



ARL-TR-8899 • JAN 2020



On the Electrical Connectivity of a 2-D, Randomly Distributed, Two-Component (Conducting/Insulating) Mixture

by Steven B Segletes

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by Steven B Segletes

Weapons and Materials Research Directorate, CCDC Army Research Laboratory

REPORT DOCUMENTATION PAGE				Form Approved OMB No. 0704-0188	
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1. REPORT DATE (DD-MM-YYYY) January 2020		2. REPORT TYPE Technical Report		3. DATES COVERED (From - To) October 2014–November 2014	
4. TITLE AND SUBTITLE On the Electrical Connectivity of a 2-D, Randomly Distributed, Two-Component (Conducting/Insulating) Mixture				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S) Steven B Segletes				5d. PROJECT NUMBER AH80	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) US Army Combat Capabilities Development Command Army Research Laboratory ATTN: FCDD-RLW-PC Aberdeen Proving Ground, MD 21005-5066				8. PERFORMING ORGANIZATION REPORT NUMBER ARL-TR-8899	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)				10. SPONSOR/MONITOR'S ACRONYM(S)	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution is unlimited.					
13. SUPPLEMENTARY NOTES primary author's email: <steven.b.segletes.civ@mail.mil>.					
14. ABSTRACT The connectivity of $n \times n$ networks are studied as an analogy to two-component mixed cells, comprising conducting and insulating components. The statistical realizations of the network and their probabilities are enumerated and tabulated in an effort to determine the manner in which the probability of individual-linkage connectivity affects the overall likelihood of network connectivity. Two methods are examined, one in which the local conduction probability of each individual linkage in the network is fixed, and a second in which the global fraction of conducting linkages in the network is constrained. The results indicate a threshold behavior, in which the probability (or global fraction) of conducting links, once reaching the threshold, are sufficient to trigger a high likelihood of connectivity across the network. As an aside, an approximate analytical approach is also shown, which becomes possible if restrictions are placed on the topology of the connecting pathway across the network.					
15. SUBJECT TERMS mixed-cell, network, connectivity, insulator, conductor					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT UU	18. NUMBER OF PAGES 48	19a. NAME OF RESPONSIBLE PERSON Steven B Segletes
a. REPORT Unclassified	b. ABSTRACT Unclassified	c. THIS PAGE Unclassified			19b. TELEPHONE NUMBER (Include area code) 410-278-6010

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Acknowledgments

I wish to sincerely thank my colleague of many years, Dr Misha Grinfeld, for drawing my attention to the metaphorical similarity between the problems of electrical and network connectivity. I further thank him for his technical review of this report. I am also indebted to Ms Carol Johnson, my editor, who has again applied her skills with diligence to improve the quality of this report.

1. Introduction

The problem of determining the electrical *conductivity* of a computational “mixed cell” is a challenging one under any circumstance, though the problem of averaging properties across heterogeneous media is a well-studied one.¹ One aspect of the mixed-cell problem that continues to vex modelers is knowing the morphology of the constituents within the mixed cell. By morphology I mean the spatial distribution and granularity of the constituents. This is especially relevant to the problem of electrical conductivity, as circuits with insulators connected in serial versus parallel configurations exhibit vastly different conductivity.

In general, based on the understanding of cell resolution, the spatial distribution of material within a mixed cell is unknown. In some treatments, for example, with the BLINT algorithm in CTH,² a heterogeneous spatial distribution of material within a mixed cell is assumed, based on the constituent fractions found in adjacent cells. In general, however, assuming a random distribution of material within the mixed cell is the norm.

The challenge becomes even more critical, yet more direct, when one mixed-cell component is a perfect insulator (*e.g.*, void). It is more critical because the net mixed-cell conductivity drops completely to zero at the point where the conducting component(s) of material cannot establish a route of connectivity across the cell. However, the problem is also more direct, in that, to begin with, one can focus on the issue of *connectivity* rather than *conductivity*.

With that perspective, we examine the issue of electrical *connectivity* across a randomly distributed two-component mixture, in which one of the components is a perfect insulator. This report does *not* propose a computational approach to addressing the larger problem of mixed-cell conductivity. Rather, it presents some relevant ideas and examines their implications in the context of assessing the probability of electrical *connectivity* between two arbitrary points on opposite boundaries of a two-dimensional (2-D), two-component mixture.

2. Granularity

In addition to the distribution of the mixed-cell components within the cell volume, which we assume as randomly distributed, another significant factor to consider is the component granularity. That is to say, the physical size of the individual material

fragments within the cell, relative to the overall cell size. The finer the granularity, the more potential pathways there exist across the cell through which connectivity can be established.

To consider this concept of granularity, we choose to model the material system within a mixed cell as a 2-D Cartesian network of nodes, connected by horizontal and vertical links to the nearest neighbors (examples shown in Fig. 1). The nodes represent fixed connectivity-monitoring stations within the cell, and the dashed links represent an abstraction of the physical material that lies between the monitoring stations. This abstraction allows us to convert the physical reality of material-component fragments within the cell into a 2-D network, with which we hope to study the electrical connectivity between opposing nodes O and X .

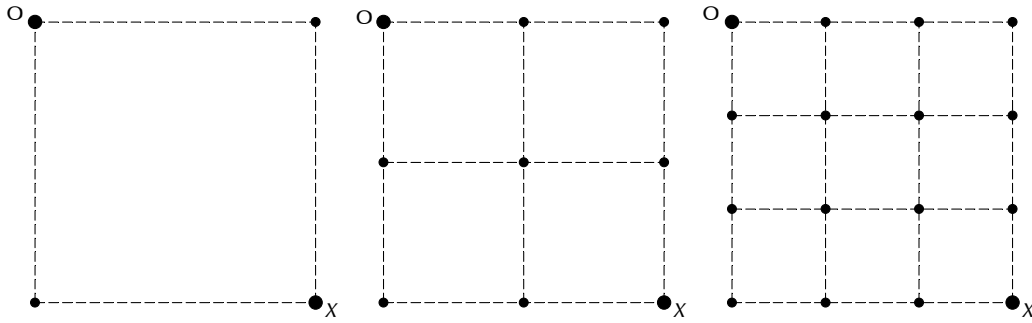


Fig. 1 Several sample representations of $n \times n$ mixed-cell granularity by way of a Cartesian nodal array (circle symbols) connected by linkages (dashed lines)

The examples provided in Fig. 1 are intended to be representative of the material granularity within the cell. However, they are in no way intended to be definitive. In the 4×4 sample array, for example, there are 24 linkages connecting the 16 nodal stations, which would indicate that each link represents approximately $1/24$ of the cell's total volume, thus providing a representation of the fragment size of the material within the cell. In contrast, each of the 12 linkages in the 3×3 net represent approximately $1/12$ of the cell's total volume.

3. Material Components

It has already been indicated that the linkages in Fig. 1 are abstract representations of the material in the mixed cell. For simplicity in this introductory report, we limit our consideration to a two-component system, in which one of the components is an electrical insulator (such as void), while the other component is a simple conductor.

A key point of understanding is that a given linkage may be composed of *either* conductor material *or* insulator material, but not both (*i.e.*, the network linkage represents the smallest indivisible quantity of material).

There are several ways to go about probabilistically assessing whether a given linkage embodies conductive or insulating material. Those methods are introduced later—at this point, one need merely comprehend that each linkage embodies exactly one of the material constituents in the mixed cell (either conductor or insulator, according to our presently considered situation).

In this way, an analysis into the probability of electrical *connectivity* between nodes O and X is an indicator of whether the *conductivity* across the cell is likely to be zero or some value on the order of the conductor’s intrinsic value. An inference of the actual nonzero *conductivity* magnitude, based on the specifics of the connectivity, is not addressed in this introductory report, which limits itself to studying the *connectivity* of the network that abstractly represents the morphological conditions within the mixed cell.

4. Network Permutations (2×2 Example)

The netc program was written (in C, see Appendix A) to methodically explore all the permutations that a given network can exhibit. Since a given network linkage contains either the conductor (1) or the insulator (0), each realization of the network can be identified by a binary number consisting of one digit for each of the network’s linkages.

