An Efficient Brownian Motion Simulation Method for the Conductivity of a Digitized Composite Medium

In Chan Kim*

School of Mechanical Engineering, Kunsan National University, Miryong-Dong 68, Kunsan Chonbuk 573-701, Korea

We use the first-passage-time formulation by Torquato, Kim and Cule [J. Appl. Phys., Vol. 85, pp. 1560~1571 (1999)], which makes use of the first-passage region in association with the diffusion tracer's Brownian movement, and develop a new efficient Brownian motion simulation method to compute the effective conductivity of digitized composite media. By using the new method, one can remarkably enhance the speed of the Brownian walkers sampling the medium and thus reduce the computation time. In the new method, we specifically choose the first-passage regions such that they coincide with two, four, or eight digitizing units according to the dimensionality of the composite medium and the local configurations around the Brownian walkers. We first obtain explicit solutions for the relevant first-passage-time equations in two- and three-dimensions. We then apply the new method to solve the illustrative benchmark problem of estimating the effective conductivities of the checkerboard-shaped composite media, for both periodic and random configurations. Simulation results show that the new method can reduce the computation time about by an order of magnitude.

Key Words : Digitized Mediam, Effective Conductivity, Brownian Motion Simulation, First-Passage-Time Method

1. Introduction

Development of the modern digital technique makes it advantageous and convenient to digitize most geometrical objects. Estimation of the effective conductivity of a composite material consisting of more than one phase is an application in which the digitization of the medium is found useful. Except for a few examples fabricated for special purposes, most natural and artificial composite materials have complex geometrical configurations. Clearly, it is easier to deal with the digitized image of a composite medium than its actual complex configuration. There exist a variety of techniques to obtain two- and three-dimensional digitized images of composite materials, including transmission electron microscopy,[1] scanning tunneling electron microscopy,[2] synchrotron based tomography[3] and confocal microscopy.[4] For a digitized image of a composite medium given by any of such techniques, a computation method is required to process this image and estimate the desired characteristic property. In an estimation of diffusive transport properties, such as thermal conductivities, diffusion coefficients, and magnetic permeabilities, a numerical method based on Brownian motion simulation has been successfully used for many different classes of composite media.[5] In this method, imaginary random (or Brownian) walkers are allowed to freely move inside the composite medium. At each step, their movements and speeds are influenced by the local phases and geometries. The effective conductivity σ_e of a d-dimensional composite medium is related to random walkers'

* **E-mail** : ickim@kunsan.ac.kr
TEL : +82-63-469-4720; **FAX** : +82-63-469-4726
School of Mechanical Engineering, Kunsan National University, Miryong-Dong 68, Kunsan Chonbuk 573-701, Korea. (Manuscript **Received** September 14, 2002; **Revised** January 17, 2003)

overall mean square displacement $\langle R^2(t)\rangle$ as follows :

$$\sigma_e = \frac{\langle R^2(t)\rangle}{2dt}\bigg|_{t\to\infty} \quad (1)$$

where t is the time and the angular bracket denotes the ensemble average.

Several different methods implementing random walkers have been developed for different applications in the computational physics. For the estimation of the effective conductivity of composite media, a method is preferred in which random walkers move around the medium as fast as possible since random walkers' movements consume major portion of the computational efforts in most computer simulations. It is well established that, among different random walk methods, the so-called first-passage-time technique is the most efficient in the estimation of the effective conductivity of composite media. Compared to the conventional random walk method that simulates the detailed zig-zag motions of walkers, the first-passage-time method has been proved to dramatically reduce the computation time.[6] Though the first-passage-time Brownian motion simulation method is generally applicable for any complex heterogeneous configuration, it can be specially tailored for a configuration consisting of geometrically identical elements such as square pixels and cubic voxels in digitized two- and three-dimensional media. Such a tailored method for digitized media was recently developed by Torquato et al.[7] They used "first-passage squares" ("first-passage cubes") to take advantage of the replicating geometry and thus speed up random walkers in a composite medium consisting of squares (cubes). It is noteworthy that the lattice walk method is inappropriate for the simulation of the conduction in a digitized medium although it may appear natural to use this method. In the lattice walk method, a random walker moves from the center of a square to one of four (eight) centers of adjacent squares (cubes). This way of moving walkers is simple, perhaps the simplest, and computationally easy. However, the lattice walk method cannot properly capture the conductive transport through corners and thus yields inexact conductivities when the conduction through corners becomes important.[8] As an illustrative benchmark problem, Torquato et al.[7] computed the effective conductivity of a checkerboard-type composite medium in which the black and white squares denote phases of different conductivities. Indeed, the checkerboard problem is a severe benchmark test when the contrast between conductivities of different phases becomes intense. When one phase, say black, is more conducting than the other phase, say white, the conductive transport through diagonally touching black squares becomes more important as the conductivity ratio becomes larger. However, in a lattice random walk method or in a conventional numerical analysis such as a finite differences method, this transport through corner could not be properly simulated.[7,8] To the author's knowledge, the first-passage-time method by Torquato et al.[7] is the only random walk method that can exactly capture the conductive transport through corners.

In this paper, we present a new first-passage-time method that improves over Torquato's algorithm. The new method incorporates the concept of imaginary "first-passage-bisquare" (first-passage-bicubes) instead of Torquato's "first-passage-square" (first-passage-cubes). Compared to Torquato's method, it reduces the computation time about by an order of magnitude while exactly capturing the conductive transport through corners. As an illustrative example, we use the new method to calculate again the effective conductivities of the checkerboard-type composite media, for both periodic and random checkerboards. We compare the calculation results with ones obtained by using Torquato's first-passage-square method.

The remainder of this article is organized as follows. In Sec. 2, we present the theoretical background for a general first-passage-time simulation. In Sec. 3, we specialize first-passage-time equations for two- and three-dimensional digitized media and solve for relevant statistical quantities using first-passage-bisquares (or first-passage-bicubes). In Sec. 4, we describe the details of the first-passage-time simulation technique. In Sec. 5, we apply the algorithm to obtain the effective conductivities of the checkerboard-type composite media. Summary is given in Sec. 6.

2. First-Passage Time Method

We summarize the general first-passage time algorithm formulated by Torquato et al.[7] They introduced the canonical probability function $P(\mathbf{r}, \mathbf{r}_B, t)$ as a fundamental construct and expressed relevant statistical quantities in terms of this canonical function. We present the formulation for the first-passage movement of a Brownian (or random) walker in homogeneous and heterogeneous regions separately.

2.1 Random walk in a homogeneous situation

Consider a random walker diffusing in a d-dimensional homogeneous medium of conductivity σ. Let us draw a first-passage region Ω around the walker and denote its bounding surface by $\partial\Omega$. Let $\mathbf{r}$ be a position inside Ω and $\mathbf{r}_B$ be a specific point on $\partial\Omega$. The canonical function $P(\mathbf{r}, \mathbf{r}_B, t)$ is defined as the probability associated with the walker hitting the surface $\partial\Omega$ in the vicinity of $\mathbf{r}_B$ for the first time at time t when the walker starts at $\mathbf{r}$. This canonical probability function is given by the solution of the transient diffusion equation

$$\begin{aligned}&\sigma\nabla^2 P(\mathbf{r}, \mathbf{r}_B, t)\\ &=\frac{\partial}{\partial t}P(\mathbf{r}, \mathbf{r}_B, t),\ \mathbf{r} \text{ in } \Omega,\ t>0\end{aligned} \tag{2}$$

subject to the following initial and boundary conditions:

$$P(\mathbf{r}, \mathbf{r}_B, t=0)=0,\ \mathbf{r} \text{ in } \Omega \tag{3}$$

$$P(\mathbf{r}, \mathbf{r}_B, t)=\delta(\mathbf{r}-\mathbf{r}_B),\ \mathbf{r} \text{ on } \partial\Omega,\ t>0 \tag{4}$$

Most relevant first-passage-time quantities are expressed in terms of $P(\mathbf{r}, \mathbf{r}_B, t)$. Following is the formulation for the quantities needed for the computer simulation.

