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LETTER TO THE EDITOR

Effective conductivity of many-component composites by a random walk method

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Abstract. An extension to the many-component case is given for a random walk algorithm which was recently introduced to calculate the effective conductivity of random mixtures with two finite conductivity components. The many-component algorithm has been tested for the case in which the conductivity distribution is generated by taking N-component conductivities and assigning them at random, with equal probability, to the sites of a lattice of size 30^3. Simulations have been done with $N = 10$, 100, 1000 and 27 000. Numerical results obtained by using the proposed random walk algorithm are shown to be in close agreement with those obtained using the conventional finite difference method.

In a recent paper [1], a random walk algorithm for calculating the effective conductivity of random mixtures of two components, each with finite conductivity, was introduced. It is an extension of the 'ant in a labyrinth' algorithm [2], which only applies when one of the components has zero conductivity. Numerical results obtained using the proposed random walk algorithm were shown to be in close agreement with those obtained using the conventional finite-difference method for a variety of conductivity distributions (both isotropic and anisotropic, but necessarily statistically homogeneous over an ensemble) on three-dimensional cubic lattices. In this letter, an extension of the algorithm to the many-component case is discussed. Again, only numerical evidence is provided to support the validity of the algorithm and it would be highly desirable to put it on a sound theoretical basis. However, the author considers the numerical results to be sufficiently suggestive, and the algorithm itself to be sufficiently important, to merit attention at this stage.

Consider a block of conducting material with an applied voltage. Ohm's law gives the relation between the electrical current at any point in the block, $j(r)$, and the voltage distribution, $V(r)$:

$$j(r) = \sigma(r)\nabla V(r) \tag{1}$$

where $\sigma(r)$ is the local electrical conductivity. If the block were made of homogeneous conducting material then $\sigma(r) = \sigma$ would be a constant over the block, giving the electrical conductivity of the material. If the block were heterogeneous then Ohm's law could still be applied in a statistical sense over the block, provided that the scale of the heterogeneities was small compared to the dimensions of the block. In that case, the relationship between the average current, $\bar{j}$, and the average voltage, $\bar{V}$, over a cross section of the block would be given by:

$$\bar{j} = \sigma^* \overline{\nabla V} \tag{2}$$

where σ^* is called the effective conductivity of the block (see e.g. Batchelor's review [3]).

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In general, σ^* is a second-order tensor. It can be anisotropic, even if the local conductivity is isotropic at each point in the block. Strictly speaking, σ^* depends on the boundary conditions for a finite block because the voltage distribution $V(r)$ is determined by the requirement that the steady-state solution satisfy:

$$\operatorname{div}(j(r)) = 0 \tag{3}$$

together with suitable boundary conditions at the ends of the block. Thus, combining Ohm's law (1) and the conservation law (3) gives:

$$\operatorname{div}(\sigma(r)\nabla V(r)) = 0. \tag{4}$$

For given boundary conditions and given conductivity distribution $\sigma(r)$, (4) can be solved numerically using the finite difference method to give the voltage distribution $V(r)$ (more precisely, to compute the voltages V_{ijk} at the node points (ijk) of the imposed finite difference grid). Then the effective conductivity σ^* can be found using (3).

The finite difference method is accurate and can be applied to a wide range of many-component conductivity distributions. However, it is limited by the size of the systems that can be solved in a reasonable amount of computing time (a maximum lattice size of about 30^3 is a good rule of thumb). The size of the system that is simulated determines the range of scales of heterogeneity that can be resolved. For example, if one wishes to simulate a medium which has an anisotropy ratio in the horizontal to vertical directions of 15 : 1 then a lattice of size at least 45^3 would be required to obtain statistically meaningful results. This is because the effective conductivity of a heterogeneous medium depends on both the boundary conditions and the distribution of heterogeneities, which in turn depends on the volume being considered.

Finite-size effects make it important to be able to treat large systems. Because of the constraints involved in using the finite-difference method, there has been an impetus towards developing more efficient algorithms for calculating the effective conductivity. Random walk algorithms, or more general diffusion algorithms, have proved to be useful in some special cases [4–6]. In particular, it has been shown (see e.g. [7]) that simulations based on Einstein's relation between the conductivity σ and the diffusion constant D provide a useful approach to the description of electrical transport in homogeneous disordered continuum systems. Until recently, this type of simulation has been restricted to two-component systems, in which one of the components has zero conductivity, using an algorithm called the 'ant in a labyrinth' algorithm [2]. In [1], it was described how to extend the simulations to the case in which both components have finite conductivity. In this paper, an extension to the many-component conductivity case is discussed.

