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# Efficient random walk algorithm for computing conductivity in continuum percolation systems

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Random walks can be used to obtain the diffusion constant and thus the conductivity for continuum percolation problems. This paper presents an efficient algorithm that allows walkers to move very large distances in one step. The algorithm uses a first-passage time distribution for  $d$ -dimensional spherical surfaces. Results are given for overlapping nonconducting disks in two dimensions. Depending on the density of disks, it is found that the present algorithm is about 5 to 50 times faster than an equivalent algorithm using fixed step lengths.

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## INTRODUCTION

Research on the diffusion and electrical conductivity through inhomogeneous materials is of interest from both an applied and fundamental point of view. In geophysics, the conductivity through porous sedimentary rocks is approximated by Archie's law<sup>1</sup>:  $\sigma \propto \phi^m$ , where  $\sigma$  is the conductivity,  $\phi$  is the porosity, and  $m$  is a number typically around 2. Recently, there has been some work on looking for realistic models for porous rocks and determining the relation between conductivity and porosity.<sup>2</sup> The field of percolation theory originated from the question of how does the conductivity depend on the random placement of conducting objects of various shapes (or the inverse problem of placing random nonconducting objects in a conducting medium).<sup>3</sup> There has been a great deal of interest in obtaining the critical exponents describing the behavior of various quantities near the percolation threshold between the conducting and nonconducting region. All exponents for static quantities have been found to be universal depending only on the dimension  $d$  of the system.<sup>4</sup> The universality of the static exponents has been shown to hold in continuum systems as well.<sup>5</sup> However, the critical exponents for transport quantities may not have the same value in certain continuum systems as they do in lattice systems.<sup>6</sup> Thus it is important to find efficient methods for working with systems that do not have an underlying lattice.

Recently, a number of researchers<sup>7</sup> have been exploring the use of random walkers to compute the diffusion constant and thus through an Einstein relation the conductivity in continuum systems. This method on a lattice frequently goes under the expression "an ant in the labyrinth."<sup>8</sup> The results thus far are generally at about the 5% to 10% accuracy level even though significant computer time has been used. Thus there is a need to improve this method since currently there does not seem to be any other comparable method. The purpose of this paper is to report a new algorithm for the random walk method which pro-

vides an improvement factor of between about 5 to 50 in running time depending on the porosity.

## I. SMALL-STEP METHOD FOR COMPUTING CONDUCTIVITY

The basic random walk method is as follows: One first lays down a configuration of nonconducting obstacles into which the walker may not step. (The inverse problem of conducting objects in a nonconducting background can also be done.) Then one puts down a walker in the conducting region and allows it to exercise a random walk. One can either have walk steps of fixed length and random directions along coordinate axes, fixed step lengths in a uniformly random direction, or steps of random size in each of  $d$  directions according to some probability distribution of step sizes (typically a uniform distribution). If the walker does not step into or through an obstacle, then the step is allowed. Otherwise, the walker is returned to its original position and the time is incremented one unit. This method is referred to as the "blind ant" boundary condition. Data on the mean-square displacement from its original position and possibly other quantities are accumulated periodically and averaged in with the results of many other walkers. The step size must be small enough to sample accurately the crevices between obstacles and the shape of the obstacles as well as ensuring that walkers rarely move through the edge of an obstacle. Simultaneously the step size must be large enough so that the walker makes some progress sampling a significant portion of the configuration space. Finally, one must produce enough configurations to sample adequately configuration space.

The ratio of  $\langle R^2 \rangle$  to the time (proportional to the number of attempted steps) in the long time limit is  $2dD$ , where  $D$  is the diffusion constant and  $\langle R^2 \rangle$  is the walkers' mean-squared distance from their starting position. Using an Einstein relation, the conductivity is proportional to  $\phi D$

where the porosity,  $\phi$ , plays the role of the number of carriers. One can show that this procedure gives the correct expression for the conductivity even though some walkers may be trapped in finite regions.

