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A Model for the Electrical Conductivity of a Mixed Computational Cell

by Steven B Segletes

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Weapons and Materials Research Directorate, CCDC Army Research Laboratory

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14. ABSTRACT A model is formulated to describe the electrical conductivity of a mixed computational cell with an arbitrary number of material species. The method treats a mixed cell as a network of linkages, in which the random distribution of different linkages throughout the network corresponds to the volume fractions of the different species composing the mixed cell. The proposed method relies on the probabilistic likelihood of connectivity across the cell, when considering electrical pathways composed of different combinations of the material species present in the cell. The contribution to the overall electrical conductivity for each material–species combination is estimated by considering both the conductivity of pathways composed of that species combination, as well as the likelihood that any given electrical pathway will be composed of that species combination.			
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1. Introduction

The problem of determining the electrical conductivity of a computational "mixed cell" is a challenging one. The result may be strongly affected by the morphology (distribution and granularity) of the constituents within the mixed cell, which nonetheless must be, at a certain level, assumed. The study of *conductivity* is closely linked with that of *connectivity*, since any pathway across a cell that hopes to conduct must, in fact, be connected. To this end, in ARL-TR-8899,[1] the point-to-point *connectivity* of various network lattices were studied as metaphors for the connectivity across a computational cell containing both conducting and insulating material. The result, when the conductor was distributed randomly across the network, was that connectivity exhibits a threshold behavior, as seen in Fig. 1 for a 4×4 network.

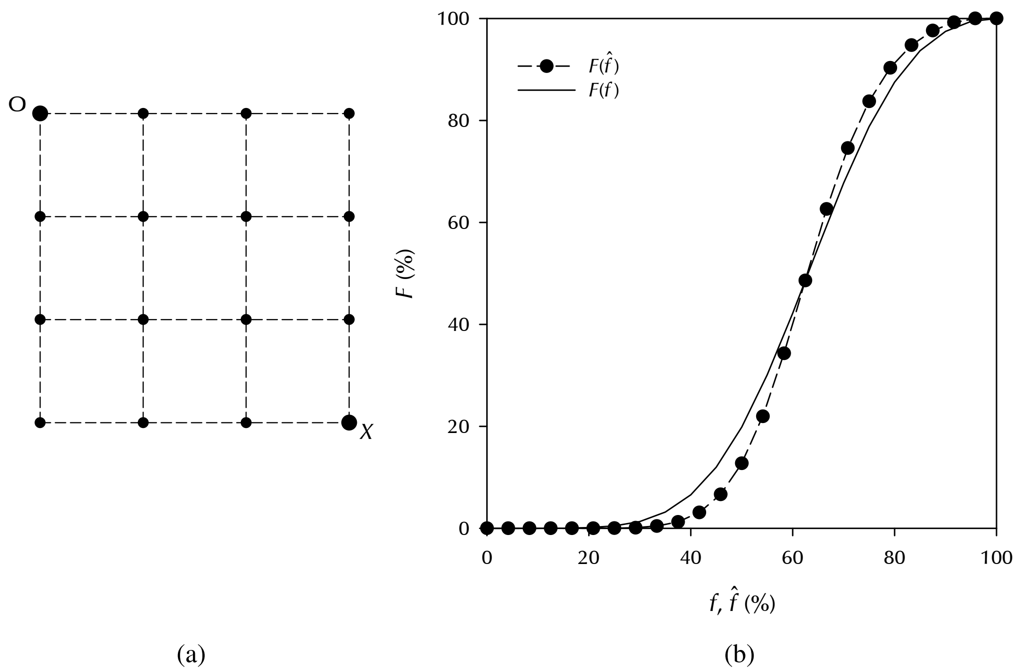

Fig. 1 For a) the given 4×4 network, b) is the likelihood of O-to-X network connectivity F, expressed as a function of either the local conduction probability f or the global conducting fraction $\hat{f}$ of the network links

The implication of Fig. 1 is that, if the fraction of conductors in the network is below the threshold (approximately 65% for this type of network), the likelihood of connectivity is quite small. In fact, below a 20% conducting fraction, the 4×4 network provides zero likelihood of connectivity. Beyond the 65% threshold, the likelihood becomes very large. Such a result is in line with conclusions from percolation theory.[2] Our goal in this report is to use that connectivity result to formulate a statement on the electrical *conductivity* of a mixed cell containing an arbitrary number of species, each with its own value of conductivity. Because of the assumptions employed in ARL-TR-8899, we are limited to an analysis in which the species composing the mixed cell (regardless of their concentration) are considered to be randomly distributed throughout the cell.