First, we need to find the mean hitting time $\tau(\mathbf{r})$, that is defined as the average time taken by the random walker to hit the surface $\partial\Omega$ for the first time when it starts from $\mathbf{r}$. This quantity is given by

$$\tau(\mathbf{r})=\int_{\partial\Omega}\int_0^\infty t\,\frac{\partial P(\mathbf{r}, \mathbf{r}_B, t)}{\partial t}\,dt d\mathbf{r}_B \tag{5}$$

The mean hitting time τ can be alternatively obtained by the solution of the steady-state diffusion equation

$$\sigma\nabla^2\tau(\mathbf{r})=-1,\ \mathbf{r} \text{ in } \Omega \tag{6}$$

subject to the absorbing boundary condition

$$\tau(\mathbf{r})=0,\ \mathbf{r} \text{ on } \partial\Omega \tag{7}$$

Next, we need the probability density function $w(\mathbf{r}, \mathbf{r}_B)$ that is defined as the probability associated with hitting the vicinity of a particular position $\mathbf{r}_B$ on the surface $\partial\Omega$ for the first time when the walker starts at $\mathbf{r}$. This quantity is obtained by integrating the time derivative of the canonical probability density function, $\partial P(\mathbf{r}, \mathbf{r}_B, t)/\partial t$, over all times, i.e.,

$$\begin{aligned}w(\mathbf{r}, \mathbf{r}_B)&=\int_0^\infty\frac{\partial P}{\partial t}\,dt\\ &=P(\mathbf{r}, \mathbf{r}_B, t=\infty)\end{aligned} \tag{8}$$

This expression in conjunction with Eqs. (2)-(4) gives the Laplace equation

$$\nabla^2 w(\mathbf{r}, \mathbf{r}_B)=0,\ \mathbf{r} \text{ in } \Omega \tag{9}$$

of which the boundary condition is given by

$$w(\mathbf{r}, \mathbf{r}_B)=\delta(\mathbf{r}-\mathbf{r}_B),\ \mathbf{r} \text{ on } \partial\Omega \tag{10}$$

Finally, another important quantity is the jumping probability $p(\mathbf{r})$ which gives the probability that a random walker starting at $\mathbf{r}$ lands on a certain portion of the first-passage surface $\partial\Omega_0$ for the first time. This is obtained by integrating the probability density function $w(\mathbf{r}, \mathbf{r}_B)$ over boundary points on $\partial\Omega_0$, i.e.,

$$p(\mathbf{r})=\int_{\partial\Omega_0} w(\mathbf{r}, \mathbf{r}_B)\,d\mathbf{r}_B \tag{11}$$

Using this expression and relations (9), (10), one can easily derive the boundary value problem for the jumping probability distribution $p(\mathbf{r})$:

$$\nabla^2 p(\mathbf{r})=0,\ \mathbf{r} \text{ in } \Omega \tag{12}$$

of which the boundary condition is given by

$$p(\mathbf{r})=\begin{cases}1, & \mathbf{r} \text{ on } \partial\Omega_0\\ 0, & \mathbf{r} \text{ not on } \partial\Omega_0\end{cases} \tag{13}$$

2.2 Random walk in a heterogeneous situation

Consider a d-dimensional two-phase medium of which the phase conductivities are σ_1 and σ_2. Let a random walker diffuse in the vicinity of the two-phase interface. Let us draw a first-passage region Ω around the walker with its bounding surface $\partial\Omega$. Let Ω_i denote the portion of Ω containing phase $i(=1, 2)$ and $\partial\Omega_i$ denote the corresponding surface of Ω_i. Interface surface is denoted by Γ.

The mean hitting time, $\tau(\mathbf{r})$, satisfies the steady-state diffusion equation,

$$\sigma_i\nabla^2\tau(\mathbf{r}) = -1, \ \mathbf{r} \text{ in } \Omega_i \tag{14}$$

subject to the absorbing boundary condition

$$\tau(\mathbf{r}) = 0, \ \mathbf{r} \text{ on } \partial\Omega \tag{15}$$

and the interface conditions

$$\tau|_1 = \tau|_2, \ \mathbf{r} \text{ on } \Gamma \tag{16}$$

$$\left.\frac{\partial\tau}{\partial n_1}\right|_1 = \frac{\sigma_2}{\sigma_1}\left.\frac{\partial\tau}{\partial n_1}\right|_2, \ \mathbf{r} \text{ on } \gamma \tag{17}$$

where n_i is the unit outward normal from region Ω_i and $|_i$ means that the approach to Γ from the region Ω_i.

The probability density function $w(\mathbf{r}, \mathbf{r}_B)$ satisfies the Laplace equation

$$\nabla^2 w(\mathbf{r}, \mathbf{r}_B) = 0, \ \mathbf{r} \text{ in } \Omega \tag{18}$$

subject to the boundary condition

$$w(\mathbf{r}, \mathbf{r}_B) = \delta(\mathbf{r}-\mathbf{r}_B), \ \mathbf{r} \text{ on } \partial\Omega \tag{19}$$

and the interface conditions

$$w|_1 = w|_2, \ \mathbf{r} \text{ on } \Gamma \tag{20}$$

$$\left.\frac{\partial w}{\partial n_1}\right|_1 = \frac{\sigma_2}{\sigma_1}\left.\frac{\partial w}{\partial n_1}\right|_2, \ \mathbf{r} \text{ on } \Gamma \tag{21}$$

Finally, let us define the probability $p_1(\mathbf{r})$ [$p_2(\mathbf{r})$] to be the probability that the random walker, initially at $\mathbf{r}$, hits the first-passage surface $\partial\Omega_1$ [$\partial\Omega_2$] for the first time. The probability p_1 is then obtained by integrating the above probability density function $w(\mathbf{r}, \mathbf{r}_B)$ over the boundary points on partial $\partial\Omega_1$, i.e.,

$$p_1(\mathbf{r}) = \int_{\partial\Omega_1} w(\mathbf{r}, \mathbf{r}_B)\, d\mathbf{r}_B \tag{22}$$

Using this expression and the relations Eq. (18)-(21), one can easily derive the boundary value problem for the jumping probability $p_1(\mathbf{r})$:

$$\nabla^2 p_1(\mathbf{r}) = 0, \ \mathbf{r} \text{ in } \Omega \tag{23}$$

subject to the boundary condition

$$p_1(\mathbf{r}) = \begin{cases} 1, \ \mathbf{r} \text{ on } \partial\Omega_1 \\ 0, \ \mathbf{r} \text{ on } \partial\Omega_2 \end{cases} \tag{24}$$

and the interface conditions

$$p_1|_1 = p_1|_2, \ \mathbf{r} \text{ on } \Gamma \tag{25}$$

$$\left.\frac{\partial p_1}{\partial n_1}\right|_1 = \frac{\sigma_2}{\sigma_1}\left.\frac{\partial p_1}{\partial n_1}\right|_2, \ \mathbf{r} \text{ on } \Gamma \tag{26}$$

Once $p_1(\mathbf{r})$ is known, the jumping probability $p_2(\mathbf{r})$ for a point on the surface containing phase 2, $\partial\Omega_2$, is simply given by the trivial relation

$$p_2(\mathbf{r}) = 1 - p_1(\mathbf{r}) \tag{27}$$

3. First-Passage Time Equations for Digitized Media

In this section, we solve the first-passage-time equations formulated in Sec. 2, to obtain the first-passage-time quantities, τ, w and p, for homogeneous and heterogeneous digitized media. In two- and three-dimensional applications, the medium is consisted of square pixels and cubic voxels, respectively. We consider the two- and three-dimensional problems separately. We solve for the first-passage region that is consisted of two adjacent squares (cubes). Choice of this first-passage region is one distinctive feature of the new simulation method, in contrast to the method by Torquato et al.[7] The other distinction is that, at each step, a random walker is positioned at a pixel (voxel) boundary, rather than an arbitrary location inside the first-passage region. We also present the solutions for the first-passage region consisted of four squares (eight cubes).

3.1 Two-dimensional digitized media

3.1.1 Random walk in a homogeneous situation

Let us consider the first-passage region that is consisted of two horizontally adjacent squares. For a first-passage region consisting of two vertically adjacent squares, the following results can

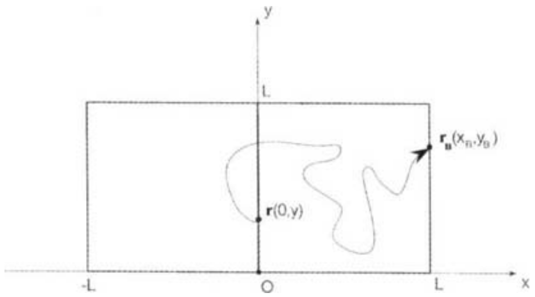


Fig. 1 First-passage-region consisted of two neighboring unit squares of area L^2. A Brownian walker diffuses from $\mathbf{r}$ at the centerline to some point $\mathbf{r}_B$ on the boundary

be used by simply interchanging x and y coordinates. Each square has an area of L^2 and the unit conductivity $(\sigma=1)$. The origin is taken to be the bottom location in the centerline, as depicted in Fig. 1. Let a random walker start to diffuse from an arbitrary location $\mathbf{r}=(x, y)$ in the first-passage region, or the "first-passage bisquare." Eventually, it lands at some point $\mathbf{r}_B=(x_B, y_B)$ in the outer boundary of this first-passage bisquare for the first time. The mean hitting time $\tau(\mathbf{r})$ taken for the displacement is easily found by solving the diffusion problem Equation (6) and (7). That is,

$$\begin{aligned}\tau(\mathbf{r})=\tau(x, y)=\frac{L^2}{4}\Bigg\{\frac{1}{2}-2\left(\frac{y}{L}\right)^2 \\ +\frac{16}{\pi^3}\sum_{n=0}^{\infty}\frac{(-1)^{n-1}}{(2n+1)^3}\frac{\cosh[(2n+1)\pi x/L]}{\cosh[(2n+1)\pi]}\cos[(2n+1)\pi y/L]\Bigg\}\end{aligned} \tag{28}$$

For the implementation of the computer simulation, we need τ only for the centerline at $\mathbf{r}=(0, y)$. If we define, for a homogeneous first-passage bisquare,

$$\tau_H(y)=\tau(0, y) \tag{29}$$

then $\tau_H(y)$ is obtained as

$$\begin{aligned}\tau_H(y)=\frac{L^2}{4}\Bigg\{\frac{1}{2}-2\left(\frac{y}{L}\right)^2 \\ +\frac{16}{\pi^3}\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{(2n+1)^3}\frac{1}{\cosh[(2n+1)\pi]}\cos[(2n+1)\pi y/L]\Bigg\}\end{aligned} \tag{30}$$

Figure 2 shows the graph of $\tau_H(y)$ as a function of y.