## II. ALGORITHM USING FIRST-PASSAGE TIMES

The above method is an inefficient use of computer time. This is because the walker spends too much time walking between obstacles without getting very close to an obstacle. To get around this waste of computer time, I have changed the basic algorithm as follows. First, find the largest  $d$ -dimensional sphere that does not overlap any obstacle centered at the present position of the walker. Our system space is divided into cells of the same size as the obstacles so that only cells near the walker need be checked. Then move the walker immediately to a random position on this sphere. (See Ref. 9 and references therein for efficient methods for doing this.) Update the time by picking it from a distribution of first-passage times to the surface of this sphere. We set both upper and lower limits on the radius of this sphere. The upper limit is set so that we limit the number of obstacles we must check. The lower limit is set because when the walker gets too close to an obstacle, the radius of this sphere tends to decrease very rapidly leading to the undesirable situation that the walker remains still. In practice, when the walker gets too close to the obstacle, we use the old algorithm until it walks away from the obstacle. Below we explain how to determine the first-passage time distribution  $\rho(a,t)dt$  defined as the probability of first reaching the surface of a  $d$ -dimensional sphere of radius  $a$  in a time between  $t$  and  $t + dt$ .

The first step toward an analytical calculation of  $\rho(a,t)dt$  is to calculate  $P(r,t)$ , the probability that a particle starting at the origin will be at a distance  $r$  from the origin at time  $t$ , having never gone a distance greater than  $a$ . This probability is determined by solving the diffusion equation:

$$D \nabla^2 P(\mathbf{r},t) = \frac{\partial P(\mathbf{r},t)}{\partial t}, \quad (1)$$

with initial condition

$$P(\mathbf{r},0) = \delta(\mathbf{r}) = \delta(r)/r \quad (2)$$

and the absorbing boundary condition

$$P(a,t) = 0. \quad (3)$$

The solution in two dimensions is

$$P(r,t) = \sum_{n=1}^{\infty} \frac{J_0(j_n r/a)}{\pi a^2 [J_1(j_n)]^2} e^{-(j_n/a)^2 Dt}, \quad (4)$$

where  $J_0$  and  $J_1$  are Bessel functions and  $j_n$  is the  $n$ th zero of  $J_0(z)$ . In three dimensions the solution is

$$P(r,t) = \sum_{n=1}^{\infty} \frac{n \sin(n\pi r/a)}{2a^2 r} e^{-(n\pi/a)^2 Dt}. \quad (5)$$

The next step is to find the probability of not being absorbed at time  $t$ . This function  $P(t)$  is obtained by integrating Eqs. (5) and (6) over the region  $r < a$ . The result in two dimensions is

$$P(t) = \sum_{n=1}^{\infty} \frac{2}{j_n J_1(j_n)} e^{-j_n^2 Dt/a^2} \quad (6)$$

and in three dimensions it is

$$P(t) = 2 \sum_{n=1}^T (-1)^{n+1} e^{-(n\pi/a)^2 Dt}. \quad (7)$$

The third step is to find the probability of being absorbed during the time  $t$  to  $t + dt$ . This is given by

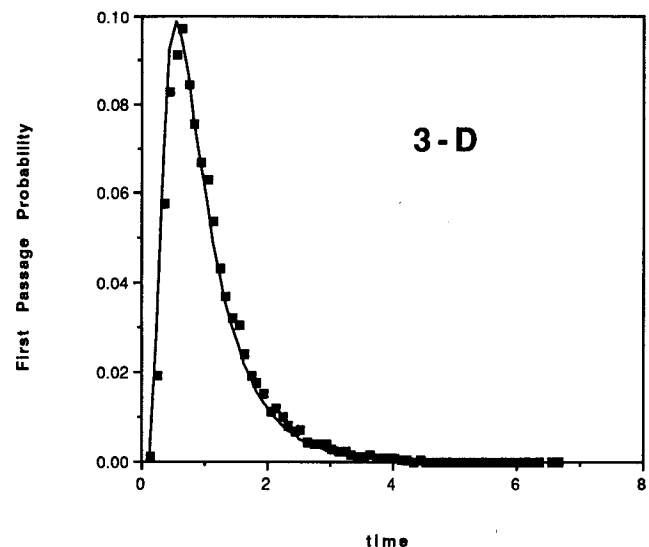
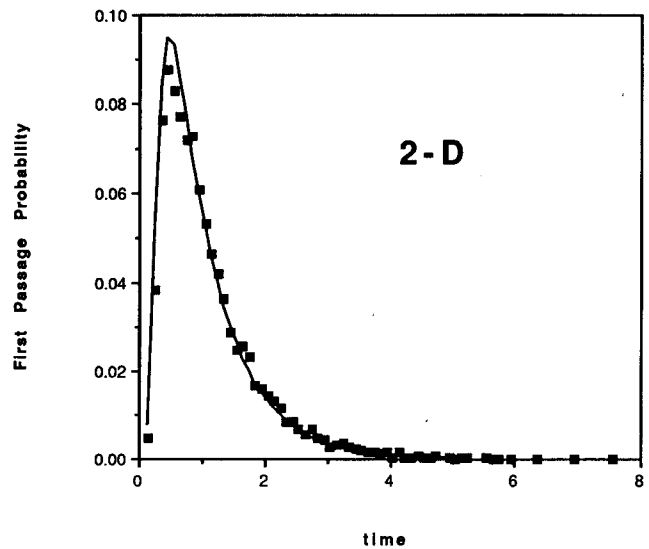