It is said that "current takes the path of least resistance". This can be restated as "current takes the path of greatest conductance". It is on this underlying principle that we build the model for mixed-cell conductivity presented in this report—when considering electrical pathways across the mixed cell, it is the most conductive pathways that govern the flow of current across the cell. Put another way, if an electron has the choice of two paths across the cell, it will choose the one that is most conductive.

2. Modeling Conductivity of a Mixed Cell

The $F(\hat{f})$ threshold curve of Fig. 1 provides the statistical backbone on which we develop relations to express the conductivity of a mixed cell. The function $F(\hat{f})$ represents the probability of establishing a connected circuit between opposite corners of a network (in this case, a 4×4 square network of linked nodes), given the fraction $\hat{f}$ of conducting linkages in the network. The numerical values for the $F(\hat{f})$ data in Fig. 1 are presented in Table 13 of ARL-TR-8899.[1]

While, technically, the $F(\hat{f})$ function represents the likelihood of corner-to-corner connectivity across the network, we treat the function as isotropic. In this way, it may be taken to represent the likelihood of point-to-point connectivity between any two arbitrary points across the breadth of the mixed cell.

Let us start heuristically in trying to establish a viable method for calculating the cross-cell conductivity. Consider the simplest of mixed cells, with $n = 2$ species. Let the conductivity of species 1 exceed that of species 2 (*i.e.*, $\kappa_1 > \kappa_2$). Designate the volume fractions of the species by v_j, which are constrained by continuity: $\sum_{j=1}^{n} v_j = 1$. The value $F(v_1)$ represents the likelihood of establishing connectivity between two arbitrary edge points that lie across the breadth of the cell, utilizing a pathway composed solely of species 1. Statistically, therefore, for a cell with a large number of pathways across it, $F(v_1)$ represents the expected fraction of pathways composed solely of species 1.

Those pathways that are *not* composed solely of species 1 must either be composed solely of species 2 or a combination of species 1 and 2 (we use the symbol $\cap$ to denote these combination or "series" pathways, as in $1\cap 2$). Since $\kappa_1 > \kappa_2$, the conductivity of the $1\cap 2$ pathways will be greater than those of the species-2 pathways. It is here that we rely on our underlying principle that current will take the path of greatest conductance—thus, the $1\cap 2$ pathways will always take conductive precedence over species-2 pathways.

With only two species present, $F(v_1 + v_2) \equiv 1$, which is to say that, if both (non-insulating*) species can be traversed, there is a 100% chance of establishing connectivity across the cell. Therefore, we conclude that, while the fraction $F(v_1)$ of the pathways will be composed solely of species 1, all remaining $1 - F(v_1)$ pathways will be $1\cap 2$ pathways.†

The conductance G of a single-element circuit is defined as $G = \kappa A/l$, where A is the cross-sectional area of the element, l is the path length across the element, and κ is the electrical conductivity of the element. We consider each pathway across our mixed cell as a circuit element. We note that for our idealized network composed of linkages, the cross section A of all pathways is the same.

While the pathlength l of individual pathways can vary depending on how much meandering occurs in the route across the cell, many of the connected pathway realizations are of comparable length. For example, ARL-TR-8899 reported[1] that the 4×4 grid of Fig. 1 has 184 unique pathways from corner to corner. Of those, 20 are six links long, 36 require eight links, 48 require ten and twelve links each, and 32 require fourteen links. However, the longer pathways are less probable. So, while it may be a stretch to assume that all pathlengths are of equal length l, our

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*For the computational models of interest to us, all material species possess some nonzero level of conductivity.

†Note that we are not saying species-2 pathways do not exist; they have a likelihood of occurrence of $F(v_2)$. Rather, we are saying that any current traveling from point A to B along a species-2 pathway will *always* detour into species 1 at every opportunity, even if temporarily. Thus, species-2 pathways play no role in determining the overall conductance of a $1\cup 2$ mixture, for which $\kappa_1 > \kappa_2$. The assumption of random distribution of species throughout the cell allows us to discount the hypothetical counter-example where a single node of species-1 material is embedded within a species-2 matrix.

calculations are greatly simplified by making this assumption nonetheless, leading to $G \propto \kappa$.

While the conductivity of pathways composed solely of species 1 or 2 are simply κ_1 or κ_2, respectively, a $1{\cap}2$ network pathway can be thought of as a *series* circuit in which species-1 linkages are v_1/v_2 times as likely to appear as those of species 2 (thus, $l_1/l_2 = v_1/v_2$). The conductivity for these $1{\cap}2$ pathways can be derived from the equation for series conductance, $1/G = \sum_{j=1}^{n} 1/G_j$, as

$$\kappa_{1\cap 2} = \frac{v_1 + v_2}{\dfrac{v_1}{\kappa_1} + \dfrac{v_2}{\kappa_2}} \quad . \tag{1}$$

For the case of $n = 2$ species, it will be the case that $v_1 + v_2 \equiv 1$.