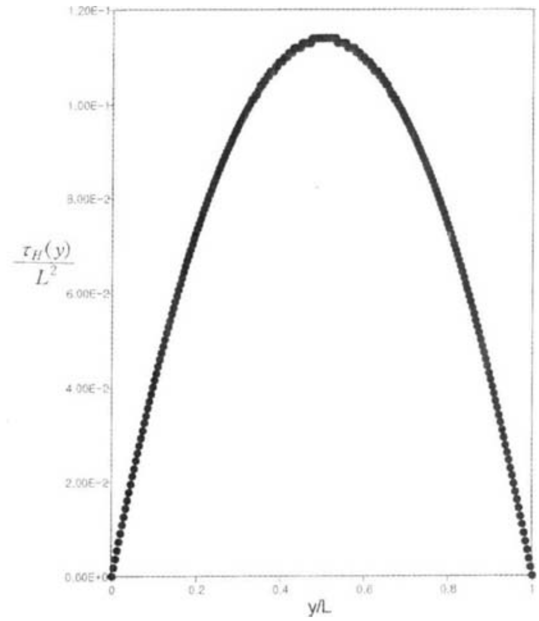


Fig. 2 Mean hitting time $\tau_H(y)$ for a Brownian walker starting from $\mathbf{r}=(0, y)$ to arrive at some point on the first-pasage-bisquare of area $2L^2$

The probability density function $w(\mathbf{r}, \mathbf{r}_B)$ is obtained by solving Eqs. (9) and (10). Let us define, for a homogeneous first-passage bisquare,

$$w_H(y, x_B, y_B)=w(0, y, x_B, y_B) \tag{31}$$

and define further, for brevity,

$$w_{H1}(y, x_B)=w_H(y, x_B, 0)=w(0, y, x_B, 0) \tag{32}$$

$$w_{H2}(y, y_B)=w_H(y, \pm L, y_B)=w(0, y, \pm L, y_B) \tag{33}$$

$$w_{H3}(y, x_B)=w_H(y, x_B, L)=w(0, y, x_B, L) \tag{34}$$

Note that w_{H1}, w_{H2}, and w_{H3} denote the probability densities for the cases that a random walker reaches at the bottom, the side, and top boundaries, respectively, of the first-passage bisquare as in Fig. 1. The probability densities, w_{H1}, w_{H2}, w_{H3}, are obtained as, for a position (x_B, y_B) at the boundary $\partial\Omega$,

$$w_{H1}(y, x_B)=\frac{1}{L}\sum_{n=1}^{\infty}\sin\left(\frac{n\pi}{2}\right)\sin\left[\frac{n\pi}{2}\left(1+\frac{x_B}{L}\right)\right]\frac{\sinh[n\pi/2(1-y/L)]}{\sinh(n\pi/2)} \tag{35}$$

$$w_{H2}(y, y_B)=\frac{2}{L}\sum_{n=1}^{\infty}\frac{\sinh(n\pi)\sin(n\pi y/L)\sin(n\pi y_B/L)}{\sinh(2n\pi)} \tag{36}$$

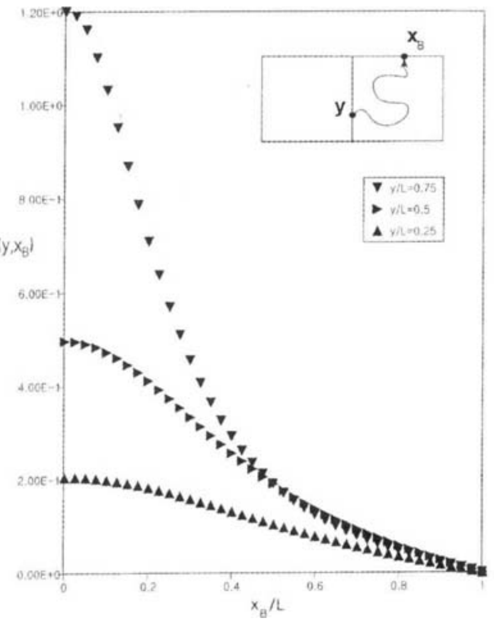


Fig. 3 Probability density w_{H1} for a Brownian walker starting from $\mathbf{r}=(0, y)$ to first hit $\mathbf{r}_B=(x_B, L)$, for $y/L=0.25$, 0.5 and 0.75

$$w_{H3}(y, x_B)=\frac{1}{L}\sum_{n=1}^{\infty}\sin\left(\frac{n\pi}{2}\right)\sin\left[\frac{n\pi}{2}\left(1+\frac{x_B}{L}\right)\right]\frac{\sinh(n\pi y/2L)}{\sinh(n\pi/2)} \tag{37}$$

respectively. The graphs of w_{H1}, w_{H2}, w_{H3} for a few values of y are drawn in Figs. 3-5.

We also need the probability p that a random walker land for the first time at a boundary section $\partial\Omega_0$. This probability is given by the solution of the Laplace problem (12), (13) but it can be alternatively obtained by integrating Eqs. (35)-(37) over $\partial\Omega_0$. For example, if $\partial\Omega_0$ is taken to be the right half boundary $(x_B\geq 0)$, then p is found to be

$$p=\int_0^L w_{H1}(y, x_B)\,dx_B+\int_0^L w_{H2}(y, y_B)\,dy_B + \int_0^L w_{H3}(y, x_B)\,dx_B=\frac{1}{2} \tag{38}$$

which understates that the random walker starts at the centerline of the symmetric bisquare.

During its diffusion, a random walker could happen to land exactly at or very close to a corner of a square pixel. A first-passage bisquare movement is inappropriate for a random walker in such circumstance, since the walker cannot move further. (The walker continues to stay at a corner

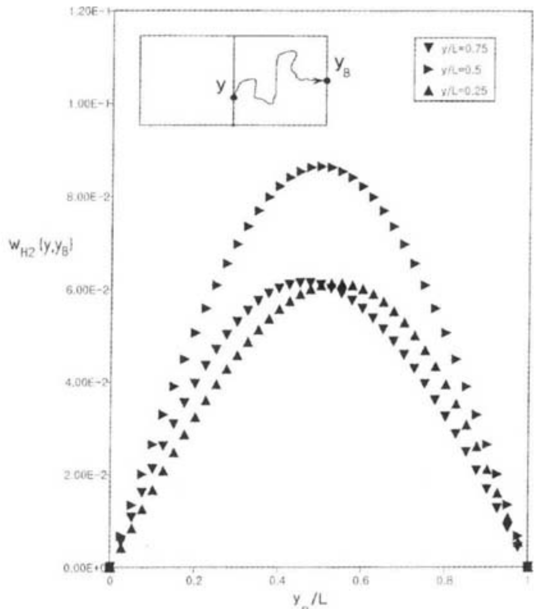


Fig. 4 Probability density w_{H2} for a Brownian walker starting from $\mathbf{r}=(0, y)$ to first hit $\mathbf{r}_B=(L, y_B)$, for $y/L=0.25$, 0.5 and 0.75