For example, consider the 2×2 matrix shown in Fig. 2, in which network nodes are numbered in **black** and network linkages are numbered in **red**. The binary identifier 1011 will identify the realization of the network in which linkages 0, 2, and 3 contain the conductor, and only linkage 1 contains the (“broken-link”) insulator.* We may deduce that such a 4-link network has a total of 16 realizations. In general, the number of realizations, N , is expressed as

$$N = 2^n \quad , \quad (1)$$

where n is the number of links in the network (in our example, $n = 4$). The netc

*We refer to insulator links as “broken” because they break the path of conductivity.

program explores each of these realizations, in search of connectivity between opposing nodes, here designated with numerals 0 and 3.

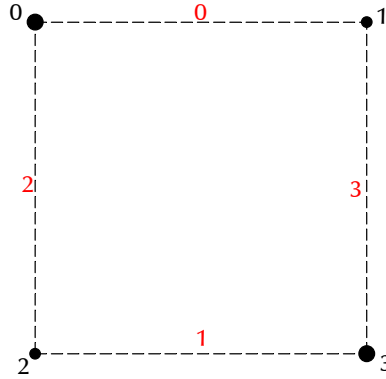


Fig. 2 A 2x2 network in which nodes and linkages have been assigned unique identification, node numbers in black and linkage numbers in red

In some realizations, such as 1010 (conductor at linkages 0 and 2), no conductive paths connect nodes 0 to 3. In other realizations, such as 0110, exactly one conductive pathway, node path 0-2-3, by way of links 2 and 1, will present itself. Finally, some realizations will exist that present more than one conductive pathway from node 0 to 3, namely, realization 1111, in which all linkages are populated with conducting material. There, both node pathways 0-1-3 as well as 0-2-3 provide connectivity between nodes 0 and 3.

Because the realization space is so limited, we present it in full in Table 1. We can then aggregate the data found in Table 1 by grouping those realizations that share a common number, k , of broken links. Such an aggregation is found in Table 2. We denote the total number of realizations possessing k broken links as N_k . The number of realizations that, with k broken links, retain electrical connectivity between nodes O and X , we denote C_k .

Table 1 Realization space for the 2×2 network

Realization	Link status	Broken links	Pathways found	Nodal path(s)
0	0000	4	0	
1	1000	3	0	
2	0100	3	0	
3	1100	2	0	
4	0010	3	0	
5	1010	2	0	
6	0110	2	1	0-2-3
7	1110	1	1	0-2-3
8	0001	3	0	
9	1001	2	1	0-1-3
10	0101	2	0	
11	1101	1	1	0-1-3
12	0011	2	0	
13	1011	1	1	0-1-3
14	0111	1	1	0-2-3
15	1111	0	2	0-1-3, 0-2-3

This topology has four nodes and four links, giving $2^4 = 16$ realizations.
We note that 43.75% or 7/16 realizations provide connectivity.

Table 2 Aggregated realization space for the 2×2 network

Broken links k	Connected realizations / Realizations C_k / N_k	Connectivity rate (%)
0	1 / 1	100
1	4 / 4	100
2	2 / 6	33.3
3	0 / 4	0
4	0 / 1	0
0-4	7 / 16	43.8

5. Statistical Analysis of Permutations

The goal here is to statistically analyze the probability, over all possible realizations, that connectivity will be maintained in the given network, as a function of the broken (insulating) links that are introduced. There are a number of ways in which the permutations of a given network may be analyzed to this end, two of which we pursue in this report.

One technique is to assign a *local* conduction probability, f , that any given (indistinguishable) linkage in the network will be a conductor. The other technique is to actually constrain the *global* fraction, \hat{f} , of the conducting linkages in the network, to an assigned value. Let us not forget that these networks we consider are being used as analogs for a two-component mixed cell, in which one of the components is a conductor and the other an insulator.

With either technique, let us infer something about the relationship of the network-conduction local/global parameter (f or \hat{f}) to the void fraction of the analogous mixed computational cell, since a material void is insulating in its nature. The total fraction of conducting material in a mixed cell is precisely represented by the global conducting fraction \hat{f} . If the total fraction of conducting material is \hat{f} , then the volume fraction of the insulating (*e.g.*, void) material is $1 - \hat{f}$.

In a similar fashion, if f , rather than \hat{f} , is our independent variable, it implies that the probability of finding conductor material at any arbitrary link in the net equals f . Correspondingly, if the void fraction of the analogous mixed cell were $1 - f$, the probability of finding *randomly distributed* conducting material at any given location in the cell would also be f .

This correspondence of \hat{f} (or f) to the mixed cell's solid fraction is drawn so that we may understand the connection between studying these hypothetical Cartesian networks and the problem of mixed-cell connectivity. Our task is to predict the probability of network connectivity, F , as a function of f or \hat{f} , whichever is given. What we find is that the relationship is highly nonlinear and reminiscent of a threshold in which the likelihood of network connectivity remains suppressed until such time that f (or \hat{f}) rises above a threshold level. This observation is reminiscent of the phenomena known as order-disorder transitions.³

5.1 $F(f)$: Connectivity as a Function of *Local* Conduction Probability

In this first approach, we do not reject the possibility of any network realization—all realizations are possible. However, the likelihood of any particular realization will vary with the probability, f , that any given (indistinguishable) link is conducting.

For a network with n links, the probability $P(k, f)$ that, for any given realization, exactly k out of the n links will be “broken” (insulating), may be given as

$$P(k, f) = f^{n-k}(1 - f)^k \quad . \quad (2)$$

In comparison, the random likelihood* that any given realization will manifest is $1/N$. Thus, $P(k, f)$ can be expressed relative to the random draw as

$$P_{\text{rel}}(k, f) = \frac{P(k, f)}{1/N} = N f^{n-k}(1 - f)^k \quad . \quad (3)$$

Equation 3 represents the normalized weight of likelihood that attaches to a realization with k broken links, for a given value of local conduction probability, f . One can understand this better, using the 2×2 network example, by examining values of $P_{\text{rel}}(k, f)$ in Table 3.

Table 3 For the 2×2 network, relative likelihood of k broken links in network, given local conduction probabilities of 0.1, 0.3, 0.5, 0.7, and 0.9, respectively

k	$P_{\text{rel}}(k, 0.1)$	$P_{\text{rel}}(k, 0.3)$	$P_{\text{rel}}(k, 0.5)$	$P_{\text{rel}}(k, 0.7)$	$P_{\text{rel}}(k, 0.9)$
0	0.002	0.130	1.000	3.842	10.498
1	0.014	0.302	1.000	1.646	1.166
2	0.130	0.706	1.000	0.706	0.130
3	1.166	1.646	1.000	0.302	0.014
4	10.498	3.842	1.000	0.130	0.002

When the single-link conduction probability is small (*e.g.*, $f = 0.1$), broken links are more likely. Thus, a single realization that has four broken links is 10.498 times more likely than the random case in which all realizations have equal likelihood. Correspondingly, in that case, the likelihood of manifesting a particular realization with only one of four links broken is quite low: 0.014 times as likely as the random case.

*By random likelihood, we mean the likelihood of a given realization with no consideration given to the value of f . That is to say, the likelihood if all realizations were equally probable, which is simply given as $1/N$, the inverse of the number of realizations.

As the local conduction probability rises to 0.5, all realizations have equal probability of occurrence. Again, as f rises above 0.5, the P_{rel} values favor the realizations having fewer numbers of broken links.

We now have all the information needed to reach our goal of assessing the probability, F , of establishing connectivity, as a function of local conduction probability, f . Each realization that exhibits connectivity must have summed its particular probability of occurring, $P(k, f)$:

$$F(f) = \sum_{k=0}^n C_k P(k, f) = \sum_{k=0}^n \frac{C_k}{N} \cdot P_{\text{rel}}(k, f) \quad . \quad (4)$$

For the 2×2 case that has been used as our example, all the information to calculate $F(f)$ is available in Tables 2 and 3. The result of applying Eq. 4 is tabulated in Table 4. Note that, because of the simplicity of the 2×2 network, without any crosslinks, the function F may be, likewise, calculated analytically as $F(f) = 2f^2 - f^4$.