We now have, for all relevant varieties of pathways (1 and $1{\cap}2$), both the conductivities (κ_1 and $\kappa_{1\cap 2}$) as well as the fractions of the overall pathway count they represent ($F(v_1)$ and $1 - F(v_1)$). These pathways operate in parallel and thus the rule for parallel conductance applies, in which $G = \sum_{j=1}^{n} G_i$, leading to the conclusion that, for a mixture of two species,

$$\kappa = \kappa_{1\cup 2} = F(v_1)\kappa_1 + \left[F(v_1 + v_2) - F(v_1)\right]\kappa_{1\cap 2} \qquad (\kappa_1 > \kappa_2) \quad , \tag{2}$$

where the notation $1{\cup}2$ refers to the set of all *parallel* pathways of conduction that incorporate species 1 and 2—namely, those that solely employ species 1 or 2, as well as those that simultaneously incorporate both species 1 and 2 (that is to say, $\{1{\cup}2\} = \{1, 2, 1{\cap}2\}$). For a two-species mixture, $F(v_1 + v_2) \equiv 1$. Introducing the notation

$$F_{1\cup 2} = F(v_1 + v_2) \quad , \tag{3}$$

we may write Eq. 2 more compactly as

$$\kappa = \kappa_{1\cup 2} = F_1\kappa_1 + \left[F_{1\cup 2} - F_1\right]\kappa_{1\cap 2} \qquad (\kappa_1 > \kappa_2)$$

This result for $\kappa_{1\cup 2}$ is plotted in Fig. 2, for three initial values of κ_1/κ_2, with $F(\hat{f})$ provided as a reference. This figure exhibits all the desired properties:

- when $v_1 = 0$, $\kappa = \kappa_2$,
- when $v_2 = 0$, $\kappa = \kappa_1$,

- the behavior of $\kappa_{1\cup 2}$ is monotonic as the volume fraction ratio is changed,
- $d\kappa/dv_1 \rightarrow 0$ in the vicinity of $v_1 \rightarrow 1$ (implying that the introduction of small quantities of species 2 are conductively bypassed),
- the trend (shape) in κ (*conductivity*) is similar to the trend in F (*connectivity*), and
- as $\kappa_2 \rightarrow 0$ (*i.e.*, insulating), the behavior of κ approaches that of F, such that $d\kappa/dv_1 \rightarrow 0$ in the vicinity of $v_1 \rightarrow 0$, *if and only if* $\kappa_2 \ll \kappa_1$.