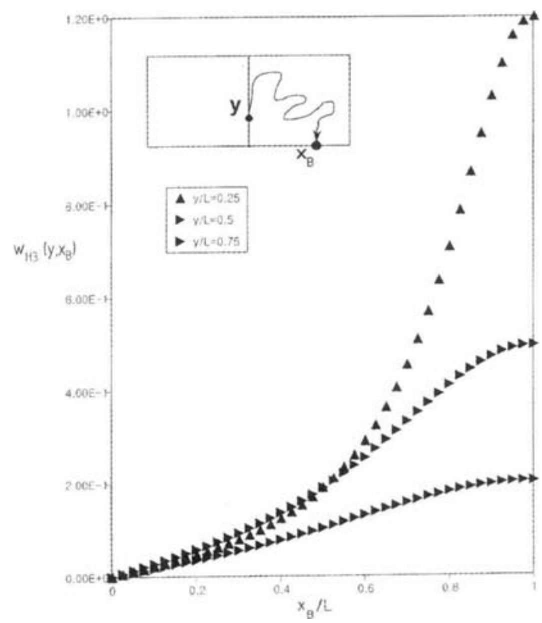


Fig. 5 Probability density w_{H3} for a Brownian walker starting from $\mathbf{r}=(0, y)$ to first hit $\mathbf{r}_B=(x_B, 0)$, for $y/L=0.25$, 0.5 and 0.75

spending no time.) In order to let such a random

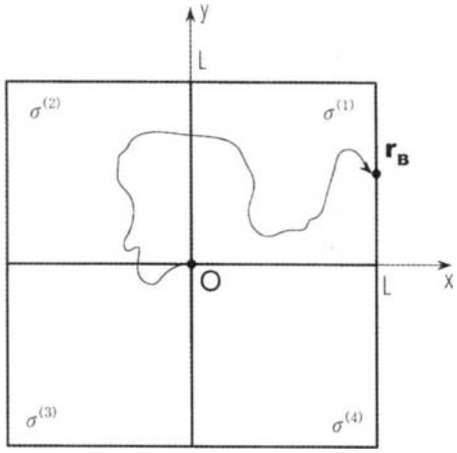


Fig. 6 First-passage-square of area $4L^2$. A Brownian walker diffuses from the center to some point $\mathbf{r}_B$ on the boundary

walker move further, we construct a first-passage region consisting of four squares encompassing the walker at the corner, instead of two squares. Consider a random walker exactly at or very close to the origin that is taken at the center of four squares, as shown in Fig. 6. Each of four squares has an area of L^2 and the unit conductivity. A random walker diffusing from the center will eventually arrive at an outer boundary of a region of four squares. The mean hitting time τ and the probability density function w in association with this displacement are again obtained as solutions of Eqs. (6) and (7) and Eqs. (9) and (10), respectively. Let us define, for a homogeneous first-passage square having the unit conductivity,

$$\tau_H = \tau(0, 0) \tag{39}$$

and

$$w_H(x_B, y_B) = w(0, 0, x_B, y_B) \tag{40}$$

The mean hitting time τ_H is obtained, for the homogenous first-passage square in Fig. 6, as

$$\tau_H \simeq 0.295L^2 \tag{41}$$

For a random walker arriving at $\mathbf{r}_B = (\pm L, y_B)$ in the left or right boundary side, w_H is obtained as

$$w_H(\pm L, y_B) = \frac{1}{2L}\sum_{n=1}^{\infty}\frac{\sin(n\pi/2)\sin[n\pi/2(y_B/L\pm 1)]}{\cosh(n\pi/2)} \tag{42}$$

For a random walker arriving at $\mathbf{r}_B = (x_B, \pm L)$ in the top or bottom boundary, w_H is obtained as

$$w_H(x_B, \pm L) = \frac{1}{2L}\sum_{n=1}^{\infty}\frac{\sin(n\pi/2)\sin[n\pi/2(x_B/L\pm 1)]}{\cosh(n\pi/2)} \tag{43}$$

The probability p that the random walker land for the first time at a boundary section $\partial\Omega_0$ can be obtained by integrating Eq. (42) or (43) over $\partial\Omega_0$. For example, the probability to land at any point along the side $x=L$, is given by

$$p = \int_{-L}^{L} w_H(L, y_B)\, dy_B = \frac{1}{4} \tag{44}$$

This result confirms that the random walker lands at each side with equal probability of 1/4.

3.1.2 Random walk in a heterogeneous situation

Consider the first-passage region consisted of two horizontally adjacent squares of different conductivities. For a first-passage region consisting of two vertically adjacent squares, the following results can be used by simply interchanging x and y coordinates. Each square has an area of L^2. The origin is again taken to be the bottom location in the centerline, as in Fig. 1. Let σ_1 and σ_2 be the conductivities of squares on the right ($x \geq 0$) and left ($x \leq 0$) sides, respectively. A random walker starts to diffuse from an arbitrary position $\mathbf{r} = (0, y)$ in the centerline and arrives at some point $\mathbf{r}_B = (x_B, y_B)$ in the outer boundary of the first-passage region for the first time. The mean hitting time $\tau(\mathbf{r})$ taken for this displacement is given by the solution of the boundary value problem Eq. (14)-(17). One can easily solve this problem and find that

$$\tau = \frac{2}{\sigma_1 + \sigma_2}\tau_H \tag{45}$$

where τ_H denotes the homogeneous solution given by Eq. (30) for a unit conductivity.

The probability density function $w(0, y, x_B, y_B)$ in association with the walker's displacement is given by the solution of the boundary value problem (18)-(21). This problem can be easily solved and its solution is obtained as

$$w(0,\, y,\, x_B,\, y_B) = \begin{cases} \dfrac{2\sigma_1}{\sigma_1+\sigma_2} w_H(y,\, x_B,\, y_B),\ x_B \geq 0 \\ \dfrac{2\sigma_2}{\sigma_1+\sigma_2} w_H(y,\, x_B,\, y_B),\ x_B < 0 \end{cases} \tag{46}$$

where w_H is defined in Eq. (31) and its explicit expression is given as w_{H1}, w_{H2}, or w_{H3} in Eqs. (35)-(37), depending on the position of $\mathbf{r}_B$. Note that w_H is obtained as w_{H1} for $\mathbf{r}_B=(x_B,\, 0)$, w_{H2} for $\mathbf{r}_B=(\pm L,\, y_B)$, or w_{H3} for $\mathbf{r}_B=(x_B,\, L)$.

The probability p_1 that a random walker land for the first time at any point along the right half boundary $\partial\Omega_1$ can be obtained by integrating Eq. (46) with the Eqs. (35)-(37) over $\partial\Omega_1$, i.e.,

$$\begin{aligned} p_1 &= \int_0^L w(0,\, y,\, x_B,\, 0)\, dx_B + \int_0^L w(0,\, y,\, L,\, y_B)\, dy_B + \int_0^L w(0,\, y,\, x_B,\, L)\, dx_B \\ &= \int_0^L w_{H1}(y,\, x_B)\, dx_B + \int_0^L w_{H2}(y,\, y_B)\, dy_B + \int_0^L w_{H3}(y,\, x_B)\, dx_B = \frac{\sigma_1}{\sigma_1+\sigma_2} \end{aligned} \tag{47}$$

It immediately follows that the probability p_2 for a random walker to first hit $\partial\Omega_2$ is obtained as

$$p_2 = 1 - p_1 = \frac{\sigma_2}{\sigma_1+\sigma_2} \tag{48}$$

This result implies that the probability p_i landing at $\partial\Omega_i$ is proportional to the local conductivity σ_i of the corresponding square.

If a random walker is exactly at or very close to a corner of a square in the course of diffusion, the walker carries out its first-passage displacement by use of a first-passage square (or four squares) instead of a first-passage bisquare. One constructs a first-passage region such that it includes four squares around the random walker, as shown in Fig. 6. Let $\sigma^{(i)}(i=1,\, 2,\, 3,\, 4)$ be the conductivity of the square at the i-th quadrant. The random walker starts from the center of the four-square region and eventually lands at the outer boundary of this first-passage region for the first time. The mean hitting time τ for this first-passage displacement is again given by the solution of the boundary value problem, Eqs. (14)-(17) and the solution is found to be

$$\tau = \frac{1}{\bar{\sigma}}\tau_H \simeq \frac{0.295 L^2}{\bar{\sigma}} \tag{49}$$

where

$$\bar{\sigma} = \frac{1}{4}\sum_{i=1}^{4}\sigma^{(i)} \tag{50}$$

and τ_H is the mean hitting time for the random walker associated with the homogeneous first-passage region of the unit conductivity, as given in Eq. (41). The jumping probability density function $w(\mathbf{r},\, \mathbf{r}_B)$ associated with this first-passage displacement is given by the solution of the boundary value problem Eqs. (18)-(21). Let $\partial\Omega^{(i)}$ denote the section of the boundary $\partial\Omega$ belonging in i-th quadrant. For a random walker arriving at the boundary $\partial\Omega^{(i)}$, the probability density is obtained as

$$w(\mathbf{r},\, \mathbf{r}_B) = \frac{\sigma^{(i)}}{\bar{\sigma}} w_H(\mathbf{r}_B),\ \mathbf{r}_B \text{ on } \partial\Omega^{(i)} \tag{51}$$

where w_H is the probability density associated with the homogeneous first-passage region, as given in Eqs. (42) and (43). The probability p that the random walker land for the first time at any point along the specific boundary side is obtained by integrating Eq. (50) with the Eqs. (42), (43). For example, the probability to land at any point along the side $x=L$, is given by

$$p = \int_{-L}^{L} w(0,\, 0,\, L,\, y_B)\, dy_B = \frac{\sigma^{(1)}+\sigma^{(4)}}{8\bar{\sigma}} \tag{52}$$

which confirms again that p is proportional to the local conductivity $\sigma^{(i)}$.