Table 4 For the 2×2 network, the probability of network connectivity, F , as a function of the local conduction probability, f

f	$F(f)$
0.0	0.000
0.1	0.020
0.3	0.172
0.5	0.438
0.7	0.740
0.9	0.964
1.0	1.000

5.2 $F(\hat{f})$: Connectivity as a Function of *Global* Conducting Fraction

With this second approach, the process is considerably simplified relative to that described in Section 5.1. However, it is also more limited in scope, for the reason that the global conducting fraction, \hat{f} , can only take on certain discrete values.

The independent variable \hat{f} signifies the global fraction of linkages in the network that are conducting. Since the number of linkages is finite and the number of con-

ducting linkages is integral, the possible values of \hat{f} are limited to

$$\hat{f} = \frac{n - k}{n} \quad (n \text{ integer, } k = 0, 1, \dots, n) \quad , \quad (5)$$

where k is the number of broken (insulating) links in the network of n links. Thus, there are only $n + 1$ possible values of \hat{f} , evenly distributed between $\hat{f} = 0$ and $\hat{f} = 1$, inclusive. For small n , this can seem quite limiting.

With this approach, realizations that do not comport to the selected value of \hat{f} (*i.e.*, the selected value of k) are excluded from consideration. Thus the result can be very simply expressed as

$$F(\hat{f}) = \frac{C_k}{N_k} \quad , \quad (6)$$

given as the last column of Table 2 directly and repeated again in Table 5.

Table 5 For the 2×2 network, the probability of network connectivity, F , as a function of the global conducting fraction, \hat{f}

\hat{f}	$F(\hat{f})$
0.00	0.000
0.25	0.000
0.50	0.333
0.75	1.000
1.00	1.000

5.3 Example: 2×2 Nodal Grid

The 2×2 case was used illustratively in Sections 5.1 and 5.2 of this report. The schematic was given in Fig. 2, while tabulated results of the aggregation of permutations were presented in Tables 2–5. We can use those results to present graphically in Fig. 3 the probability of network connectivity as a function of either the local conductivity probability, f , or the global conducting fraction, \hat{f} .

We see that $F(f)$ begins to take on an “S”-shaped aspect. The $F(\hat{f})$ result shows a steeper transition from insulating ($F = 0$) to conducting ($F = 1$). However, the dearth of valid domain points, brought about by the small number of links in the mesh, is quite apparent.

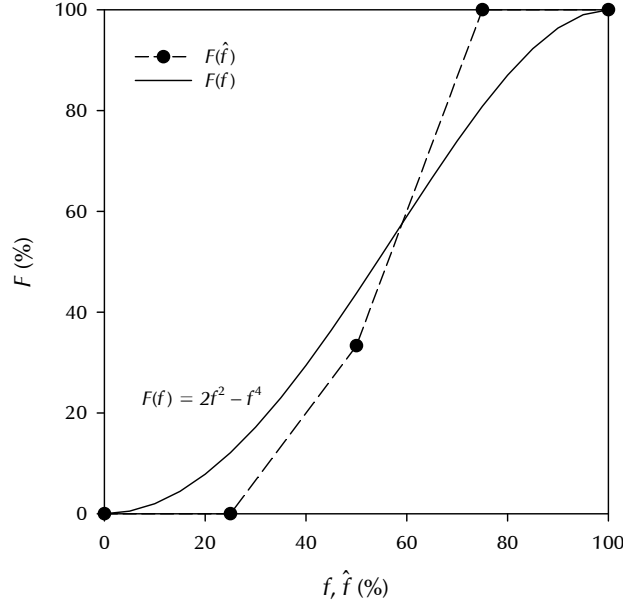


Fig. 3 For the 2×2 network, the probability of network connectivity, F , with either f or \hat{f} as the independent variable

5.4 Example: 3×3 Nodal Grid

In the 3×3 grid, there are 9 nodal points and 12 linkages, as seen in the schematic of Fig. 4. With $n = 12$ linkages, the number of realizations involving conducting and insulating link combinations is $N = 2^{12} = 4096$. In addition, for every one of these 4096 realizations, the netc program must search out each of the many pathways for connecting node 0 to node 8. For the 3×3 grid, netc determines that there are 12 unique pathways for traversing from node 0 to 8 (6 paths involving 5 nodes, 4 paths involving 7 nodes, and 2 paths involving all 9 nodes).

The raw data are too voluminous to tabulate in the space of this report, so instead, we jump to the aggregated data found in Table 6. Because four links are the minimum to achieve connectivity in the 3×3 grid, any realizations with fewer than four conducting links will always fail to connect.

As the enabler for calculating $F(f)$, we need to calculate the values of P_{rel} for various numbers of broken links (k) and local conduction probability (f). Since the number of links, n , is larger than for the 2×2 case, the enumeration in Table 7 is, likewise, longer. Because P_{rel} is based on fractions to the power n , the relative likelihoods take on more extreme values, than in the 2×2 case. The values showing

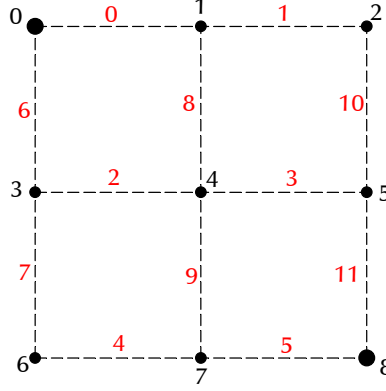


Fig. 4 A 3×3 network in which nodes and linkages have been assigned unique identification, node numbers in black and linkage numbers in red

in the table as 0.000 are, in fact, very small positive numbers with large negative exponents. They are presented in truncated decimal form merely to emphasize the relative weights placed on realizations for differing values of k . They are not truncated by the netc program (except to the limit of machine precision).

The content of Tables 6 and 7 may be used in accordance with Eq. 4 to calculate $F(f)$. Those results are presented in Table 8, for a number of specified values of f .

The alternative to specifying the local-conduction probability f is to specify the global conducting fraction, \hat{f} . The data for this $F(\hat{f})$ probability are generated in accordance with Eq. 6, come from the right-hand column of Table 6 and are represented again in Table 9. Recall that \hat{f} is not a continuous domain, but evenly spaced across $n + 1$ values in the range 0 to 1, according to Eq. 5.

The results of Tables 8 and 9 are presented graphically in Fig. 5. The “S”-shaped character of the probability distribution is more distinct as compared to Fig. 5. We further see that the $F(\hat{f})$ result, while still valid only over the discrete domain indicated by circles in the figure, is also developing into a steep “S”-shaped curve. These curves represent the probability F that network connectivity is achieved.

Table 6 Aggregated realization space for the 3×3 network

Broken links k	Connected realizations C_k / N_k	Realizations	Connectivity rate (%)
0	1 / 1		100
1	12 / 12		100
2	64 / 66		97.0
3	192 / 220		87.3
4	334 / 495		67.5
5	312 / 792		39.4
6	166 / 924		18.0
7	48 / 792		6.1
8	6 / 495		1.2
9	0 / 220		0
10	0 / 66		0
11	0 / 12		0
12	0 / 1		0
0–12	1135 / 4096		27.7

Table 7 For the 3×3 network, relative likelihood of k broken links in network, given local conduction probabilities of 0.1, 0.3, 0.5, 0.7, and 0.9, respectively

k	$P_{\text{rel}}(k, 0.1)$	$P_{\text{rel}}(k, 0.3)$	$P_{\text{rel}}(k, 0.5)$	$P_{\text{rel}}(k, 0.7)$	$P_{\text{rel}}(k, 0.9)$
0	0.000	0.002	1.000	56.694	1156.831
1	0.000	0.005	1.000	24.297	128.537
2	0.000	0.012	1.000	10.413	14.282
3	0.000	0.028	1.000	4.463	1.587
4	0.000	0.065	1.000	1.913	0.176
5	0.000	0.151	1.000	0.820	0.020
6	0.002	0.351	1.000	0.351	0.002
7	0.020	0.820	1.000	0.151	0.000
8	0.176	1.913	1.000	0.065	0.000
9	1.587	4.463	1.000	0.028	0.000
10	14.282	10.413	1.000	0.012	0.000
11	128.537	24.297	1.000	0.005	0.000
12	1156.831	56.564	1.000	0.002	0.000

