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A Method for Systematic Site-to-Bond Conversion of Directed Graphs

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A graph-theoretic method for the complete derivability of bond graphs from their site counterparts is described. Bond perimeter, valence, and cyclomatic number distributions as well as spatial extent measures can be systematically generated when coupled with a site valence partition in the original graph. Relevant consequences for bond configurations include the facts that (i) percolation perimeter and cyclomatic number distributions are equivalent, (ii) geometrical susceptibilities are not independent, and (iii) a critical site/bond ratio exists.

KEY WORDS: Percolation perimeter; dilute polymers; site valence.

1. INTRODUCTION

The study of fully directed animals both in a percolation context(1) and as diluted polymers(2) has mostly dealt with site problems in all enumerative approaches involving systematic counting, although both types of problems have led to precise estimates in two dimensions when treated through subgraph expansions.(1,8)

For a polymer-type approach this has always had to do with the use of recurrence relations that greatly reduce the amount of configurations to be counted. Bond graphs, or rather their lattice embeddings, for which no equivalent relations have ever been discovered, have the edge on percolation problems, where series expansions are better behaved than their site counterparts.(1,8)

In spite of this, the initial effort of Redner and Yang(3) uncovered a disturbing discrepancy between site and bond polymers, most noticeable in

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the critical exponent estimates, which the later exact solutions in 2D and 3D left unexplained.$^{(2)}$

In the present paper a graph-theoretic method for the derivation of bond configurations from the corresponding site animals is detailed. Originally devised as a strategy to exploit the recurrence relation properties, this conversion method has enabled us to establish several additional results concerning properties of the bond percolation perimeter and the cyclomatic number partition of directed bond configurations.

2. THE SITE-TO-BOND CONVERSION METHOD

The idea of site-to-bond conversion (or yield) techniques is not new and has been applied to undirected graphs in the past.$^{(4)}$ But the task is always cumbersome, basically involving the knowledge of the full connectivity of the underlying graph and systematic checks every time a bond between sites of the original graph is deleted (and thus, in a percolation context, added to the perimeter). Consider a partition of the sites s, according to the number of neighbors (their valence). For undirected graphs

$$s = \sum_{v=1}^{z} s_v \tag{1a}$$

$$2b = \sum_{v=1}^{z} v s_v \tag{1b}$$

$$c = b - s + 1 \tag{1c}$$

$$f = zs - 2b \tag{1d}$$

with s_v the number of sites with valence v, b the number of bonds, c the cyclomatic number, and f the number of adjacent external bonds. For directed graphs, Eqs. (1a)–(1c) are valid [but not (1d)] if the orientation of bonds connected to a given site is taken as irrelevant. The valence v divides naturally into a forward (w-outgoing bonds) and a backward (u-incident bonds) valence. For any of these, the linkage rules (1a)–(1c) must be written as ($\tilde{z} = z/2$)

$$s = \sum_{0}^{\tilde{z}} s_u = \sum_{0}^{\tilde{z}} s_w \tag{2a}$$

$$b = \sum_{u=0}^{\tilde{z}} u s_u = \sum_{w=0}^{\tilde{z}} w s_w \tag{2b}$$

$$e = \tilde{z} s - b \tag{2c}$$

with e measuring the adjacent external bonds according to the axis orientation. Single-site valence, however, is useless for undirected graph conversion because complete correlations between neighboring valences are still required. The same applies to forward valence in directed graphs. But for the backward valence partition (Fig. 1), each of the u-incident bonds (but not all of them) can be removed (and thus transferred to the bond perimeter). The spatial correlations can then be treated locally, and connectivity will never be violated provided one incident bond is left per site other than the graph origin (for normal one-rooted graphs).

At this level, all possible spanning directed bond trees of the original graph have been generated. The conversion factor associated with it is

$$C(G)=\prod_{u=2}^{\tilde{z}}\left[1+\sum_{i=1}^{u-1}\binom{u}{i}(q/p)^{i}\right]^{s_u} \tag{3}$$

where p and $q=1-p$ are the occupation (absence) probabilities, with the weight of G equal to $p^b q^e$. The same conversion factor applies to all graphs with the same valence partition, and we see that the bond percolation distribution, as well as the valence partition, is automatically derived from it. With the latter, the loop partition of bond graphs follows from Eq. (2b).