3.2 Three-dimensional digitized media

3.2.1 Random walk in a homogeneous situation

Consider the first passage region that is consisted of two neighboring cubes in z-direction. The first passage region consisting of two neighboring cubes in x-or y-directions can be treated similarly. Each cube has a volume of L^3. Let assume the cube has the unit conductivity, $\sigma=1$. The origin is taken to be the corner location in the center-cutting plane between two cubes such that the center-cutting plane coincide with the plane in which $z=0$, as depicted in Fig. 7. Let the random walker start to diffuse from the location $\mathbf{r}=(x,\, y,\, 0)$. Using the separation of variables technique, one can easily solve the boundary

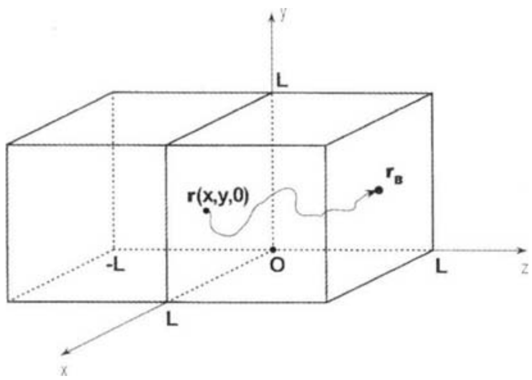


Fig. 7 First-passage-region consisted of two neighboring unit cubes of volume L^3. A Brownian walker diffuses from $\mathbf{r}$ at the center-cutting plane to some point $\mathbf{r}_B$ on the boundary

value problem, Eqs. (6), (7) to obtain the mean hitting time $\tau(\mathbf{r})$. The mean hitting time τ for a random walk starting from a point $\tau=(x, y, 0)$ on the center-cutting plane is obtained as

$$\tau(x, y, 0)=\frac{L^2}{6}\left\{T_1(x, y, 0)+T_2(x, y, 0)+T_3(x, y, 0) -\frac{3}{2}\left[\left(\frac{x}{L}+\frac{1}{2}\right)^2+\left(\frac{y}{L}+\frac{1}{2}\right)^2\right]+\frac{3}{4}\right\} \tag{53}$$

where

$$T_1(x, y, 0)=\frac{3}{2\pi^4}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{(-1)^{m+n+1}}{(m+1/2)^3(m+1/2)}\frac{\cosh[k_1(2x/L+1)]}{\cosh(k_1)} \times\cos\left[\left(m+\frac{1}{2}\right)\pi\left(\frac{2y}{L}+1\right)\right] \tag{54}$$

$$T_2(x, y, 0)=\frac{3}{2\pi^4}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{(-1)^{m+n+1}}{(m+1/2)^3(n+1/2)}\frac{\cosh[k_1(2y/L+1)]}{\cosh(k_1)} \times\cos\left[\left(m+\frac{1}{2}\right)\pi\left(\frac{2x}{L}+1\right)\right] \tag{55}$$

$$T_3(x, y, 0) =\frac{3}{2\pi^2}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}(-1)^{m+n+1}\left[\frac{2}{(m+1/2)(n+1/2)}-\frac{1}{(m+1/2)(n+1/2)^3\pi^2}\right] \times\cos\left[\left(m+\frac{1}{2}\right)\pi\left(\frac{2x}{L}+1\right)\right]\cos\left[\left(n+\frac{1}{2}\right)\pi\left(\frac{2y}{L}+1\right)\right]\frac{1}{\cosh(2k_1)} \tag{56}$$

$$k_1=\left[\left(m+\frac{1}{2}\right)^2+\left(n+\frac{1}{2}\right)^2\right]^{1/2}\pi \tag{57}$$

The jumping probability density function $w(\mathbf{r}, \mathbf{r}_B)$ is obtained by solving Eqs. (9) and (10). Let us define, for a homogeneous first-passage bicube,

$$w_H(x, y, x_B, y_B, z_B)=w(x, y, 0, x_B, y_B, z_B) \tag{58}$$

and define further, for brevity,

$$\begin{aligned} w_{H1}(x, y, x_B, y_B)&=w_H(x, y, x_B, y_B, \pm L)\\ &=w(x, y, 0, x_B, y_B, \pm L)\end{aligned} \tag{59}$$

$$\begin{aligned} w_{H2}(x, y, y_B, z_B)&=w_H(x, y, 0, y_B, z_B)\\ &=w(x, y, 0, 0, y_B, z_B)\end{aligned} \tag{60}$$

$$\begin{aligned} w_{H3}(x, y, x_B, x_B)&=w_H(x, y, x_B, 0, z_B)\\ &=w(x, y, 0, x_B, 0, z_B)\end{aligned} \tag{61}$$

$$\begin{aligned} w_{H4}(x, y, y_B, z_B)&=w_H(x, y, L, y_B, z_B)\\ &=w(x, y, 0, L, y_B, z_B)\end{aligned} \tag{62}$$

$$\begin{aligned} w_{H5}(x, y, x_B, z_B)&=w_H(x, y, x_B, L, z_B)\\ &=w(x, y, 0, x_B, L, z_B)\end{aligned} \tag{63}$$

Then w_H's are obtained as, for a position (x_B, y_B, z_B) at the boundary $\partial\Omega$ of the first-passage bicube,

$$w_{H1}(x, y, x_B, y_B)=\frac{4}{L^2}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{m\pi x_B}{L}\right)\sin\left(\frac{n\pi y}{L}\right)\sin\left(\frac{n\pi y_B}{L}\right) \times\frac{\sinh(k_2)}{\sinh(2k_2)} \tag{64}$$

$$w_{H2}(x, y, y_B, z_B)=\frac{2}{L^2}\sum_{m=1}^{\infty}\sum_{n=0}^{\infty}\sin\left(\frac{m\pi y}{L}\right)\sin\left(\frac{m\pi y_B}{L}\right)\cos\left[\frac{(n+1/2)\pi z_B}{L}\right] \times\frac{\sinh[k_3(1-x/L)]}{\sinh(k_3)} \tag{65}$$

$$w_{H3}(x, y, x_B, z_B)=\frac{2}{L^2}\sum_{m=1}^{\infty}\sum_{n=0}^{\infty}\sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{m\pi x_B}{L}\right)\cos\left[\frac{(n+1/2)\pi z_B}{L}\right] \times\frac{\sinh[k_3(1-y/L)]}{\sinh(k_3)} \tag{66}$$

$$w_{H4}(x, y, y_B, z_B)=\frac{2}{L^2}\sum_{m=1}^{\infty}\sum_{n=0}^{\infty}\sin\left(\frac{m\pi y}{L}\right)\sin\left(\frac{m\pi y_B}{L}\right)\cos\left[\frac{(n+1/2)\pi z_B}{L}\right] \times\frac{\sinh(k_3 x/L)}{\sinh(k_3)} \tag{67}$$

$$w_{H5}(x, y, x_B, z_B)=\frac{2}{L^2}\sum_{m=1}^{\infty}\sum_{n=0}^{\infty}\sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{m\pi x_B}{L}\right)\cos\left[\frac{(n+1/2)\pi z_B}{L}\right] \times\frac{\sinh(k_3 y/L)}{\sinh(k_3)} \tag{68}$$

where k_2 and k_3 are defined as

$$k_2=(m^2+n^2)^{1/2}\pi \tag{69}$$

$$k_3=[m^2+(n+1/2)^2]^{1/2}\pi \tag{70}$$

respectively.

The probability p that a random walker land for the first time at a boundary section $\partial\Omega_0$ is obtained by integrating Eqs. (64)-(68) over $\partial\Omega_0$.

For example, if $\partial\Omega_0$ is taken as the right half boundary $(z_B \geq 0)$, then p is obtained as

$$p=\int_0^L\int_0^L w_{H1}(x, y, x_B, y_B)\,dx_B dy_B+\int_0^L\int_0^L w_{H2}(x, y, y_B, y_B)\,dy_B dz_B$$
$$+\int_0^L\int_0^L w_{H3}(x, y, x_B, z_B)\,dx_B dz_B+\int_0^L\int_0^L w_{H4}(x, y, y_B, z_B)\,dy_B dz_B \quad (71)$$
$$+\int_0^L\int_0^L w_{H5}(x, y, x_B, z_B)\,dx_B dz_B=\frac{1}{2}$$

which understates that the random walker starts at the center-cutting plane of the symmetric bicube.