Table 8 For the 3×3 network, the probability of network connectivity, F , as a function of the local conduction probability, f

f	$F(f)$
0.0	0.000
0.1	0.001
0.3	0.045
0.5	0.277
0.7	0.691
0.9	0.973
1.0	1.000

Table 9 For the 3×3 network, the probability of network connectivity, F , as a function of the global conducting fraction, \hat{f}

\hat{f}	$F(\hat{f})$
0.000	0.000
0.083	0.000
0.167	0.000
0.250	0.000
0.333	0.012
0.417	0.066
0.500	0.180
0.583	0.394
0.667	0.675
0.750	0.873
0.833	0.970
0.917	1.000
1.000	1.000

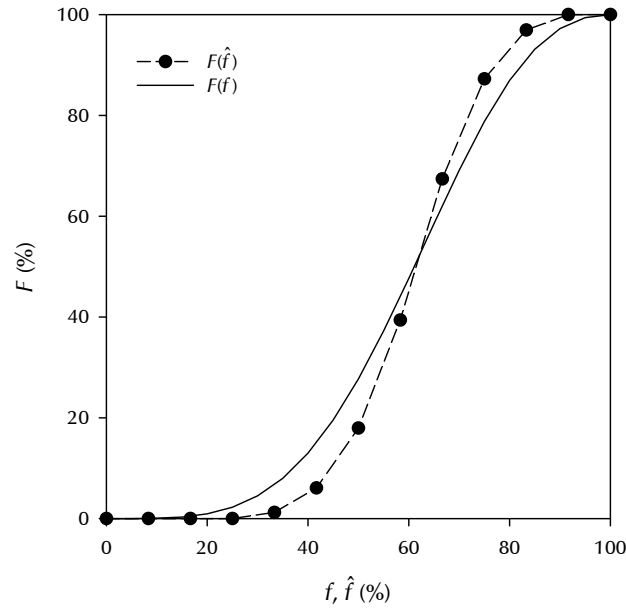


Fig. 5 For the 3×3 network, the probability of network connectivity, F , with either f or \hat{f} as the independent variable

5.5 Example: 4×4 Nodal Grid

In the 4×4 grid, there are 16 nodal points and 24 linkages, as seen in the schematic of Fig. 6. With $n = 24$ linkages, the number of realizations involving conducting and insulating link combinations is $N = 2^{24} = 16,777,216$. In addition, for every one of these nearly 17 million realizations, the netc program must search out each of the many pathways for connecting node 0 to node 15. For the 4×4 grid, netc determines that there are 184 unique pathways for traversing from node 0 to 15 (ranging from 7- to 15-node paths).

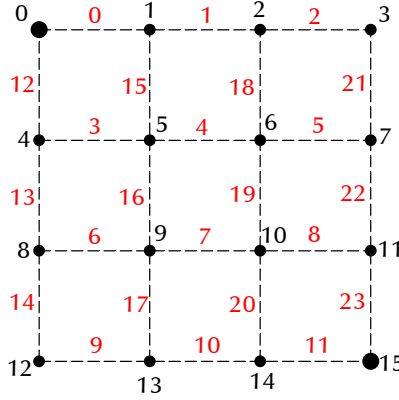


Fig. 6 A 4×4 network in which nodes and linkages have been assigned unique identification, node numbers in black and linkage numbers in red

The raw data are far too voluminous to tabulate in the space of this report, so instead, we jump to the aggregated data found in Table 10. Because six links are the minimum to achieve connectivity in the 4×4 grid, any realizations with fewer than six conducting links will always fail to connect.

As the enabler for calculating $F(f)$, we need to calculate the values of P_{rel} for various numbers of broken links (k) and local conduction probability (f). Since the number of links, n , is larger than for the 3×3 case, the enumeration in Table 11 is, likewise, longer than that presented in Table 7. Because P_{rel} is based on fractions to the power n , the relative likelihoods take on more extreme values, than those found in the 3×3 case. The values showing in the table as 0.000 are, in fact, very small positive numbers with large negative exponents. The netc program, unlike the table, does not truncate their values (below machine resolution) when using them in calculations. The tabulated results are left in decimal form to emphasize the relative magnitude of weight placed on realizations with differing numbers of broken links.

Table 10 Aggregated realization space for the 4×4 network

Broken links k	Connected realizations / Realizations C_k / N_k	Connectivity rate (%)
0	1 / 1	100
1	24 / 24	100
2	274 / 276	99.3
3	1976 / 2024	97.6
4	10071 / 10626	94.8
5	38392 / 42504	90.3
6	112742 / 134596	83.8
7	258144 / 346104	74.6
8	460680 / 735471	62.6
9	635632 / 1307504	48.6
10	672928 / 1961256	34.3
11	547944 / 2496144	22.0
12	344033 / 2704156	12.7
13	165956 / 2496144	6.7
14	60670 / 1961256	3.1
15	16332 / 1307504	1.3
16	3066 / 735471	0.4
17	360 / 346104	0.1
18	20 / 134596	≈0
19	0 / 42504	0
20	0 / 10626	0
21	0 / 2024	0
22	0 / 276	0
23	0 / 24	0
24	0 / 1	0
0–24	3329245 / 16777216	19.8

The content of Tables 10 and 11 may be used in accordance with Eq. 4 to calculate $F(f)$. Those results are presented in Table 12, for a number of specified values of f .

The alternative to specifying the local-conduction probability f is to specify the global conducting fraction, \hat{f} . The data for this $F(\hat{f})$ probability are generated in accordance with Eq. 6, come from the right-hand column of Table 10, and are represented again in Table 13. Recall that \hat{f} is not a continuous domain, but evenly spaced across $n + 1$ values in the range 0 to 1, according to Eq. 5.

Table 11 For the 4×4 network, relative likelihood of k broken links in network, given local conduction probabilities of 0.1, 0.3, 0.5, 0.7, and 0.9, respectively

k	$P_{\text{rel}}(k, 0.1)$	$P_{\text{rel}}(k, 0.3)$	$P_{\text{rel}}(k, 0.5)$	$P_{\text{rel}}(k, 0.7)$	$P_{\text{rel}}(k, 0.9)$
0	0.000	0.000	1.000	3214.200	1338258.845
1	0.000	0.000	1.000	1377.514	148695.427
2	0.000	0.000	1.000	590.363	16521.714
3	0.000	0.000	1.000	253.013	1835.746
4	0.000	0.000	1.000	108.434	203.972
5	0.000	0.000	1.000	46.472	22.664
6	0.000	0.001	1.000	19.916	2.518
7	0.000	0.002	1.000	8.536	0.280
8	0.000	0.004	1.000	3.658	0.031
9	0.000	0.010	1.000	1.568	0.003
10	0.000	0.023	1.000	0.672	0.000
11	0.000	0.053	1.000	0.288	0.000
12	0.000	0.123	1.000	0.123	0.000
13	0.000	0.288	1.000	0.053	0.000
14	0.000	0.672	1.000	0.023	0.000
15	0.003	1.568	1.000	0.010	0.000
16	0.031	3.658	1.000	0.004	0.000
17	0.280	8.536	1.000	0.002	0.000
18	2.518	19.916	1.000	0.001	0.000
19	22.664	46.472	1.000	0.000	0.000
20	203.972	108.434	1.000	0.000	0.000
21	1835.746	253.013	1.000	0.000	0.000
22	16521.714	590.363	1.000	0.000	0.000
23	148695.427	1377.514	1.000	0.000	0.000
24	1338258.845	3214.200	1.000	0.000	0.000

Table 12 For the 4×4 network, the probability of network connectivity, F , as a function of the local conduction probability, f

f	$F(f)$
0.0	0.000
0.1	0.000
0.3	0.013
0.5	0.198
0.7	0.678
0.9	0.975
1.0	1.000

Table 13 For the 4×4 network, the probability of network connectivity, F , as a function of the global conducting fraction, \hat{f}

\hat{f}	$F(\hat{f})$
0.000	0.000
0.042	0.000
0.083	0.000
0.125	0.000
0.167	0.000
0.208	0.000
0.250	≈0.000
0.292	0.001
0.333	0.004
0.375	0.013
0.417	0.031
0.458	0.067
0.500	0.127
0.542	0.220
0.583	0.343
0.625	0.486
0.667	0.626
0.708	0.746
0.750	0.838
0.792	0.903
0.833	0.948
0.875	0.976
0.917	0.993
0.958	1.000
1.000	1.000

The results of Tables 12 and 13 are presented graphically in Fig. 7. The “S”-shaped character of the probability distribution is much more distinct, even as compared to that in Fig. 5. We further see that the $F(\hat{f})$ result, while still valid only over the discrete domain indicated by circles in the figure, is more fully developed into a steep “S”-shaped curve. Recall, these curves represent the probability F that network connectivity is achieved.