Several significant corollaries can be derived from this method:

(i) On fully directed lattices with constant coordination number $\tilde{z}$, the percolation perimeter partition at fixed size b, g_{bt}, is just the cyclomatic

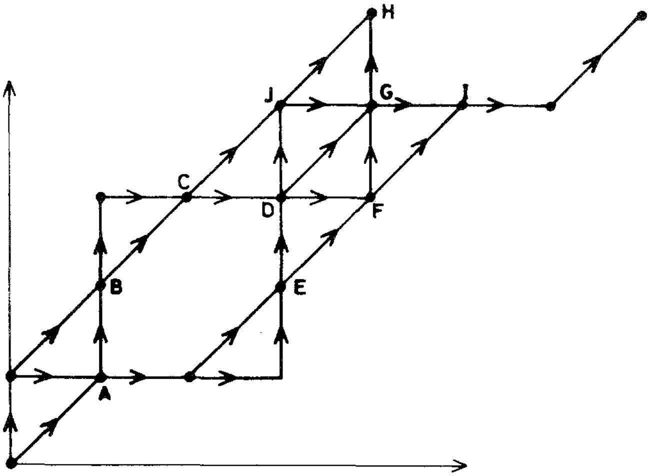

Fig. 1. A directed-site triangular graph. All sites marked with a letter contribute to the conversion factor, Eq. (3). Site G is the only one with backward valence 3. In addition, the contributions of sites A, D, and G to the spatial measures along the preferred axis would be common to all bond graphs generated by the conversion factor.

number distribution g_{bs} (with s the number of sites). From Eqs. (2) and (3), a bond graph with d converted bonds has perimeter $e+d$ and size $b-d$. With these two values, Eq. (2c) is still valid and with

$$t-(\tilde{z}-1)\,b=\tilde{z}(1-c) \tag{4}$$

the spacing between perimeter values is equal to $\tilde{z}$, and t fixes the cyclomatic number c at fixed b.

(ii) The mean size and site susceptibility expansions for bond percolation are not independent. Averaging size moments, we have

$$1=\sum_{b=0} g_{bt}\,p^b q^t \tag{5}$$

$$S(p)=\sum_{i=1} d_i\,p^i=\sum bg_{bt}\,p^b q^t \tag{6}$$

where $S(p)$ is the mean size (or first moment) of the cluster size distribution. For the site susceptibility,[1] which, according to the fluctuation-dissipation theorem, is given by the sum of the pair connectedness between the origin and all its other sites,

$$R(p)=1+\sum_i c_i\,p^i=\sum_{s=1} sg_{bt}\,p^b q^t \tag{7}$$

$$=\tilde{z}\sum_{b=0}(t+b)\,g_{bt}\,p^b q^t \tag{8}$$

Using Eq. (5) and equating powers of p, we have

$$d_i=\tilde{z}c_{i-1}(d_0=0,\ c_0=1) \tag{9}$$

Note that for the site problem, as for undirected percolation, these two susceptibilities are independent.[5]

(iii) There exists a critical site/bond ratio for directed bond animals. This follows from the asymptotic shape of the bond perimeter distribution g_{bt}, and from the singularity structure at fixed loop number, both of which closely parallel the behavior found for site problems.[6,7] Such a limiting shape is described by a function $\lambda(t/b)$ which gives the growth value for a given perimeter-to-size ratio when the discrete g_{bt} are smoothed into a continuous distribution. Trees are then the maximum-perimeter configurations and share the same growth constant as 1-loop,..., i-loop animals. In the asymptotic limit there is a critical perimeter-to-size ratio $a_c=(1-p_c)/p_c$ below which the growth constant $\lambda(a)$ of animals at a fixed ratio is given by $(a=t/b)$

$$\lambda(a)=(a+1)^{a+1}/a^a \qquad (a<a_c) \tag{8a}$$

where $a = \tilde{z} - 1 + (\tilde{z}/b) - (\tilde{z}c/b)$, while for higher a,

$$\lambda(a) = [(a+1)^{a+1}/a^{a}]\, e^{-k(a)} \qquad (a > a_c) \tag{8b}$$

where $k(a)$ is positive and measures the separation from the critical growth value.

On the other hand, with the limiting logarithmic shape of the perimeter [given by $n \log \lambda(a)$] distribution linear in the bond size, the total growth constant for animals, which should be taken as strictly higher than that for trees, occurs at a smaller cycle/size ratio.

3. FINAL REMARKS

We have applied the method to several lattices and dimensionalities, extending both the data of Redner and Yang(3) and the percolation results of ref. 1 for dimensions 2 to 5, while duplicating the susceptibilities in ref. 8 to order 25—square, s. cubic (to order 16), and 4D hypercubic (to order 14) that appear elsewhere.(9) This conversion method is on the other hand trivially applicable to measures of spatial extent (center-of-mass location and radius of gyration(3)), which are, of course, inherited by all terms in the conversion factor [Eq. (3)] if present in the original graph.

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