In case that a random walker happens to land exactly at or very close to a corner of a cubic voxel, the walker moves further by use of a first-passage cube, rather than a first-passage bicube. One constructs a first-passage region consisting of eight cubes encompassing the random walker at the corner, instead of two cubes. Consider a random walker exactly at or very close to the origin that is taken at the center of eight cubes, as shown in Fig. 8. Each of eight cubes has a volume of L^3 and the unit conductivity. A random walker diffusing from the center will eventually arrive at an outer boundary of the first-passage region of eight cubes. The mean hitting time τ and the probability density function w in association with this displacement are obtained as solutions of Eqs. (6), (7) and Eqs. (9), (10), respectively. Let us define, for a homogeneous first-passage cube having the unit conductivity,

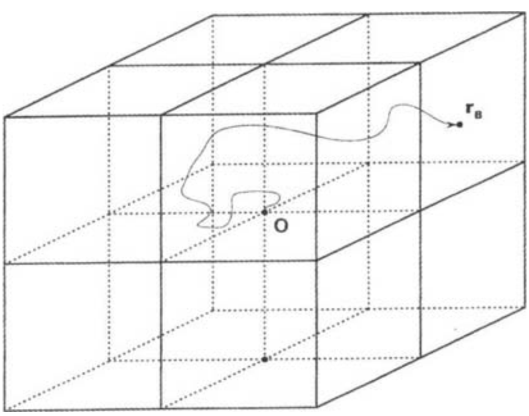


Fig. 8 First-passage-cube of volume $8L^3$. A Brownian walker diffuses from the center to some point $\mathbf{r}_B$ on the boundary

$$\tau_H=\tau(0, 0) \quad (72)$$

and

$$w_H(x_B, y_B, z_B)=w(0, 0, 0, x_B, y_B, z_B) \quad (73)$$

The mean hitting time τ_H is obtained, for the homogenous first-passage-cube in Fig. 8, as

$$\tau_H \simeq 0.22485L^2 \quad (74)$$

The expressions for w_H can be also obtained. For a random walker arriving at $\mathbf{r}_B=(\pm L, y_B, z_B)$ in the x-boundary surface, w_H is obtained as

$$w_H(\pm L, y_B, z_B)$$
$$=\frac{1}{2L^2}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{\sin(m\pi/2)\sin[m\pi/2(y_B/L\pm 1)]\sin(n\pi/2)\sin[n\pi/2(z_B/L\pm 1)]}{\cosh(k_2/2)} \quad (75)$$

For a random walker arriving at $\mathbf{r}_B=(x_B, \pm L, z_B)$ in the y-boundary surface, w_H is obtained as

$$w_H(x_B, \pm L, z_B)$$
$$=\frac{1}{2L^2}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{\sin(m\pi/2)\sin[m\pi/2(x_B/L\pm 1)]\sin(n\pi/2)\sin[n\pi/2(z_B/L\pm 1)]}{\cosh(k_2/2)} \quad (76)$$

For a random walker arriving at $\mathbf{r}_B=(x_B, y_B, \pm L)$ in the z-boundary surface, w_H is obtained as

$$w_H(x_B, y_B, \pm L)$$
$$=\frac{1}{2L^2}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{\sin(m\pi/2)\sin[m\pi/2(x_B/L\pm 1)]\sin(n\pi/2)\sin[n\pi/2(y_B/L\pm 1)]}{\cosh(k_2/2)} \quad (77)$$

The probability that the random walker land for the first time at any point in the specific boundary surface is obtained by integrating Eq. (75), (76) or (77) over the corresponding range. For example, the probability to land at any point in the surface $x=L$, is given by

$$p=\int_{-L}^{L}\int_{-L}^{L} w_H(L, y_B, z_B)\,dy_B dz_B=\frac{1}{6} \quad (78)$$

This result confirms that the random walker lands at each surface with equal probability of 1/6.

3.2.2 Random walk in a heterogeneous situation

Consider the first passage region that is consisted of two cubes of different conductivities, neighboring in z-direction. The first passage region consisting of two neighboring cubes in x- or y- directions can be treated similarly. Each cube has a volume L^3. The origin is again taken to be the corner location in the center-cutting plane between two cubes. The center-cutting plane coincides with the plane in which $z=0$, as depicted in Fig. 7. Let σ_1 and σ_2 be the conductivities of the cubes located at the positive and the negative sides along the z-axis, respectively. A random walker starts to diffuse from a location $\mathbf{r}=(x,\ y,\ 0)$. Using the separation of variables technique, one can solve the boundary value problem, Eqs. (14)-(17) to obtain the mean hitting time $\tau(\mathbf{r})$. For a random walker diffusing from an arbitrary location $\mathbf{r}=(x,\ y,\ 0)$ and landing at some point $\mathbf{r}_B=(x_B,\ y_B,\ z_B)$ in the outer boundary of the first-passage bicube for the first time, the mean hitting time $\tau(\mathbf{r})$ is obtained as

$$\tau=\frac{2}{\sigma_1+\sigma_2}\tau_H \tag{79}$$

where τ_H denotes the homogeneous solution given by Eq. (74) for a unit conductivity.

The probability density function $w(x,\ y,\ 0,\ x_B,\ y_B,\ z_B)$ in association with the walker's displacement is given by the solution of the boundary value problem, Eqs. (18)-(21). This problem can be solved and its solution is obtained as

$$w(x,\ y,\ 0,\ x_B,\ y_B,\ z_B)=\begin{cases}\dfrac{2\sigma_1}{\sigma_1+\sigma_2}w_H(x,\ y,\ x_B,\ y_B,\ z_B),\ \text{for } z_B\geq 0\\[2mm] \dfrac{2\sigma_2}{\sigma_1+\sigma_2}w_H(x,\ y,\ x_B,\ y_B,\ z_B),\ \text{for } z_B\geq 0\end{cases} \tag{80}$$

where w_H is defined in Eq. (58) and its explicit expression is given as w_{H1}, w_{H2}, w_{H3}, w_{H4}, or w_{H5} in Eqs. (64)-(68), depending on the position of $\mathbf{r}_B$. Note that w_H is obtained as w_{H1} for $\mathbf{r}_B=(x_B,\ y_B,\ \pm L)$, w_{H2} for $\mathbf{r}_B=(0,\ y_B,\ z_B)$, w_{H3} for $\mathbf{r}_B=(x_B,\ 0,\ z_B)$, w_{H4} for $\mathbf{r}_B=(L,\ y_B,\ z_B)$, or w_{H5} for $\mathbf{r}_B=(x_B,\ L,\ z_B)$.

The probability p_1 that a random walker land for the first time at any point along the right half $\partial\Omega_1$ of the boundary surface is obtained by integrating Eq. (80) with Eqs. (64)-(68) over $\partial\Omega_1$, i.e.,

$$\begin{aligned}p_1=&\int_0^L\int_0^L w(x,\ y,\ 0,\ x_B,\ y_B,\ L)\,dx_B dy_B+\int_0^L\int_0^L w(x,\ y,\ 0,\ 0,\ y_B,\ z_B)\,dy_B dz_B\\&+\int_0^L\int_0^L w(x,\ y,\ 0,\ x_B,\ 0,\ z_B)\,dx_B dz_B+\int_0^L\int_0^L w(x,\ y,\ 0,\ L,\ y_B,\ z_B)\,dy_B dz_B\\&+\int_0^L\int_0^L w(x,\ y,\ 0,\ x_B,\ L,\ z_B)\,dx_B dz_B\end{aligned} \tag{81}$$

$$\begin{aligned}&=\int_0^L\int_0^L w_{H1}(x,\ y,\ x_B,\ y_B)\,dx_B dy_B+\int_0^L\int_0^L w_{H2}(x,\ y,\ y_B,\ z_B)\,dy_B dz_B\\&+\int_0^L\int_0^L w_{H3}(x,\ y,\ x_B,\ z_B)\,dx_B dz_B+\int_0^L\int_0^L w_{H4}(x,\ y,\ y_B,\ z_B)\,dy_B dz_B\\&+\int_0^L\int_0^L w_{H5}(x,\ y,\ x_B,\ z_B)\,dx_B dz_B\\&=\frac{\sigma_1}{\sigma_1+\sigma_2}\end{aligned}$$

It follows that p_2 for $\partial\Omega_2$ is obtained as

$$p_2=1-p_1=\frac{\sigma_2}{\sigma_1+\sigma_2} \tag{82}$$

implying that the probability p_i landing at Ω_i is proportional to the local conductivity σ_i of the corresponding cube.

In case that a random walker happens to land exactly at or very close to a corner of a cubic voxel, the walker moves further by use of a first-passage cube, rather than a first-passage bicube. One constructs a first-passage region consisting of eight cubes encompassing the random walker at the corner, instead of two cubes. Consider a random walker exactly at or very close to the origin that is taken at the center of eight cubes, as shown in Fig. 8. Each of eight cubes has a volume of L^3. Let $\sigma^{(i)}(i=1,\ 2,\ \cdots,\ 8)$ be the conductivity of the cube at the i-th octant. A random walker diffuses from the center and eventually arrives at an outer boundary of a region of eight cubes. The mean hitting time τ in association with this displacement are obtained as solutions of Eqs. (14)-(17). The solution is found to be

$$\tau=\frac{1}{\bar{\sigma}}\tau_H\simeq\frac{0.22485L^2}{\bar{\sigma}} \tag{83}$$

where

$$\bar{\sigma}=\frac{1}{8}\sum_{i=1}^{8}\sigma^{(i)} \tag{84}$$

and τ_H is the mean hitting time taken for a random walker associated with the homogeneous first-passage region of a unit conductivity, as given in Eq. (73). The probability density function $w(\mathbf{r},\ \mathbf{r}_B)$ associated with this first-passage displacement is given by the solution of the boundary value problem, Eqs. (18)-(21). Let $\partial\Omega^{(i)}$ denote the section of the boundary $\partial\Omega$ belonging in the i-th octant. For a random walker arriving at the boundary at $\partial\Omega^{(i)}$, the probability density is obtained as

$$w(\mathbf{r}, \mathbf{r}_B) = \frac{\sigma^{(i)}}{\bar{\sigma}} w_H(\mathbf{r}_B), \ \mathbf{r}_B \text{ on } \partial\Omega^{(i)} \quad (85)$$

where $w_H(\mathbf{r})$ is the probability density associated with the homogeneous first-passage region, as given in Eqs. (75), (76) and (77). The probability p that the random walker land for the first time at any point along the specific boundary side can be obtained by integrating (85) with the Eqs. (75), (76) and (77).