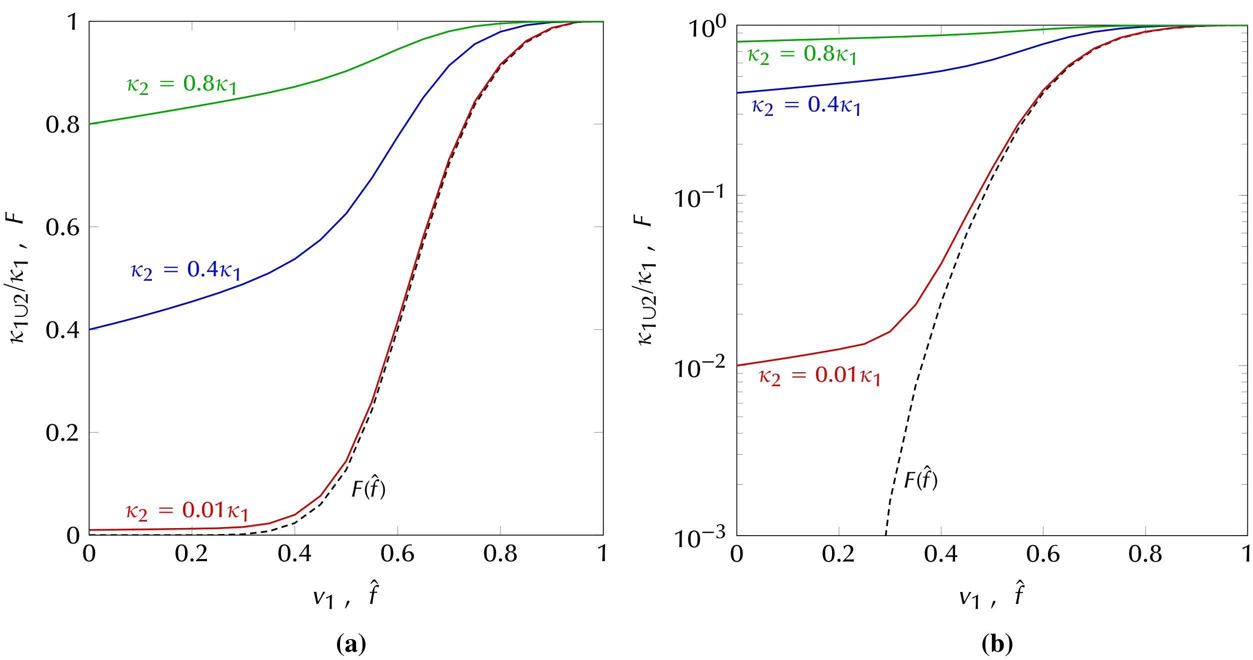

Fig. 2 The net conductivity $\kappa_{1\cup 2}$ of a two-species mixed cell, as a function of the volume fraction v_1, for different ratios of κ_2/κ_1, in both a) linear and b) semilog scales. Reference curve, $F(\hat{f})$, provided for comparison.

It is imperative to understand that one of the principal approximations, in what has been presented to this point, is the assumption that all $1\cap 2$ pathways (those involving species 1 and 2 in series) are characteristically identical. This is true not only of the estimate for pathlength, from which we infer $G \propto \kappa$, but also for the uniformity of ratio l_1/l_2 that is taken to apply to all $1\cap 2$ pathways, which allows a uniform value of $\kappa_{1\cap 2}$ to be calculated.

The Tyranny of Geometric Combinations

It has been said, "In theory, theory and practice are the same. In practice, they are not."[3] When there are multiple species that occupy a mixed cell, one should, *in theory*, consider all the possible conductive pathways across the cell. Unfortunately, this approach necessarily entails a method that incorporates the combinations of those species (including the partial combinations).

When there are three species, pathways will come in a greater number of varieties, composed of the following material combinations: 1, 2, 3, 1∩2, 2∩3, 1∩3, and 1∩2∩3—seven pathway types in total. For four species: 1, 2, 3, 4, 1∩2, 1∩3, 1∩4, 2∩3, 2∩4, 3∩4, 1∩2∩3, 1∩2∩4, 1∩3∩4, 2∩3∩4, and 1∩2∩3∩4—15 pathway varieties total. We deduce that for n species in a cell, there are $2^n - 1$ unique material combinations that make up the pathway varieties. As the number of mixed-cell species grows, the pathway combinations can quickly become unmanageable.

In the mixed cell previously considered, composed of two species, there are combinatorically three pathway types: 1, 2, and 1∩2. However, on the basis of heuristic argument, we were able to eliminate species-2 pathway types from consideration. Therefore, *in practice*, we would like to avoid any procedure that requires the full combinatorial enumeration of all possible pathways, even if the resulting practice involves a further measure of approximation.

3. Approximately Modeling Conductivity of a Mixed Cell

To aid the algorithm that we now propose, when considering an arbitrary number of material species in a mixed cell, we choose to order the species from greatest conductivity to least conductivity, in the manner of Fig. 3.

At the risk of sacrificing some accuracy, we propose an approach to avoid the necessity of exhaustively considering all the material combinations that can compose a given pathway.

For the hypothetical situation summarized in Fig. 3, the preferred path of conduction (that of least resistance) would traverse those pathways composed solely of species 1, the most conductive material. The conductivity of those pathways is simply κ_1. However, the overall fraction of such pathways, $F(v_1) = F_1$, may be quite

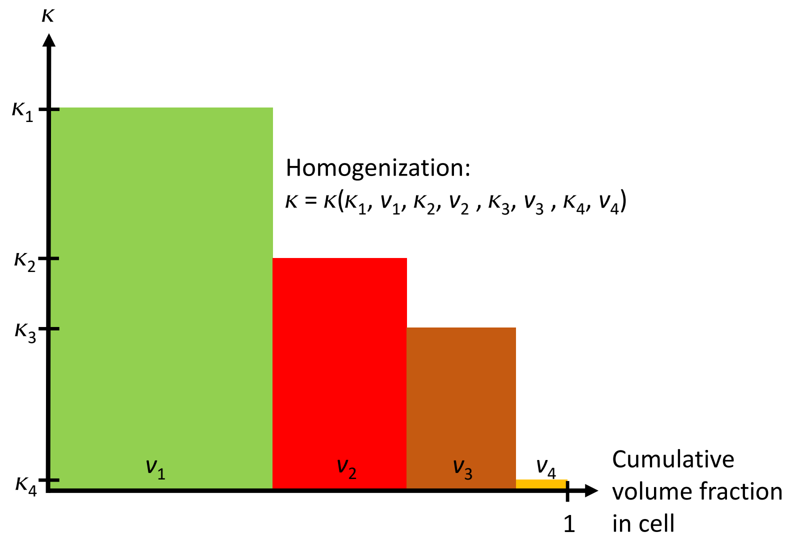

Fig. 3 An expression of the conductivities κ_j and volume fractions v_j of the species within a given mixed cell, where the species have been organized in the order of most conductive (species 1) to least conductive (species n = 4)

small, especially if the volume fraction v_1 of that constituent is below the probabilistic threshold value alluded to in Fig. 1b.