It is clear that, in a region in which $\sigma(r) = \sigma$ is constant, (4) reduces to Laplace's equation:

$$\sigma\nabla^2 V = 0. \tag{5}$$

For the purposes of numerical simulation (see [4]), it is useful to consider the diffusion problem associated with (5), namely

$$\sigma\nabla^2 V = \frac{\partial V}{\partial t} \tag{6}$$

where t is an artificial simulation time, distinct from real time, so far as the conductivity

problem is concerned. Any solution of (6) which satisfies the physical boundary conditions of the original problem will relax to the correct solution of (5) as $t \to \infty$. The diffusivity of a homogeneous region can be calculated numerically, without actually solving for the distribution $V(r)$ explicitly, by using lattice random walks. The diffusivity is given by the slope D of the line defined by the equation:

$$\langle R^2(t) \rangle = Dt \tag{7}$$

at large times, where $\langle R^2(t) \rangle$ is the mean square distance travelled by the random walkers at time t, with the average being taken over an ensemble of random walkers.

The algorithm [1] proposed for the two-component conductivity case involves a random walker which performs a lattice random walk on each component separately, with the jump rate slowed down by a factor of σ_2/σ_1 in the low conductivity, σ_2, region as compared with the high conductivity, σ_1, region, and with an appropriate probability, the 'interface' probability, defined for jumping from one component to another when starting from an interface site. The interface probability corresponds to the drift term which appears in the governing differential equation (4) when the conductivity gradient is non-zero.

In the proposed algorithm the conductivities are scaled so that $\sigma_1 = 1$ and $\sigma_2 = \sigma_2/\sigma_1$. The random walker at site i chooses one of its nearest neighbours, say j, at random and moves there with a probability given by:

$$\Pi_{ij} = \frac{2\sigma_i\sigma_j}{\sigma_i + \sigma_j} \tag{8}$$

or stays put with probability $(1 - \Pi_{ij})$. In either case, the simulation time is incremented by one unit.

As required, this algorithm reduces to the 'ant in a labyrinth' algorithm in the case when one of the conductivities is zero. Also, if both conductivities have the same value, it reduces to a simple lattice random walk, as required for the homogeneous case described above. Furthermore, it was shown numerically in [1], by comparison with results obtained using the finite difference method, that the algorithm gives very accurate results for the effective conductivity of random, uncorrelated two-component systems over a wide range of conductivity contrast ratios, $\alpha = \sigma_2/\sigma_1$.

The algorithm has an obvious extension to the many-component case. The N values of the conductivity must be scaled so that

$$\sigma_i = \frac{\sigma_i}{\sigma_{\max}} \qquad i = 1, \ldots, N \tag{9}$$

where $\sigma_{\max} = \max\{\sigma_i, i = 1, \ldots, N\}$. Then the jump probability Π_{ij} is defined to be given by (8), as before.

Notice that if $\sigma_i = \sigma_j = \sigma$, then $\Pi_{ij} = \sigma$. Hence, in a region of constant conductivity, the random walker performs a simple random walk with the jump rate slowed down by a factor σ compared with its rate in the highest conductivity region. If $\sigma_i \neq \sigma_j$, then Π_{ij} is given by the harmonic mean of the two conductivities. This is suggested by the fact that for flow in one dimension, or for flow perpendicular to the layers in a layered medium, the effective conductivity is given by the harmonic mean of the constituent conductivities. A rigorous justification is yet to be provided. The aim is that, over a large ensemble of random walkers, the relative time spent in each conductivity region, σ_i, will be such as to give that conductivity its correct weight, λ_i, in a weighted

mean, σ_m:

$$\sigma_m = \sum_{i=1}^{N} \lambda_i \sigma_i \tag{10}$$

so that σ_m will be equal to the effective conductivity, σ^*, defined in (2).