4. Simulation Details

The effective conductivity σ_e of a conductive medium is directly proportional to random walkers' mean square displacements $\langle R^2(t) \rangle$ in their long-time limit $t \to \infty$, regardless of the homogeneity of the medium. In the computer simulation, one releases sufficiently many random walkers on the digitized medium and keeps track of their displacements for a sufficiently long time interval. First-passage time quantities considered in Sec. 3 are used in letting random walkers move around the medium in an efficient fashion. We describe some simulation details in the language of two dimensions for concreteness. Three-dimensional problems are merely obvious extensions of two-dimensional problems.

Consider a digitized medium that is consisted of square pixels of area L^2. In order to sample the medium, one first chooses an initial location of a random walker such that this initial location is right at a boundary of a square pixel. In our new simulation method, a random walker always jumps from a pixel boundary to another pixel boundary, unlike in previous first-passage-time methods. Thus, at the beginning of each step, a random walker is at the inner boundary (or the centerline) of two adjacent squares, such as $\mathbf{r}$ in Fig. 1. These two neighboring squares are taken as a "first-passage-bisquare," or FPBS, in association with the random walker's displacement. Let us assume that the FPBS is horizontally long, as in Fig. 1. For the random walker's displacement in association with the vertically long FPBS, the following description can be applied by merely interchanging the horizontal and the vertical axes. The FPBS is either homogeneous or heterogeneous, depending on the local geometry around the walker. We describe a random walker's displacement with a homogeneous FPBS and a heterogeneous FPBS, separately.

4.1 Random walker in a homogeneous situation

If a random walker is at the centerline of the homogeneous FPBS, then the walker jumps from the centerline to the outer boundary of the FPBS in one step. For the homogeneous FPBS with the conductivity σ, this jump takes an average amount of time τ_H/σ, where τ_H is given by Eq. (30). The probability density to land at a point on the outer boundary of the FPBS is not uniform along the boundary, but symmetric about the centerline. One first chooses either one of the two boundary sides, left or right, of the FPBS with equal probability of 1/2, and then picks up an arbitrary point at the chosen boundary side according to the probability distribution w_{H1}, w_{H2}, or w_{H3}, given by Eqs. (35)-(37). The walker jumps to this point in one step. One repeats this FPBS jump, unless the walker gets too close to a corner of the FPBS or reaches at the interface boundary of two squares having different conductivities.

If the random walker happens to land at a point right at or very close to the corner, the walker cannot move further by use of the FPBS, since it continues to stay there spending no time. In the computer simulation, one uses a simulation parameter δ to avoid this. If a random walker is within the prescribed small distance δ (that is typically less than 10^{-8} of the pixel size) from the corner, one constructs a first-passage region consisted of four squares of area $4L^2$, instead of two squares of area $2L^2$, in association with the walker's next jump. This jump takes an average amount of time τ_H/σ, where τ_H is given by Eq. (41). One first chooses one of four outer boundary sides of the first-passage square with equal probability of 1/4 and then picks up an arbitrary point at the chosen side according to the probability distribution w_H, given by Eqs. (42) and (43). The walker jumps to this point in one step.

4.2 Random walker in a heterogeneous situation

For a random walker at the interface boundary between two squares having different conductivities, one constructs a first-passage region consisted of these two heterogeneous squares, or a heterogeneous FPBS. The walker jumps from the centerline to the outer boundary of the heterogeneous FPBS. For the FPBS consisted of squares of the conductivity σ_1 at its positive x-side and σ_2 at its negative x-side, this jump takes an average amount of time τ, as much as given by Eq. (45). The probability density to land at a point on the boundary is not uniform along the boundary, nor symmetric about the centerline. One first chooses either one of the two boundary sides, left or right, of the FPBS, with the probability p_1 or p_2, where p_1 and p_2 are given in Eqs. (81) and (82), respectively. Note that this landing probability is proportional to the local conductivity, or $p_i \sim \sigma_i$. One then picks up an arbitrary point at the chosen boundary according to the probability distribution w_H, given by Eq. (46). The walker jumps to this point in one step.

If the random walker happens to land at a point right at or very close to the corner (within δ) and four squares about the corner are not homogeneous, then one needs to use the first-passage square of area $4L^2$, instead of the FPBS of area $2L^2$. For the first-passage region consisted of four squares having conductivities $\sigma^{(i)}$ at its i-th quadrant, this jump takes an average amount of time τ, as much as given by Eq. (49). One first chooses the boundary side of the first-passage square of area $4L^2$ with the probability proportional to the local conductivity and then picks up an arbitrary point at the chosen boundary according to the probability distribution w, given by Eq. (51). The walker jumps to this point in one step.

At each step, the squared displacement is recorded as a function of time. By repeated use of homogeneous or heterogeneous first-passage bisquares of area $2L^2$ (and first-passage squares of area $4L^2$), one can let the random walker continue to displace in the digitized medium as long as needed. Fig. 9 conceptually demonstrates how the FPBS's are used in the random walker's displacement. An ensemble mean is obtained over sufficiently many walkers' displacements for sufficiently long times. The effective conductivity σ_e for a particular configuration of the digitized medium is trivially related to the slope of the mean square displacement versus time, as given in Eq. (1). For disordered media, one should average over sufficiently many configurations.

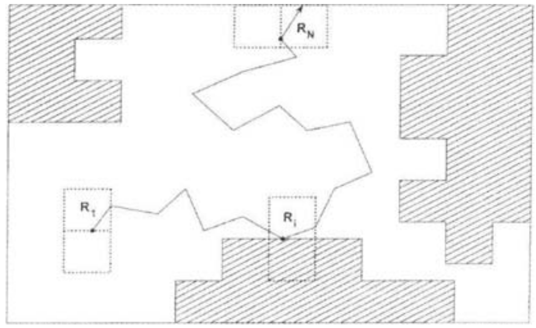


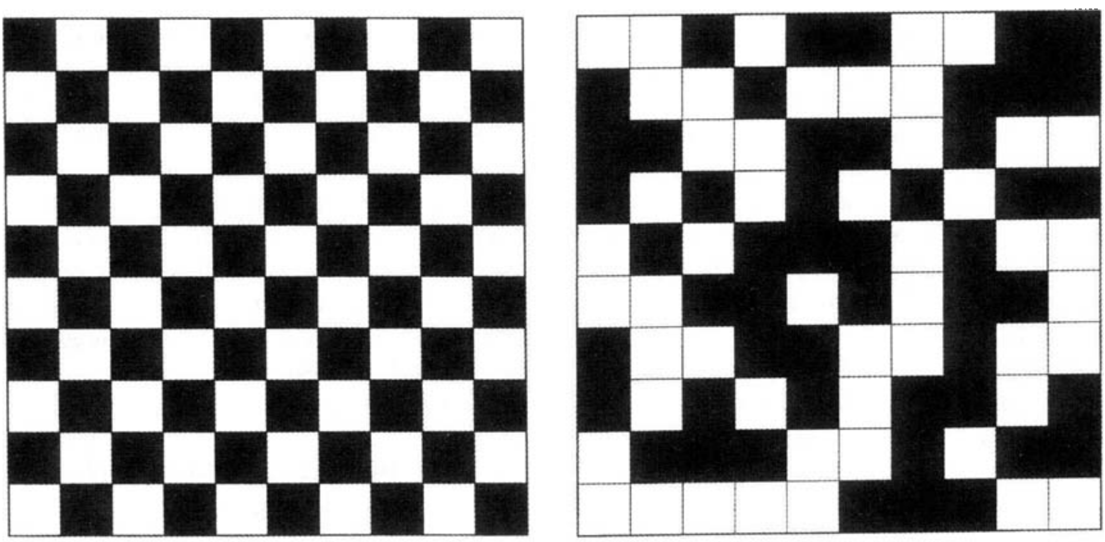
Fig. 9 Brownian walker makes an initial jump of distance R_1 to the boundary of the first-passage-bisquare. It crosses the two-phase interface for the first time in the i-th jump and reaches the sample boundary at the N-th jump

5. Simulation Results and Discussions

In order to illustrate the efficiency of the new algorithm, we carried out computer simulations to compute the effective conductivity σ_e of two-dimensional digitized heterogeneous media. We first considered the periodic and then the random checkerboards. Representative configurations of both checkerboards are shown in Fig. 10. In the following, we use the notation that black squares belong to the more conducting phase, or phase 2, of which the conductivity is σ_2 and the volume fraction is ϕ_2. The less conducting phase, or phase 1, is denoted by white squares with its conductivity σ_1 and volume fraction ϕ_1.