The next most conductive pathway sets across the cell will generally be those composed solely of species 1 and 2 in series (*i.e.*, the 1∩2 pathways, which we know will always be more conductive than the species-2 pathways). The approximation proposed here is to neglect the possibilities by which the 1∩3 pathway conductivity equals or exceeds that of 1∩2, even as $\kappa_3 \leq \kappa_2$.*

With this approximation in place, the number of pathway types to be considered for a mixed cell of n species reduces from $2^n - 1$ to merely n. For $n = 3$, the viable pathways are now 1, 1∩2, and 1∩2∩3; the 1∩3 inversion, if it exists, is essentially subsumed into the 1∩2∩3 pathways. For $n = 4$, the viable pathways become 1, 1∩2, 1∩2∩3, and 1∩2∩3∩4.

*There can exist situations when $\kappa_3 = \kappa_2$, for which both 1∩2 and 1∩3 pathways are conductively uniform and thus equally viable *in reality*, but for which the current method will still prefer the 1∩2 pathways.

Likewise, when $v_3 < v_2$ and $\kappa_3 \approx \kappa_2 - \varepsilon$, the 1∩3 pathways can result in a larger value of conductivity than 1∩2 pathways (and are thus electrically preferable). However, because v_3 must be small for this inversion to arise, the net fraction of 1∩3 pathways will likewise be small (taking a value of $F_{1\cup 3} - F_1$), so that [we hope] the error introduced by ignoring this unusual inversion will be negligible.

See the Appendix for more discussion of conductively uniform as well as inverted pathways.

The net conductivity for $1 \cap 2$ pathways can be directly obtained from Eq. 1; however, note that the difference in the current application of Eq. 1 is that, when $n > 2$, $v_1 + v_2 < 1$. The conductivity associated with pathways that traverse species 1 through j can be generalized (for all $j > 0$) as

$$\kappa_{1\cap\cdots\cap j} = \frac{\sum_{i=1}^{j} v_i}{\sum_{i=1}^{j} \frac{v_i}{\kappa_i}} \quad . \tag{4}$$

As with Eq. 1, the generalized Eq. 4 follows directly from the basic definitions of series conductance G, in which $1/G_{\text{series}} = \sum 1/G_i$, where $G = \kappa A/l$.

To formulate the net conductivity for the multi-species mixture, not only is the conductivity needed for each of the pathway types (available via Eq. 4), but the fraction of the overall conducting pathways that each type comprises is needed, as well.

With the simplification afforded by our approximation that prohibits inversions, these fractions become straightforward to calculate:

$$F_{1\cap\cdots\cap j} = F_{1\cup\cdots\cup j} - F_{1\cup\cdots\cup j-1} \quad , \tag{5}$$

where Eq. 3 may be generalized as

$$F_{1\cup\cdots\cup j} = F\left(\textstyle\sum_{i=1}^{j} v_i\right) \quad . \tag{6}$$

These different sets of pathways across the cell coexist as parallel circuits. Therefore, the conductance that arises from the sum of the connectable pathways is obtained by adding the conductances of all the pathways (*i.e.*, $G_{\text{parallel}} = \sum G_i$). In assuming that each pathway is of comparable pathlength and cross-sectional area, we deduce that the conductivity is likewise derived as a weighted sum of the pathway conductivities. The mixed-cell conductivity κ can thus be generalized across a mixed cell of n species as

$$\kappa = \kappa_{1\cup\cdots\cup n} = \sum_{j=1}^{n} F_{1\cap\cdots\cap j}\, \kappa_{1\cap\cdots\cap j} \quad . \tag{7}$$

The set of equations (Eqs. 4–7) represent the approximate model put forth here for the electrical conductivity of mixed computational cells, where the statistically based $F(\hat{f})$ function is provided from a suitable external source, such as that in Fig. 1.

This model embodies characteristics of both series and parallel circuitry. The conductivity of individual pathways, $\kappa_{1\cap\cdots\cap j}$, defined in Eq. 4 and employed in Eq. 7, is derived for conduction through a series of material species peculiar to that pathway. Nonetheless, the summation in Eq. 7 represents the parallel nature of the conductivity circuit, in which different conductive pathways contribute to the overall conductance across the mixed cell.