FIG. 1. Probability of a walker first reaching the surface of a sphere (3-D) or circle (2-D) of unit radius at time  $t$ . Units of time are chosen such that  $\langle r^2 \rangle = t$ . The curves are the analytical results and the squares are the results of simulating 10 000 random walkers starting at the origin of a sphere (3-D) or circle (2-D).

$\rho(a,t)dt = -\partial P(t)/\partial t dt$ . Thus we finally obtain in two dimensions

$$\rho(a,t)dt = 2D \sum_{n=1}^{\infty} \frac{j_n}{J_1(j_n)} e^{-j_n^2 Dt/a^2} \frac{dt}{a^2} \quad (8)$$

and in three dimensions

$$\rho(a,t)dt = 2D \sum_{n=1}^{\infty} (-1)^{n+1} (n\pi)^2 e^{-(n\pi)^2 Dt/a^2} \frac{dt}{a^2}. \quad (9)$$

Note that in both cases  $\rho(a,t)dt$  is a function of  $t/a^2$  and  $dt/a^2$ . Thus one function suffices for first passage to circles (spheres) of any radius. The three-dimensional result can be easily evaluated numerically. In two dimensions, if one uses the approximations<sup>10</sup>

$$j_n \approx (n - 0.25)\pi$$

and

$$J_1(z) \approx \sim (2/\pi z)^{1/2} \cos(z - 3\pi/4),$$

then one can get results to within a few percent. I found it easier simply to simulate the first passage walks directly and numerically determined  $\rho(a,t)dt$  in two dimensions. This procedure, for instance, guarantees that  $\rho(a,t)dt$  is normalized. Plots of these functions are shown in Fig. 1.

Once one has  $\rho(a,t)dt$ , one still must reformulate it as a nonuniform probability distribution. This is done by creating an array  $FP(i)$ , where  $i$  runs, for example, from 1 to 1000.  $FP(i)$  is defined by numerically integrating  $\rho(1,t)dt$  until the integral equals  $i/1000$ . Then the mean of the time at this point in the integration and the end of the previous point is put in the array  $FP(i)$ . Thus, if we choose a random integer between 1 and 1000,  $FP(i)$  will provide the first-passage time for moving randomly to a circle or sphere of unit radius. To obtain the actual increment in time, we must multiply this time by  $a^2$ .

### III. RESULTS

In this paper we will illustrate the new algorithm by presenting results in two dimensions of the conductivity between random overlapping nonconducting disks. The

TABLE I. Properties characterizing the efficiency of the present algorithm. All data are for a typical run of 1000 walkers walking for 400 time units using a Sun 3/75 computer. The maximum big step size is 1.

$\phi$	CPU time (h)	Improvement over fixed method	No. of fixed small steps per walker	No. of big steps per walker	Root-mean-square of big step size
0.9	2.0	47	6130	2840	0.37
0.8	3.8	28	13 180	5570	0.27
0.7	6.1	18	20 680	8380	0.22
0.6	9.4	14	30 060	11 630	0.18
0.5	13.5	11	40 450	15 380	0.16
0.4	19.2	8	54 600	19 410	0.14
0.3	27.0	7	68 220	24 150	0.12

conductivity,  $\sigma$ , is given relative to the conductivity with no disks. Preliminary results in three dimensions have also been obtained and they seem promising as well. Table I lists the CPU times to run the present algorithm on a 3/75 Sun computer and the ratios of running times between this algorithm and the fixed step length algorithm. Results are given as a function of porosity. In all cases, the fixed step length was 0.02 where the disk radius provides the unit of length. This same step length was used in the present algorithm for fixed step walks near the obstacles (within 0.04 of the surface of an obstacle). Table I also lists the number of small fixed steps that occur near the surface of obstacles, the number of big steps, and the root-mean-squared step size for the large steps. These numbers show how the fraction of time spent by the walkers near the obstacles grows as the porosity decreases.