The next in the series, a 5×5 network, proved too computationally challenging to achieve. However, a slight variation on the 5×5 network, clipped at the corners in order to reduce the number of linkages, was accomplished. Because it was not a true $n \times n$ network, we relegate the results to Appendix B.

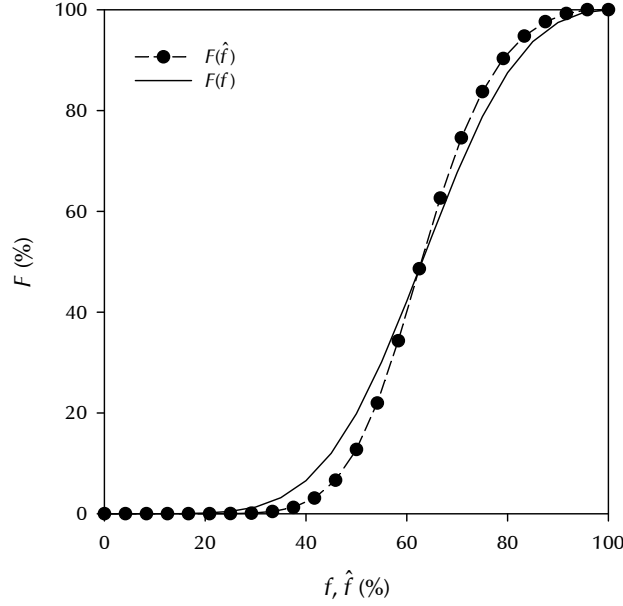


Fig. 7 For the 4×4 network, the probability of network connectivity, F , with either f or \hat{f} as the independent variable

6. Discussion

The results of this analysis are interesting from a variety of perspectives. First, as the granularity of the grid is increased, from 2×2 to 3×3 and then to 4×4 , the data more sharply transition from low F to high F , occurring over a smaller change in either f or \hat{f} . In addition, the domain of transition is shifting rightward, to higher values of both f and \hat{f} . This trend can be seen clearly in Fig. 8.

What is to be concluded by this sharp transition from low to high values of F ? Recall, these graphs represent the probability of network connectivity as a function of either the local conduction probability of each indistinguishable link in the network (f) or, alternately, as a function of the global fraction of links that are conducting (\hat{f}).

To the left side of the transition (low f or \hat{f}), the conclusion is that there is a very low likelihood of achieving network connectivity. Conversely, to the right side of the transition (high f or \hat{f}), the likelihood of connectivity is almost assured. Recall also that both f and, more directly, \hat{f} , represent analogies to the fraction of conducting material within a mixed computational cell (*i.e.*, the cell's void fraction corresponds to $1 - f$ or $1 - \hat{f}$).

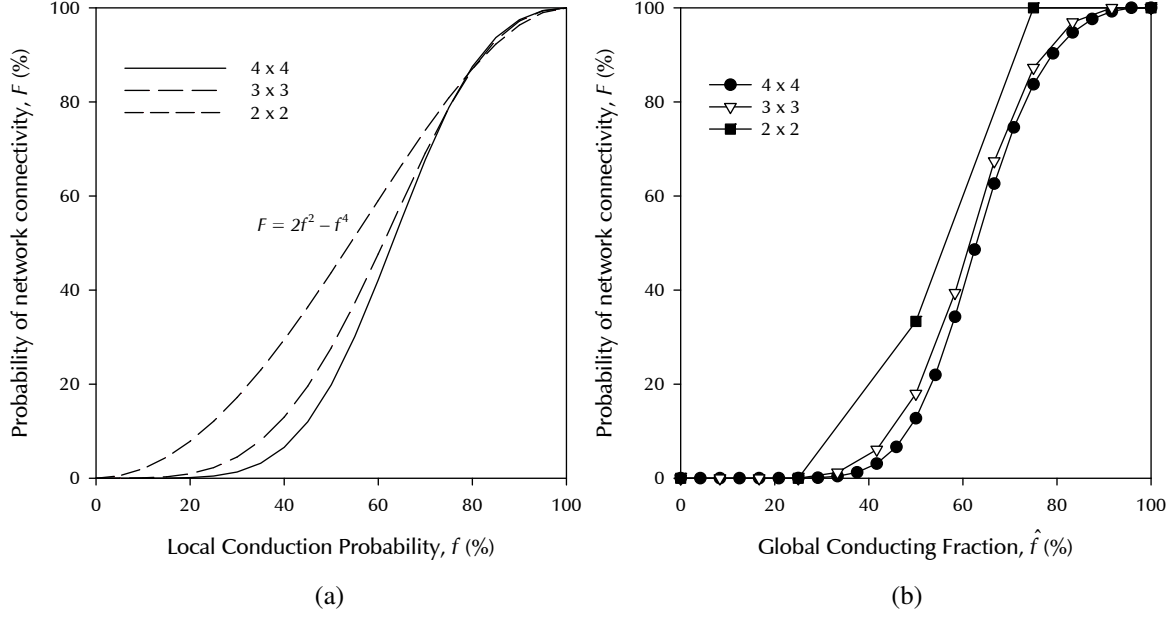


Fig. 8 For $n \times n$ networks, the probability of network connectivity as a function of either a) the local conduction probability or b) the global conducting fraction

The steep gradient represents a threshold—a fractional quantity of conducting material that is apparently required to bring the network into a highly probable conducting configuration. Too little conducting material results, not in a lower proportional conductivity, but in a high likelihood of zero conductivity. At the other end of the spectrum, the very high F values indicate that the network possesses enough redundant pathways of electrical connection, that the introduction of a small fraction of nonconducting (void) material is highly unlikely to disrupt the overall number of pathways necessary to establish a solid electrical connection.

As an aside, an alternate (approximate) analytical method of establishing $F(f)$ is shown in Appendix C.

7. Conclusion

In this report, we use the construct of an $n \times n$ network to serve as an analogy to the problem of a computational, two-component mixed cell. In the network, linkages between the Cartesian nodes were considered to be in one of two possible states: conducting or insulating. A direct metaphor was drawn between the probability that an individual network link would be conducting (or, alternately, the overall fraction of conducting links in the network) and the fraction of conducting material found

in the mixed cell.

In this way, studying the connectivity behavior of the network in a statistical way provides us an understanding of the likelihood that electrical connectivity within a mixed cell can be maintained, expressed as a function of the nonconducting void content present in the cell.

In a real mixed cell, the morphological arrangement of the void will play a significant role in establishing the connectivity. In this simplified approach to the problem, the insulating links in the network (representative of void in the mixed cell) were randomly distributed throughout the cell.

The resulting analysis, which was performed on networks of size 2×2 , 3×3 , and 4×4 , exhibited noteworthy trends. In particular, the likelihood of connectivity in no way was expressed in any manner proportional to the global fraction of conducting links, nor the local (per-link) probability of conduction. Rather, a steep threshold was noted, such that if the fraction of conducting links fell below the threshold, the probability of establishing connectivity dropped precipitously toward zero. Conversely, if the fraction of conducting links was above the threshold, there arose a very strong probability of connectivity across the network.