Table 1 Simulation results and the computation times for two different first-passage-time methods. Simulations were carried out to obtain the effective conductivity σ_e of two dimensional periodic checkerboard-type heterogeneous media, in which black (phase 2) and white (phase 1) square pixels are alternately located such that the volume fraction of each phase is equal, i.e., $\phi_1=\phi_2=0.5$. Included in the Table the theoretical values given by the phase interchange theorem. Computation times were measured in 1.7 GHz machine

	New method		FPS method		Theoretical
σ_2/σ_1	σ_e/σ_1	CPU minutes	σ_e/σ_1	CPU minutes	σ_e/σ_1
4	2.0	2	2.0	17	2.0
9	3.1	3	3.0	34	3.0
16	4.1	6	4.0	58	4.0
25	5.2	9	5.0	89	5.0
36	6.2	13	6.0	127	6.0
49	7.2	17	7.0	171	7.0
64	8.2	22	8.0	223	8.0
81	9.2	28	9.0	281	9.0
100	10.1	34	10.0	345	10.0



(a) (b)

Fig. 10 (a) Portion of a periodic checkerboard in which $\phi_1=\phi_2=0.5$. (b) Portion of a random checkerboard in which $\phi_1=\phi_2=0.5$.

5.1 Periodic checkerboard

In the digitized medium of the periodic checkerboard, as shown in Fig. 10(a), the volume fractions of both phases are equal, i.e, $\phi_1=\phi_2=0.5$. The problem of determining the effective conductivity σ_e of this checkerboard-type heterogeneous medium can be exactly solved by using Keller's phase change theorem[9] and the solution is given by

$$\sigma_e=\sqrt{\sigma_1\sigma_2} \tag{86}$$

Eguation (86) appears simple. However, this benchmark problem is one of the most severe tests of a computer simulation algorithm for moderate to high conductivity ratio σ_2/σ_1. We solved this problem for σ_2/σ_1 ranging from 1 to 100, first by using the new simulation method and then the first-passage square (FPS) method. For the simulation, we used 100,000 random walkers. Each walker has been allowed to travel for the total time of $t_{max}=5L^2$ and δ was taken to be $10^{-16}L$, where L is the size of the unit square. The simulation results are summarized in Table 1, where the computation times are also shown for comparison. It is evident that both methods yield virtually exact results but the new algorithm spends the computation time as much as about an order of magnitude smaller than that of FPS method.

5.2 Random checkerboard

In the digitized medium of the random checkerboard, as shown in Fig. 10(b), the square pixels of conductivities σ_1 and σ_2 are randomly blended. For the random checkerboard, we considered three different volume fractions : $\phi_2=0.3$, 0.5 and 0.7 and conductivity ratios σ_2/σ_1 ranging from 1 to 100. We compared again our simulation results to the theoretical values given by Keller's phase interchange theorem.[9] The theorem states that, for two-dimensional, two-phase, isotropic, composite media,

$$\sigma_e(\sigma_1, \sigma_2)\,\sigma_e(\sigma_2, \sigma_1)=\sigma_1\sigma_2 \tag{87}$$

where $\sigma_e(\sigma_1, \sigma_2)$ and $\sigma_e(\sigma_2, \sigma_1)$ are the effective conductivities of composite media in which the phases are interchanged from each other.

For the case of $\phi_2=0.5$, we carried out computer simulations using new method and FPS method. We first generated 10 different configurations of infinite size, which are replicating blocks of 100×100 squares. At each configuration, 100,000 walkers were released. Each walker has freely traveled for the total time of $t_{max}=20L^2$, where L is the size of the unit square. The simulation parameter δ was taken to be $10^{-8}L$. The simulation results are summarized in Table 2, where the computation times are also shown for comparison. One can see that, as in the periodic checkerboard, both methods yield virtually exact results but the new algorithm spends the computation time as much as about an order of magnitude smaller than that of FPS method. Table 2 also shows the theoretical result given by Keller's phase change theorem. The theorem states that, for this particular case of $\phi_1=\phi_2=0.5$, σ_2 is given again by the Eq. (86).

For the case of $\phi_2=0.3$ and 0.7, we carried out computer simulations using the new method. The simulation results are summarized in Table 3. We also include the quantity $\sigma_e(\phi_2=0.3)\cdot\sigma_e(\phi_2=0.7)$ in the Table, in order to compare to Keller's phase change theorem, Eq. (87), which gives, for this particular case,

$$\sigma_e(\phi_2=0.3)\cdot\sigma_e(\phi_2=0.7)=\sigma_1\sigma_2 \tag{88}$$

Table 2 Simulation results and the computation times for two different first-passage-time methods. Simulations were carried out to obtain the effective conductivity σ_e of two dimensional random checkerboard-type heterogeneous media, in which black (phase 2) and white (phase 1) square pixels are randomly blended such that the volume fraction of each phase is equal, i.e., $\phi_1=\phi_2=0.5$. Included in the Table the theoretical values given by the phase interchange theorem. Computation times were measured in 1.7 GHz machine

	New method		FPS method		Theoretical
σ_2/σ_1	σ_e/σ_1	CPU minutes	σ_e/σ_1	CPU minutes	σ_e/σ_1
1	1.0	2	1.0	19	1.0
4	2.0	5	2.0	48	2.0
9	3.0	11	3.0	96	3.0
16	4.0	18	4.0	162	4.0
25	5.0	28	5.0	248	5.0
36	6.0	39	6.0	353	6.0
49	7.0	53	7.0	477	7.0
64	8.0	68	8.0	621	8.0
81	9.0	86	9.0	784	9.0
100	10.0	106	10.0	966	10.0

Table 3 Comparison of simulation results for the quantity $\sigma_e(\phi_2=0.3)\,\sigma_e(\phi_2=0.7)$ and $\sigma_1\sigma_2$, for various values of σ_2/σ_1

σ_2/σ_1	$\sigma_e(\phi_2=0.3)/\sigma_1$	$\sigma_e(\phi_2=0.7)/\sigma_1$	$\sigma_e(\phi_2=0.3)\,\sigma_e(\phi_2=0.7)/\sigma_1^2$
4	1.5	2.7	4.0
9	1.9	4.9	9.1
16	2.1	7.7	16.3
25	2.3	11.0	25.4
36	2.5	14.9	36.7
49	2.6	19.2	49.8
64	2.7	24.1	64.6
81	2.8	29.4	81.6
100	2.9	35.1	100.3

One can see from the Table 3, the simulation results of $\sigma_e(\phi=0.3)\cdot\sigma_e(\phi=0.7)$ are very close to $\sigma_1\sigma_2$, with the maximum error less than 2 per cents, confirming again the exactness of the new method.

We have also compared our results with the four-point Milton bounds,[10] which is the most rigorous bounds for the cases of two-dimensional heterogeneous media considered in this paper. We note that all of our simulation results lie within the lower and the upper bounds.

6. Summary

We have considered the problem of computationally determining the effective conductivity of random heterogeneous digitized media. The digitization simplifies the usually complex configuration of a random heterogeneous medium into a readily accessible one by use of geometrically identical pieces, such as square pixels in a two-dimensional application. The simplified configuration of the digitized medium typically contains sharp edges or corners. As the configuration becomes more random and the contrast between the phase conductivities becomes larger, the conductive transport through touching corners becomes more important. In order for a computation method to be successfully applicable, the method should be able to correctly capture this conductive transport through touching corners. The first-passage-time formulation by Torquato et al., which addresses a Brownian motion simulation technique, provides a theoretical basis by which one can devise a computation method having the desired capability to correctly capture the conductive transport through touching corners. Indeed, they developed a computation method that makes use of the square-shaped first-passage region, or the first-passage square, for a two-dimensional application, and the cube-shaped first-passage region, or the first-passage cube, for a three-dimensional application. To the author's knowledge, this is the only existing computation method by which one can exactly simulate the conductive transport through touching corners. In this study, we have developed a more efficient version of the first-passage-time method that makes use of the first-passage region consisted of two digitizing units, or the first-passage bisquare and the first-passage bicube for a two- or three-dimensional application. The new method speeds up the Brownian walkers traveling in the composite medium and consequently results in the reduced computation time to compute the effective conductivity of the medium. For the illustration, we have considered the problem of determining the effective conductivities of the two-dimensional checkerboard-type heterogeneous media, first for the periodic and then for the random configurations. We computed the effective conductivities using both the first-passage square and the first-passage bisquare methods, for the wide range of conductivity ratios and volume fractions. For the periodic checkerboard, where the exact theoretical value is given by the phase interchange theorem, both methods gave virtually exact results while the proposed new method saved the computation time by about an order of magnitude. For the random checkerboard, where the relation between the conductivities at two different volume fractions is given by the phase interchange theorem, both methods gave virtually identical results while the proposed new method saved the computation time by about an order of magnitude.

Acknowledgment

The author gratefully acknowledges the support of the Korea Science Foundation under Grant No. 2000-1-30400-003-2.

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