The many-component algorithm was tested for conductivity distributions which were generated by taking N components with conductivities between 0 and 1 and assigning them at random, with equal probability, to the sites of a lattice of size 30^3 (note: in this way, it was assured that the conductivity distributions were statistically homogeneous over an ensemble. For an inhomogeneous distribution, such as a layered system, it would have been necessary to use some sort of biased diffusion algorithm, as was done by Schwartz *et al* in their study of electrical transport in inhomogeneous continuum systems [8]). Simulations were done with $N = 10$, 100, 1000 and 27 000. The values of the conductivities were chosen using a uniform random number generator and three different sets were used for each N. Two additional sets of conductivities were used for $N = 10$, one with a bias towards low values and one with a bias towards high values. The exact values chosen were

$$\sigma_{low} = (0.05, 0.06, 0.95, 0.85, 0.91, 0.005, 0.5, 0.11, 0.87, 0.01)$$

and (11)

$$\sigma_{high} = (0.95, 0.85, 0.75, 0.92, 0.82, 0.72, 0.98, 0.88, 0.78, 0.99)$$

but this was quite arbitrary. An average over 10 different conductivity distributions was taken for each set, with 10^5 random walkers for each distribution, starting at arbitrary locations, and walking for 10^3 steps. The results for the effective conductivity, σ^*_{rw}, are shown in table 1, alongside the results, σ^*_{fd}, obtained using the finite difference method (averages were taken over the same ensemble of conductivity distributions). The two sets of results are in good agreement, even for the case $N = 27\,000$.

Table 1. This table shows the values of the effective conductivity, σ^*_{rw}, obtained using the random walk algorithm compared with the results obtained using the finite difference method, σ^*_{fd}, for a variety of N-component conductivity distributions. The conductivity distributions were generated by taking N components with conductivities between 0 and 1 and assigning them at random, with equal probability, to the sites of a lattice of size 30^3.

N	σ^*_{rw} (±0.003)	σ^*_{fd} (±0.003)
10	0.295	0.295
	0.213	0.213
	0.279	0.281
(low)	0.173	0.175
(high)	0.860	0.858
100	0.366	0.368
	0.354	0.355
	0.392	0.394
1000	0.383	0.384
	0.409	0.410
	0.396	0.398
27 000	0.381	0.382
	0.380	0.382
	0.380	0.381

It is interesting to note that it has been shown theoretically for a log-normal distribution of conductivities in two dimensions, that the effective conductivity is given exactly by the value of the geometric mean, σ_{gm}, in the infinite volume limit [9]. In three dimensions, no exact result is known, but first-order perturbation theory gives:

$$\sigma^* = \sigma_{gm} \exp\left(\frac{\lambda^2}{6}\right) > \sigma_{gm} \tag{12}$$

for the log-normal distribution given by:

$$\sigma(\phi) = \exp(\lambda\phi) \tag{13}$$

where ϕ is a Gaussian random variable with zero mean and unit variance [4, 10]. To the author's knowledge, no theoretical result is available for a uniform distribution, but it can be observed that the results of table 1 for the three different sets of N uniformly distributed random conductivities appear to be converging to a value of 0.381 ± 0.003, for large values of N. This is consistent with the result of (12), in that it is close to (but greater than) the value of the geometric mean:

$$\sigma_{gm} = \exp\left(\int_0^1 \ln(\phi)\, d\phi\right) \approx 0.368. \tag{11}$$

In conclusion, an extension to the many-component case has been given for a random walk algorithm which was recently introduced to calculate the effective conductivity of random mixtures with two finite conductivity components. The many-component algorithm has been tested for the case in which the conductivity distribution is generated by taking N component conductivities and assigning them at random, with equal probability, to the sites of a lattice of size 30^3. Simulations have been done with $N = 10$, 100, 1000 and 27 000. Numerical results obtained by using the proposed random walk algorithm have been shown to be in close agreement with those obtained using the conventional finite difference method.

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References

[1] McCarthy J F 1990 *J. Phys. A: Math. Gen.* **23** L445
[2] de Gennes P 1976 *Recherche* **7** 919
[3] Batchelor G K 1974 *Ann. Rev. Fluid Mech.* **6** 227
[4] Drummond I and Horgan R 1987 *J. Phys. A: Math. Gen.* **20** 4661
[5] Haus J and Kehr K 1987 *Phys. Rep.* **150** 263
[6] Havlin S and Ben-Avraham D 1987 *Adv. Phys.* **36** 695
[7] Schwartz L and Banavar J 1989 *Phys. Rev.* B **39** 11965
[8] Schwartz L, Banavar J and Halperin B *Phys. Rev.* B **40** 9155
[9] Matheron G 1967 *Rev. de l'IFP Rueuil* **22** 443
[10] King P 1987 *J. Phys. A: Math. Gen.* **20** 3935