The observed threshold \pm width was found to be, for both f and \hat{f} , approximately 0.65 ± 0.1 . Indications are that the threshold center might increase and that the threshold width might narrow further if networks more finely granulated than 4×4 were considered.

This modeling approach does not provide the means to interpret how mixed-cell conductivity should vary with void content. It was not intended to do so. However, it does reveal that the mixed-cell connectivity (directly related to the presence of nonzero conductivity) is very much driven by a threshold phenomenon. If the conducting fraction of material in a cell falls below some critical threshold, the probability of connectivity drops very rapidly toward zero.

8. References

1. Dykhne A. Conductivity of a two-dimensional two-phase system. Soviet Phys. JETP. 1971;32(1):63–65.
2. Silling S. CTH reference manual: boundary layer algorithm for sliding interfaces in two dimensions. Albuquerque (NM): Sandia National Laboratory; 1994 Jan. Report No.: SAND93-2487.
3. Wikipedia. Order and disorder. San Francisco (CA): Wikimedia Foundation, Inc.; 2019 May 23 [accessed 2019 Nov 21]. https://en.wikipedia.org/wiki/Order_and_disorder.

Appendix A. C99 Program to Assess Network Connectivity

The C99 program source code, netc, is given. It is designed to handle up to 64 links in the simulation network.

```
#include <stdio.h>
#include "netbuild64.c"
int    main();
void    topologysummary();
void    setlinkstatus();
int     expandfromnode();
int     alreadyinnet();
void    printlayout();
double  likelihoodanalysis();
/*
OUTPUT MASKING:
0 = No masking
1 = Mask nodal paths
2 = and mask # of paths found, and mask broken-link count
3 = and mask Realization # & Link status
*/
int masklevel = 3;
/*****
int main()
{
    long long linkcases, linkcase, connectcases,
        linkstatus[99], brokenlinkcases[99], brokenlinkconnected[99];
    int i, j, netnodes, brokenlinks, netnode[99];
    double caselikelihood, Xlikelihood, brokenlikelihood,
        linklikelihood;
    int pathfound;
    for (i = 0; i < 99; i++)
    {
        brokenlinkcases[i] = 0LL;
        brokenlinkconnected[i] = 0LL;
    }
    printlayout (layout);
    linkcases = 1LL << linkcount; /*Same as 2^linkcount*/
    connectcases = 0LL;
    for (linkcase = 0LL; linkcase < linkcases; linkcase++)
    {
        if (masklevel < 3)
            printf("***Realization #d: Links status = ", linkcase);
        setlinkstatus(linkcase, linkcount, &linkstatus, &brokenlinks);
        brokenlinkcases[brokenlinks] += 1LL;
        pathfound = expandfromnode(0,0,&netnode,&linkstatus);
        if (pathfound > 0)
        {
            if (masklevel < 2) printf (" (%d paths found)\n", pathfound);
            connectcases += 1LL;
            brokenlinkconnected[brokenlinks] += 1LL;
        }
    }
    topologysummary(linkcases, connectcases);
    /* for (linklikelihood = 0.1; linklikelihood <= 1.0;
```

```

        linklikelihood += 0.2)*/
for (linklikelihood = 0.05; linklikelihood <= 1.0;
    linklikelihood += 0.05)
{
    Xlikelihood = likelihoodanalysis(linklikelihood, linkcases,
        &brokenlinkconnected, &brokenlinkcases);
    printf ("Probability of connectivity = %3.2f%%\n", Xlikelihood);
}
Xlikelihood = likelihoodanalysis(-1., linkcases,
    &brokenlinkconnected, &brokenlinkcases);
}
/*****/
void topologysummary(linkcases, connectcases)
long long linkcases, connectcases;
{
    double fraccases;
    printf ("\n");
    printf ("This topology has %d nodes and %d links, ",
        nodes, linkcount);
    printf ("giving 2^%d = %jd realizations.\n",
        linkcount, linkcases);
    fraccases = (100.*connectcases)/linkcases;
    printf ("\n%3.2f%% or %jd/%jd realizations provide"
        " connectivity.\n", fraccases, connectcases, linkcases);
    return;
}
/*****/
void setlinkstatus(linkcase, linkcount, plinkstatus, pbrokenlinks)
long long linkcase, *plinkstatus;
int linkcount, *pbrokenlinks;
{
    int L;
    *pbrokenlinks = 0;
    if (masklevel < 3) printf("[");
    for (L = 0; L < linkcount; L++)
    {
        *(plinkstatus+L) = linkcase >>L & 1LL;
        if (*(plinkstatus+L) != 1LL) *pbrokenlinks+= 1;
        if (masklevel < 3) printf("%jd", *(plinkstatus+L));
    }
    if (masklevel < 3) printf("]");
    if (masklevel < 2) printf(" (%d broken links)", *pbrokenlinks);
    if (masklevel < 3) printf ("\n");
    return;
}
/*****/
int expandfromnode(n, netnodes, pnetnode, plinkstatus)
long long *plinkstatus;
int n, netnodes, *pnetnode;
{
    int path, L, k, NN, pathfound, nestpf;
    *(pnetnode+netnodes) = n;
    netnodes++;
    if (n == (nodes-1))

```



```

{
    if (masklevel < 1)
    {
        printf(" %d-node path: ", netnodes);
        for (k=0; k < netnodes; k++)
        {
            if (k != 0) printf (" ,");
            printf("%d", *(pnetnode+k));
        }
        printf("\n");
    }
    pathfound = 1;
    return (pathfound);
}
pathfound = 0;
path = 0;
for (path=0; path < nlinks[n]; path++)
{
    L = link[n][path];
    if (*(plinkstatus+L) == 1LL)
    {
        for (k=0; k<2; k++)
        {
            if (k==0)
                NN = nA[L];
            else
                NN = nB[L];
            if (alreadyinnet(NN, netnodes, pnetnode) == 0)
            {
                nestpf = expandfromnode(NN, netnodes, pnetnode, plinkstatus);
                pathfound += nestpf;
            }
        }
    }
}
return (pathfound);
}

/*****
int alreadyinnet(NN, netnodes, pnetnode)
int NN, netnodes, *pnetnode;
{
    int status, i;
    status = 0;
    for (i=0; i<netnodes; i++)
    {
        if (*(pnetnode+i) == NN)
            status = 1;
    }
    return (status);
}

*****/
void printlayout (layout)
char layout[][50];
{

```

```

int i, j;
for (i=0; layout[i][0] != '\0'; i++)
{
    for (j=0; layout[i][j] != '\0'; j++)
    {
        printf("%c", layout[i][j]);
    }
    printf ("\n");
}
printf ("\n\n");
}
/*****/
double likelihoodanalysis(linklikelihood, linkcases,
                          pbrokenlinkconnected, pbrokenlinkcases)
long long linkcases, *pbrokenlinkconnected, *pbrokenlinkcases;
double linklikelihood;
{
    int i, j;
    double Xlikelihood, brokenlikelihood, casellikelihood;
    if (linklikelihood >= 0)
        printf ("\nFor a single-link likelihood (SL) of %4.2f:\n",
                linklikelihood);
    else
        printf ("\nCumulative-link likelihood (CLL) analysis:\n");
    Xlikelihood = 0.;
    for (i=0; i < linkcount + 1; i++)
    {
        brokenlikelihood = 100. *
            (*(pbrokenlinkconnected+i)) / (*(pbrokenlinkcases+i));
        printf ("With %d broken links, %jd/%jd realizations (%3.2f%%)"
                " connect",
                i, *(pbrokenlinkconnected+i), *(pbrokenlinkcases+i),
                brokenlikelihood);
        if (linklikelihood >= 0){
            casellikelihood = 1.0;
            for (j=0; j < linkcount; j++)
            {
                if (j < i)
                    casellikelihood *= (1.-linklikelihood)/0.5;
                else
                    casellikelihood *= linklikelihood/0.5;
            }
            printf (" at %5.3fx random likelihood\n",
                    casellikelihood);
            Xlikelihood += *(pbrokenlinkconnected+i) * casellikelihood;
        }
        else
        {
            Xlikelihood = 1. * (linkcount - i) / linkcount;
            printf (" with CLL = %1.3f\n", Xlikelihood);
        }
    }
    Xlikelihood *= 100. / linkcases;
    return Xlikelihood;
}

```

```
}  
/*****/
```

The `#included` file `netbuild64.c`, defines the net connectivity for the cases considered. Different versions exist for each of the three networks considered in this report.