4. Example with Three Species

To demonstrate the results of this model, when there exist more than two species of material within the mixed cell, we consider the following problem as an example. There are three species, with the following respective conductivities (ordered from largest to smallest), as shown in Table 1. We use the approach provided by Eqs. 4–7 to estimate the electrical conductivity of this material set for various combinations of v_1, v_2, and v_3.

Table 1 Conductivities of three material species in mixed cell for the sample problem

j	κ_j
1	1.0
2	0.6
3	0.01

We present the resulting conductivity "map" in Fig. 4. This figure is similar to that shown previously for two species in Fig. 2, in that the net electrical conductivity, κ, is presented as a function of species-1 volume fraction v_1. However, to account for the extra species in Fig. 4, we present multiple curves, parameterized such that each colored curve corresponds to a fixed value of v_2 (taking on v_2 values of 0, 0.2, 0.4, 0.6, and 0.8; the value of $v_2 = 1$, not shown, would result in a single point solution at $(0, 0.6)$ on the graph). The black curves in Fig. 4 correspond to the extremum cases, wherein $v_2 = 0$ and $v_3 = 0$, respectively. The slight overlap (rather than asymptote) of the colored curves with the extremum, $v_3 = 0$, is an artifact related to the topic of conductive inversion, discussed in the Appendix.

Whereas, in Fig. 2, we deduce that $v_2 = 1 - v_1$, we have, in the case of Fig. 4, that $v_3 = 1 - v_1 - v_2$. In both cases, these are statements of n-species continuity.

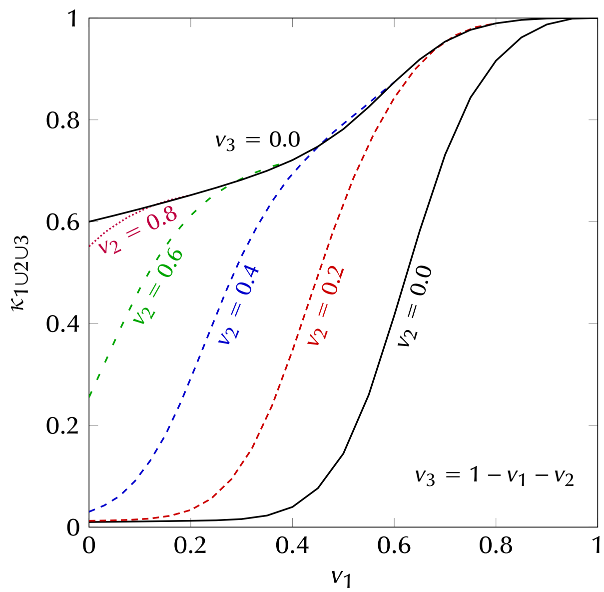

Fig. 4 Example conductivity map, with three material species, of conductivities 1.0, 0.6, and 0.01, respectively

5. Conclusion

In this report, we presented a model to estimate the net conductivity of a mixed computational cell. An important basis for the model is the function $F(\hat{f})$, the probabilistic likelihood of achieving point-to-point *connectivity* across a finite network of conductors and insulators, which is used as a metaphor for a mixed cell. This function, which was detailed in ARL-TR-8899,[1] is presently used to provide the weights assigned to the conductivities of various electrical-pathway configurations.

For each relevant pathway configuration (defined by the material species that compose it), the model estimates the local conductivity as well as the fraction of the total pathways constituted by the particular configuration. The material species that constitute a given pathway configuration are taken to represent a set of *series* electrical pathways, whereas the pathways of each different material configuration are assumed to operate in *parallel* with the other configurations.

The model does entail assumptions:

- A mixed cell is treated as a metaphorically equivalent electrical network (intrinsic to the use of the $F(\hat{f})$ function[1]).
- The underlying connectivity function, $F(\hat{f})$, is assumed to be spatially isotropic.
- The various electrical pathways across the network are nominally treated as having identical pathlength, even though we know this to be not strictly true.
- Current chooses pathways of least resistance.
- All $1\cap\ldots\cap j$ pathways (pathways including each of the species 1 through j) are uniformly conductive, which allows the solution to be expressed in terms of series, rather than integrals.
- If two species in a mixed-cell possess identical conductivity, they are nonetheless treated distinctly, rather than combined as a single pseudo-species (see the discussion of conductive uniformity in the Appendix).
- In a matrix of high-conductivity material, a pathway containing a small fraction of low-conductivity inclusion will never take conductive preference over a pathway with a larger fraction of moderately conductive material (see the discussion of conductive inversion in the Appendix).

