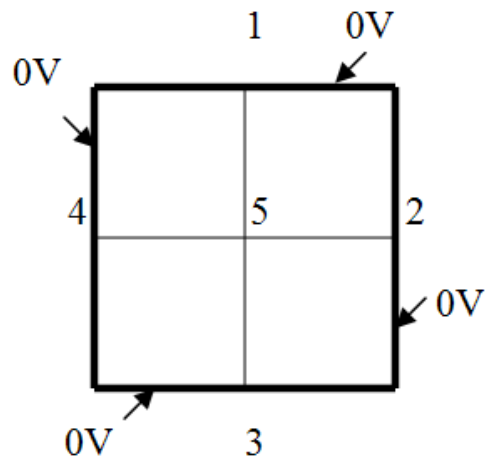


Fig. 2 For Example 1.

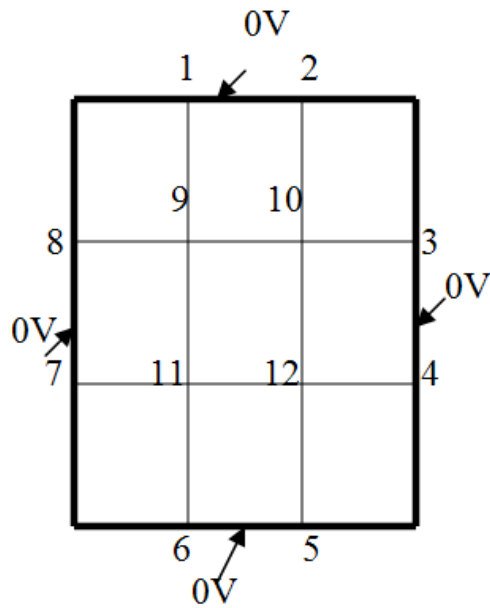


Fig. 3 For Example 2.