`netbuild64.c` (2×2 case)

```

/**2x2*****/
static char layout[][50] ={
"4 NODES:",
" ",
"0 +---+ 1",
" |   |",
" |   |",
" |   |",
"2 +---+ 3",
" ",
"4 LINKS:",
" ",
" +--+",
" |   |",
" 2   3",
" |   |",
" +--+",
"",
};
static int linkcount = 4;
static int nodes = 4;
static int nA[] = {0,2,0,1};
static int nB[] = {1,3,2,3};
static int link[][2] = {{0,2},
                        {0,3},
                        {1,2},
                        {1,3}};
static int nlinks[] = {2,2,2,2};

```

netbuild64.c (3×3 case)

```
/**3x3*****  
static char layout[][50] =(  
"9 NODES:",  
" ",  
"    1",  
"0 +---+---+ 2",  
" |   |   |",  
"3 +---+4---+ 5",  
" |   |   |",  
"6 +---+---+ 8",  
"    7",  
" ",  
"12 LINKS:",  
" ",  
"  +0-+-1-+",  
"  6   8  10",  
"  +2-+-3-+",  
"  7   9  11",  
"  +4-+-5-+",  
""  
);  
static int linkcount = 12;  
static int nodes = 9;  
static int nA[] = {0,1,3,4,6,7,0,3,1,4,2,5};  
static int nB[] = {1,2,4,5,7,8,3,6,4,7,5,8};  
static int link[][4] = {{0,6},  
                        {0,1,8},  
                        {1,10},  
                        {2,6,7},  
                        {2,3,8,9},  
                        {3,10,11},  
                        {4,7},  
                        {4,5,9},  
                        {5,11}};  
static int nlinks[] = {2,3,2,3,4,3,2,3,2};
```

netbuild64.c (4×4 case)

```
/**4x4*****/
static char layout[][50] ={
"16 NODES:",
" ",
"      1   2",
" 0 +---+---+---+ 3",
"   |   |   |   |",
" 4 +---+5---+6---+ 7",
"   |   |   |   |",
" 8 +---+9---+10---+ 11",
"   |   |   |   |",
"12 +---+---+---+ 15",
"      13  14",
" ",
"24 LINKS:",
" ",
" +-0-+-1-+-2-+",
" 12  15  18  21",
" +-3-+-4-+-5-+",
" 13  16  19  22",
" +-6-+-7-+-8-+",
" 14  17  20  23",
" +-9-+-10+-11+",
""
};

static int linkcount = 24;
static int nodes = 16;
static int nA[] =
    {0,1,2,4,5,6,8, 9,10,12,13,14,0,4, 8,1,5, 9,2, 6,10,3, 7,11};
static int nB[] =
    {1,2,3,5,6,7,9,10,11,13,14,15,4,8,12,5,9,13,6,10,14,7,11,15};
static int link[][4]= {{0,12},
                        {0,1,15},
                        {1,2,18},
                        {2,21},
                        {3,12,13},
                        {3,4,15,16},
                        {4,5,18,19},
                        {5,21,22},
                        {6,13,14},
                        {6,7,16,17},
                        {7,8,19,20},
                        {8,22,23},
                        {9,14},
                        {9,10,17},
                        {10,11,20},
                        {11,23}};

static int nlinks[] = {2,3,3,2,3,4,4,3,3,4,4,3,2,3,3,2};
```

Appendix B. Example: A 5×5 (Clipped) Nodal Grid

This example is not included directly in the report, because it does not represent a pure $n \times n$ network. Instead, it is a 5×5 network with the two lateral corner nodes clipped from the network, as shown in Fig. B-1. As it is, the network contains 36 linkages, which translates to $2^{36} = 68,719,476,736$ (68.7 billion) statistical realizations, each of which requires checking for all of the 2746 possible pathways from node O to X (amounting to over 188 trillion pathways that must be checked).

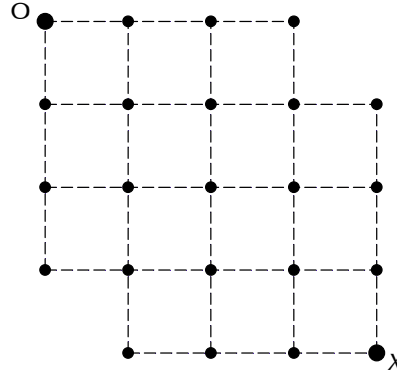


Fig. B-1 A 5×5 nodal network, clipped at corners, containing 23 nodes and 36 linkages

Retaining the clipped corner nodes, while desirable, proved to be computationally prohibitive. Thus, the corner clipping was introduced to get a sense of how the true 5×5 network might behave. Because the tabulated results are voluminous, they are omitted. We instead jump directly to the graphical result shown in Fig. B-2. We see, as n increases, the $F(f)$ and $F(\hat{f})$ behavior become more closely aligned with each other, compared with, for example, Figs. 3 or 5.

We may add these graphs atop the summaries for $F(f)$ and $F(\hat{f})$, in order to observe the trend as the network width n is increased. We do so, in red, in Fig. B-3. We observe that the expected trend continues that, as n increases, the threshold to activate F becomes both steeper and shifts toward the direction of increasing f and \hat{f} .

Finally, we present the netbuild64.c input file employed by the netc program, for the case of the clipped 5×5 network.

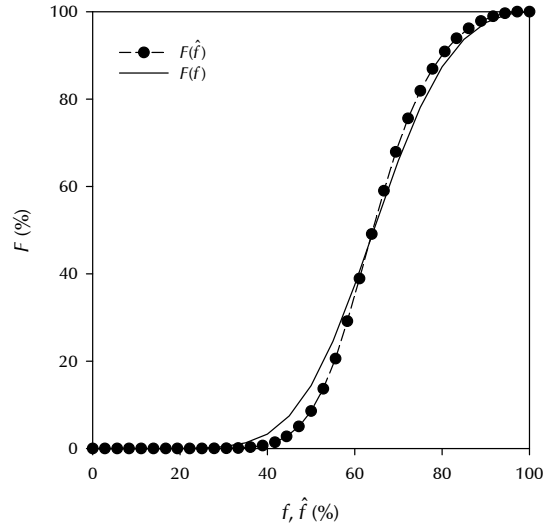


Fig. B-2 For the 5×5 (clipped) network, the probability of network connectivity, F , with either f or \hat{f} as the independent variable