The model, under these assumptions, constitutes a set of four algebraic equations (Eqs. 4–7), used to estimate the net conductivity of the mixed cell. In these equations, properties of the species within the mixed cell are weighted and summed to achieve the net result. The model is formulated to simultaneously exhibit properties of both series (multi-material pathways) and parallel circuits (different pathways for different material combinations).

The behavior of the model is in accordance with expectations, in that it limits to the proper values with expected slopes as material concentrations vary; monotonically varies with material concentrations; and follows the behavior of the $F(\hat{f})$ function for the case of a two-species mixture, in which one of the species approaches the behavior of a perfect insulator. It is the author's hope that the model may provide some utility for computational methods requiring the calculation of electrical conductivity in mixed computational cells.

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Appendix. Conductive Uniformity and Inversions

A.1 Conductive Uniformity

By conductive uniformity, we refer to the situation where two species in a mixed cell share the same value of conductivity. For discussion, let us say that species 2 and 3 in a mixed cell share a common conductivity, even though they may be different materials. Logically, this would indicate that, after species-1 pathways, the next most preferable should really be $1\cap(2\cup3)$ pathways rather than separate $1\cap2$ or $1\cap3$ pathways.

Because the method adopted forces the consideration of separate $1\cap2$ and $1\cap3$ pathways, the answer will differ from that in which species 2 and 3 act in concert. Consider an example containing four species, in which species 2 and 3 share the same conductivity, as shown in Table A-1.

Table A-1 Example mixed cell to demonstrate the effect of conductive uniformity

i	v_i	κ_i
1	0.4	1.0
2	0.3	0.8
3	0.1	0.8
4	0.2	0.1

versus

i	v_i	κ_i
1	0.4	1.0
$2\cup3$	0.4	0.8
4	0.2	0.1

The report proposes an algorithm in which the conductively uniform species are treated separately, as shown in Table A-2. By comparison, one could argue that the proper way to treat the situation is to treat the conductively uniform species as a joint species, such as that shown in Table A-3.

Table A-2 Net conductivity using the proposed algorithm, in the presence of a conductively uniform species

j	$\sum_{i=1}^{j} v_i$	$F_{1\cup\cdots\cup j}$ Eq. 6	$F_{1\cap\cdots\cap j}$ Eq. 5	$\kappa_{1\cap\cdots\cap j}$ Eq. 4	$\kappa_{1\cup\cdots\cup j}$ Eq. 7
1	0.40000	0.02345	0.02345	1.00000	0.02345
2	0.70000	0.72258	0.69913	0.90323	0.65493
3	0.80000	0.91198	0.18940	0.88889	0.82328
4	1.00000	1.00000	0.08802	0.34483	$\boxed{0.85363}$

Table A-3 Net conductivity when conductively uniform species (2 and 3) combine pathways

j	$\sum_{i=1}^{j} v_i$	$F_{1\cup\cdots\cup j}$ Eq. 6	$F_{1\cap\cdots\cap j}$ Eq. 5	$\kappa_{1\cap\cdots\cap j}$ Eq. 4	$\kappa_{1\cup\cdots\cup j}$ Eq. 7
1	0.40000	0.02345	0.02345	1.00000	0.02345
$2\cup3$	0.80000	0.91198	0.88853	0.88889	0.81326
4	1.00000	1.00000	0.08802	0.34483	$\boxed{0.84361}$

The right-most column, labeled $\kappa_{1\cup\cdots\cup j}$, associated with Eq. 7, represents the partial accumulations of conductivity from each of the different pathways, culminating in the total conductivity, boxed in the final row entry. Most of the conductivity is accumulated from the pathway whose $\sum v_i$ passes the conductivity threshold of Fig. 1 (approximately, $\sum v_i = 0.65$). As can be seen from Tables A-2 and A-3, the net conductivity using the two different approaches gave the nearly identical results of 0.85 and 0.84, respectively. This result is supportive toward a claim of suitability for the approach proposed in the report.

A.2 Conductive Inversions

The method proposed in this report orders n viable pathways of electrical conduction, denoted as 1, $1\cap 2$, ..., $1\cap\cdots\cap n$, containing n species that have been pre-ordered from highest to lowest conductivity. This will result in pathways that are also ordered from most to least conductive (which is the goal). However, if one considers pathways composed of all *possible* species combinations (of which there are $2^n - 1$, rather than the n employed by the proposed method), there can arise situations in which a conductively preferable pathway is not chosen by the proposed method. We refer to these unexpectedly preferable pathways as "conductive inversions".

Consider, for example, the mixed-cell distribution described in Table A-4. While the individual species, 1–4, are numbered in order of decreasing conductivity, we can show that, because of the low volume fraction of species 3, the $1\cap 3$ pathway will actually be conductively preferable to the $1\cap 2$ pathway. This "inversion" is ignored by the proposed method of this report. Yet, we wish to understand the extent of the difference when accounting for versus ignoring the inversion in the calculation of electrical conductivity.