In Fig. 2 are shown the data for the reduced conductivity as a function of porosity. The porosity can be determined from the density of disks,  $n$ , of radius  $R$  by the formula<sup>11</sup>

$$\phi = e^{-n\pi R^2}. \quad (10)$$

The time over which  $\langle r^2 \rangle$  is computed varied, depending on  $\phi$ , from  $t = 400$  to  $t = 1500$ . For a fixed step length  $l$ , the number of steps equals  $t/l^2$ . Thus, using our small fixed step size, a time of 400 corresponds to  $10^6$  small steps. The data shown were generated by an average over at least 1000 walkers, each of which walked in a new configuration of disks. Changing the configuration for each walker gave the most reproducible results and one is guaranteed that each walk is totally independent of previous ones.

The effective medium result and an extrapolation formula due to Xia and Thorpe<sup>11</sup> are also shown in Fig. 2. This latter formula has built in the correct slope of  $\sigma$  vs  $\phi$  near  $\phi = 1$ , the correct critical porosity,  $\phi_c \approx 0.33$ , and the accepted value for the critical exponent for the conductivity,  $\mu \approx 1.3$ .<sup>12</sup> As can be seen, our results fit the extrapolation formula very well.

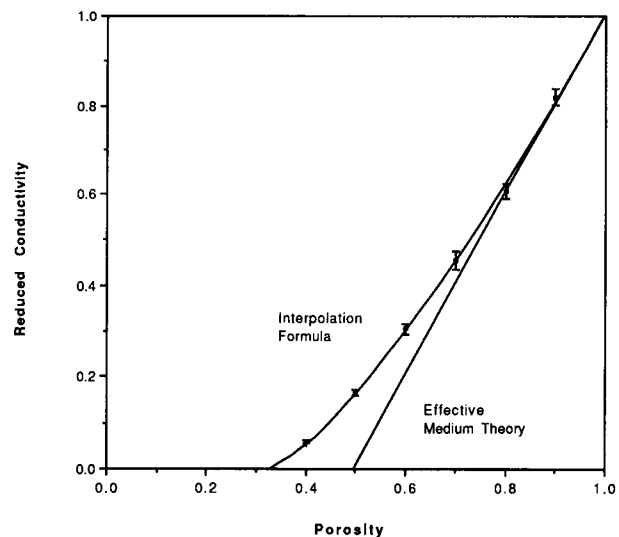


FIG. 2. Conductivity versus porosity for systems of overlapping nonconducting disks. Units are chosen such that the conductivity is unity for  $\phi = 1$ . The interpolation formula is from Xia and Thorpe.<sup>11</sup>

We have also computed the anomalous diffusion exponent  $\alpha$ , defined by  $\langle r^2 \rangle \propto t^\alpha$  for  $\phi = \phi_c$  or for distances less than the connectivity length for  $\phi < \phi_c$ . At  $\phi = 0.33$  we found  $\alpha = 0.70 \pm 0.03$  for  $t = 1$  to 1000. For  $\phi = 0.30$  we found  $\alpha = 0.67 \pm 0.03$  for  $t = 1$  to 400,  $\alpha = 0.70 \pm 0.02$  for  $t = 1$  to 200, and  $\alpha = 0.64 \pm 0.05$  for  $t = 200$  to 400. Using a scaling hypothesis<sup>13</sup> (including walks on finite as well as the infinite cluster), one can show that  $\alpha = (2\nu - \beta)/(2\nu + \mu - 2\beta) \approx 0.69$ . The numerical value is obtained by using the accepted values for the critical exponents:  $\beta = \frac{5}{36}$  and  $\nu = \frac{4}{3}$ . Our numerical results are very close to the predicted value for  $\alpha$ .

#### IV. POSSIBLE FURTHER APPLICATIONS

The algorithm presented in this paper can be used in any continuum percolation problem where it is easy to determine the intersection of a  $d$ -dimensional sphere with non-conducting obstacles.<sup>14</sup> One can also use it on the inverted problem where the walkers move on the objects instead of between them. In this case, one simply makes sure that the maximum step is within the conducting object whose center is closest to the walker. Improvements in the algorithm may be generated by optimizing the cutoff distance within which the fixed step length algorithm is used.

This algorithm may also be useful in Monte Carlo simulations of liquids when calculating the diffusive properties of individual molecules. Using the present algorithm, particles that find themselves in relatively dilute regions can move further, thus sampling a greater portion of configuration space.

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