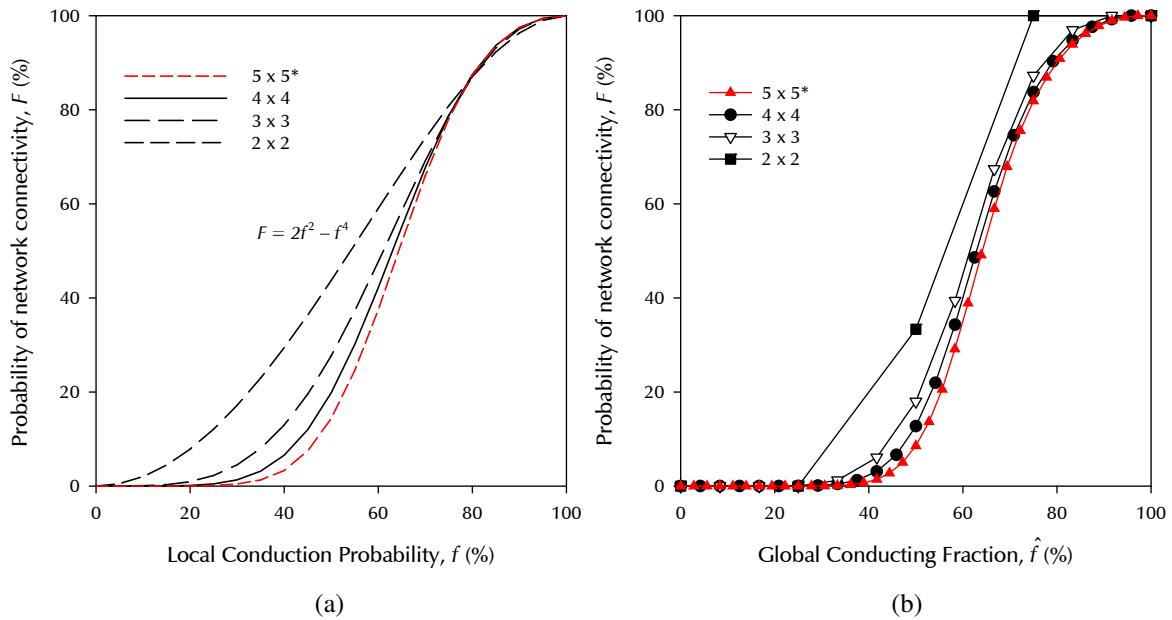


Fig. B-3 For $n \times n$ networks (including the clipped 5×5 network), the probability of network connectivity as a function of either a) the local conduction probability or b) the global conducting fraction

netbuild64.c (5×5 (clipped) case)

```
/**5x5(corners removed)*****/
static char layout[][50] ={
"23 NODES:",
" ",
" +0---+1---+2---+3   ",
" |   |   |   |   |   ",
" +4---+5---+6---+7---+8",
" |   |   |   |   |   ",
" +9---+10---+11---+12---+13",
" |   |   |   |   |   ",
" +14---+15---+16---+17---+18",
"      |   |   |   |   ",
"      +19---+20---+21---+22",
" ",
"36 LINKS:",
" ",
" +-0-+-1-+-2-+",
" 18 21 25 29",
" +-3-+-4-+-5-+-6-+",
" 19 22 26 30 33",
" +-7-+-8-+-9-+-10-+",
" 20 23 27 31 34",
" +-11-+-12-+-13-+-14-+",
"      24 28 32 35",
"      +-15-+-16-+-17-+",
""
};

static int linkcount = 36;
static int nodes = 23;
static int nA[] =
    {0,1,2, 4,5,6,7, 9,10,11,12, 14,15,16,17, 19,20,21,
     0,4,9, 1,5,10,15, 2,6,11,16, 3,7,12,17, 8,13,18};
static int nB[] =
    {1,2,3, 5,6,7,8, 10,11,12,13, 15,16,17,18, 20,21,22,
     4,9,14, 5,10,15,19, 6,11,16,20, 7,12,17,21, 13,18,22};
static int link[][4]= {{0,18},
                       {0,1,21},
                       {1,2,25},
                       {2,29},
                       {3,18,19},
                       {3,4,21,22},
                       {4,5,25,26},
                       {5,6,29,30},
                       {6,33},
                       {7,19,20},
                       {7,8,22,23},
                       {8,9,26,27},
                       {9,10,30,31},
                       {10,33,34},
                       {11,20},
                       {11,12,23,24},
```

```
        {12,13,27,28},
        {13,14,31,32},
        {14,34,35},
        {15,24},
        {15,16,28},
        {16,17,32},
        {17,35}};
static int nlinks[] =
    {2,3,3,2, 3,4,4,4,2, 3,4,4,4,3, 2,4,4,4,3, 2,3,3,2};
```

Appendix C. Approximate (Analytical) Evaluation of $F(f)$

The approaches derived in this report examine each permutative realization of the network (which represents an analogy to a mixed cell). While providing an exact tabulation of those realizations, the method is not very scalable, as the number of permutations, N , grows as 2^n , where n is the number of linkages in the network. The value of 2^n quickly exceeds computational capacity as n grows, since the method employed uses a brute-force approach to the examination.

The approach can be streamlined and even evaluated analytically, if an approximation is made. We demonstrate the approximation for the 3×3 network, whose topology is repeated for convenience as Fig. C-1. We seek to evaluate the probability of connectivity between nodes 0 and 8.

For the approximation, let us *assume* that the connectivity path across the network is precluded from experiencing “reversals”. Here, a reversal is defined as a nodal pathway that locally moves upward and/or leftward to reach the terminus. If all valid pathways are limited to those that traverse the network in a rightward and/or downward direction, in the process of connecting node 0 to node 8, then straightforward analytical methods can be brought to bear.

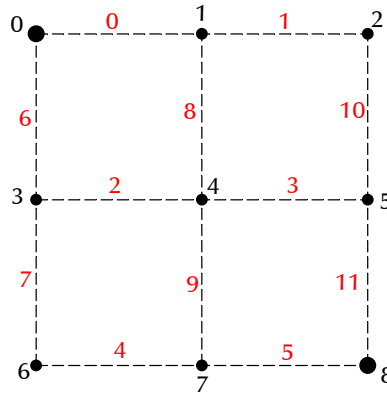


Fig. C-1 A 3×3 network in which nodes and linkages have been assigned unique identification, node numbers in black and linkage numbers in red

The preclusion of reversals means that the network can be analyzed as a standard probability tree, with the probability of each linkage specified as f . If the probability of connectivity between nodes 0 and A is F_A , and node C can only be reached directly from node A , then $F_C = fF_A$. If, on the other hand, node C can be reached directly from two separate nodes, A and B , then $F_C = fF_A + fF_B - f^2F_AF_B$.

Using this approach, the probability of connectivity between node 0 and each successive node in the 3×3 network can be established until, at last, node 8 is reached to establish the probability, F , that node 0 connects to node 8.

$$\begin{aligned}
F_0 &= 1 \\
F_1 &= F_3 = f \\
F_2 &= F_6 = f^2 \\
F_4 &= f(F_1 + F_3) - f^2 F_1 F_3 \\
&= 2f^2 - f^4 \\
F_5 &= F_7 = f(F_2 + F_4) - f^2 F_2 F_4 \\
&= f^3(3 - f^2 - 2f^3 + f^5) \\
F(f) = F_8 &= f(F_5 + F_7) - f^2 F_5 F_7 \\
&= 2fF_5 - (fF_5)^2 \\
&= 2f^4(3 - f^2 - 2f^3 + f^5) - f^8(3 - f^2 - 2f^3 + f^5)^2
\end{aligned}$$

This analytical, yet approximate, estimation of $F(f)$, which excludes reversals, can be directly compared with the exact result established in Section 5.4 of this report.

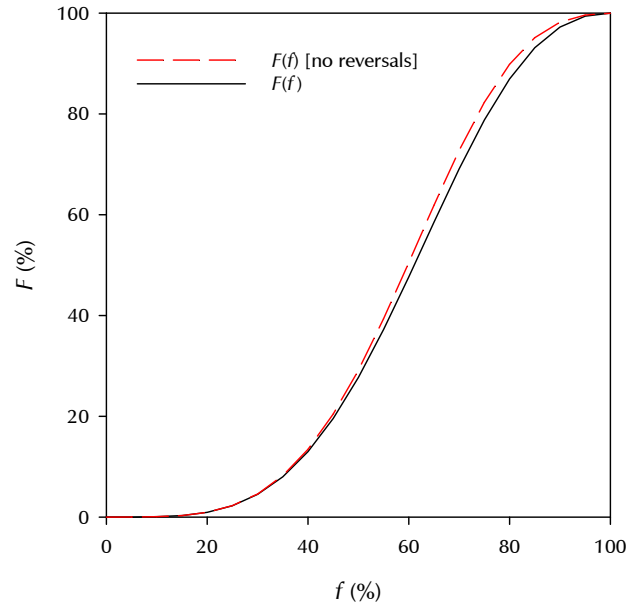


Fig. C-2 For the 3×3 network, the probability of network connectivity, $F(f)$, comparing exact and approximate methods

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