Table A-4 Example mixed cell to demonstrate the effect of conductive inversion

i	v_i	κ_i
1	0.4	1.00
2	0.3	0.80
3	0.1	0.75
4	0.2	0.10

If we use the approach proposed in this report, we ignore the inversion and calculate the cell's net conductivity using Eqs. 4–7. The result of that approach is shown in Table A-5. The predicted conductivity of the mixed cell, using the proposed method, is 0.852.

Table A-5 Net conductivity using the present algorithm, which ignores the presence of conductive inversion

j	$\sum_{i=1}^{j} v_i$	$F_{1\cup\cdots\cup j}$ Eq. 6	$F_{1\cap\cdots\cap j}$ Eq. 5	$\kappa_{1\cap\cdots\cap j}$ Eq. 4	$\kappa_{1\cup\cdots\cup j}$ Eq. 7
1	0.40000	0.02345	0.02345	1.00000	0.02345
2	0.70000	0.72258	0.69913	0.90323	0.65493
3	0.80000	0.91198	0.18940	0.88073	0.82174
4	1.00000	1.00000	0.08802	0.34483	$\boxed{0.85200}$

On the other hand, if we wish to account for the inversion, a different procedure is required. We must first tabulate all $2^4 - 1 = 15$ pathway combinations and order them in rank of decreasing conductivity, as shown in Table A-6. Then, a number of pathways can be excluded on the basis that the species that compose them would instead be incorporated into more conductive (preferred) alternatives. For example, species 2 is subsumed into $1\cap 2$ pathways, rather than simple species-2 pathways. Likewise, $2\cap 3$ pathways are preferentially incorporated as $1\cap 2\cap 3$ pathways.

Table A-6 Net conductivity accounting for the presence of conductive inversion

$\{J\}$	$\sum_{i\in J} v_i$	$F_{\cup J}$	$F_{\cap J}$	$\kappa_{\cap J}$	$\kappa_{\cup J}$
1	0.40000	0.02345	0.02345	1.00000	0.02345
Inversion→ 1,3	0.50000	0.12720	0.10375	0.93750	0.12072
1,2	0.70000	0.72258	0.69913	0.90323	0.75219
1,2,3	0.80000	0.91198	0.08565	0.88073	0.82763
2	0.30000	0.00162	—	0.80000	12 preferred
2,3	0.40000	0.02345	—	0.78689	123 preferred
3	0.10000	0.00000	—	0.75000	123 preferred
1,2,3,4	1.00000	1.00000	0.08802	0.34384	$\boxed{0.85789}$
1,2,4	0.90000	0.98612	—	0.32432	1234 preferred
1,3,4	0.70000	0.72258	—	0.27632	1234 preferred
1,4	0.60000	0.40098	—	0.25000	1234 preferred
2,3,4	0.60000	0.40098	—	0.23920	1234 preferred
2,4	0.50000	0.12720	—	0.21053	1234 preferred
3,4	0.30000	0.00162	—	0.14063	1234 preferred
4	0.20000	0.00000	—	0.10000	1234 preferred

Once these exclusions are made, the ordered set of pathways that remain are the conductive pathways that constitute the mixed cell. In our example, there is a $1\cap3$ inversion with a higher conductivity than either $1\cap2$ or $1\cap2\cap3$ pathways. Any percentage of paths arising for the $1\cap3$ inversion ($F_{1\cap3}$) are essentially borrowed from the available reservoir of $1\cup2\cup3$ paths. Thus, in comparison to Table A-5, the fraction of $1\cap2\cap3$ paths (0.18940) is diminished by the value of $1\cap3$ inversions (0.10375), leaving only a fraction of 0.08802 $1\cap2\cap3$ pathways in the allocation of Table A-6.

Despite the presence of this inversion, the net result on the calculated conductivity, when accounting for the inversion, is quite small, raising the conductivity from 0.852 to only 0.858. This result is, again, supportive toward a claim of suitability for the approach proposed in the report.

A proper resolution would involve integrations in v, rather than summations in v_i, in Eqs. 4–7. It would follow along the lines of

$$\kappa_{\cup} = \int_0^1 \kappa_{\cap}\, dF = \int_0^1 \kappa_{\cap}(v)\, \frac{dF}{dv}\, dv \quad .$$

However, such an approach would defeat the simplicity required to achieve an algebraic mixed-cell conductivity model. The result is that we are forced to accept some approximation brought about by assuming pathway uniformity (*e.g.*, wherein we assume that all $1\cap\ldots\cap j$ pathways are uniformly conductive, in the manner of Eq. 4).

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