

The cluster structure in collapsing animals

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2000 J. Phys. A: Math. Gen. 33 3653

(<http://iopscience.iop.org/0305-4470/33/19/303>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.118

The article was downloaded on 02/06/2010 at 08:07

Please note that [terms and conditions apply](#).

The cluster structure in collapsing animals

E J Janse van Rensburg

Department of Mathematics and Statistics, York University, Toronto, Ontario, Canada M3J 1P3

Received 1 February 2000

Abstract. In this paper I revisit the connection between edge percolation and the collapse transition in lattice animals. It was shown by Domb (1976 *J. Phys. A: Math. Gen.* **9** L141) that the critical percolation point is a θ -transition in a certain model of self-interacting animals. I extend this result by showing that the free energy of lattice animals in the cycle–contact model is non-analytic in contact- and cycle-activities at points other than the critical percolation point. This correspondence between percolation and collapsing animals suggests that the collapse transition in this model may be related to percolation. Contact–collapse in animals is then studied from a percolation of clusters of contacts perspective. I first argue that there is a critical activity for percolation of clusters of contacts, and then investigate this numerically.

1. Introduction

Lattice animals are commonly used as a model of a branched polymer in a dilute solution (Lubensky and Isaacson 1979). The definition of a lattice animal as a connected subgraph of a lattice dates back to cell-growth problems (Harary 1960). Of particular interest are models of self-interacting animals (see, for example, Derrida and Hermann 1983, Gaunt and Flesia 1990, 1991, Flesia and Gaunt 1992), which undergoes a *collapse transition* (θ -transition) under suitable conditions. The collapse transition has been studied in models of both linear and branched polymers over a period of several decades. The interest in these models started with Mazur and McCrackin (1968), and subsequent investigations includes the studies by Mazur and McIntyre (1975), Sun *et al* (1980), Park *et al* (1992), Flesia *et al* (1993, 1994), Tesi *et al* (1996) and Madras and Janse van Rensburg (1997).

An *edge animal* is a connected subgraph of a lattice, and is also said to be weakly embedded in the lattice. Let a_n be the number of edge animals, consisting of n edges, counted up to translational equivalence, in the square lattice. It can be checked that $a_0 = 1$, $a_1 = 2$, $a_2 = 6$, $a_3 = 14$ and so on. The asymptotic behaviour of a_n has been investigated in studies of percolation (Stauffer 1979, Essam 1980), and more recently in high dimensions within the context of the lace expansion (Hara and Slade 1990, 1995). There is significant evidence that

$$a_n \simeq n^{-\theta} \lambda^n \quad (1.1)$$

where λ is the *growth constant* of lattice animals which defines the exponential rate of growth in a_n . The existence of the limit $\lim_{n \rightarrow \infty} [\log a_n]/n = \lambda$ is also known, and is a consequence of the superadditive nature of $\log a_n$ (Klarner 1967, Klein 1981). The power-law correction to the exponential nature of a_n involves the *entropic exponent* θ , and while the existence of θ has been established in high dimensions (Hara and Slade 1990), numerical evidence strongly suggests that the asymptotic behaviour in equation (1.1) is also valid in two dimensions (Whittington *et al* 1983).

A typical model of animal collapse can be defined by introducing a nearest-neighbour interaction in a model of animals. A *contact* is a pair of vertices in the animal, which are adjacent in the lattice, but not adjacent in the animal. Let $a_n(k)$ be the number of animals counted by a_n , but with exactly k contacts in each animal. A model of contact-collapse in animals is defined by the partition function

$$Z_n(z) = \sum_{k \geq 0} a_n(k) z^k \quad (1.2)$$

where $z = e^\beta$ is an *activity* conjugate to the number of contacts. The *limiting free energy* in this model is defined by

$$\mathcal{F}(z) = \lim_{n \rightarrow \infty} \frac{1}{n} \log Z_n(z) \quad (1.3)$$

and its existence is known (see, for example, Flesia and Gaunt 1992). The collapse transition in the model is exhibited as a non-analyticity in $\mathcal{F}(z)$ at the critical point $z = z_c$. The description of critical behaviour in $\mathcal{F}(z)$ is generally the consequence of an assumption that the θ -point is a tricritical point (this was argued by de Gennes (1975)). In these circumstances, a good starting point is to treat n and z as scaling fields, and to introduce scale invariance in $Z_n(z)$ by assuming that the partition function is only a function of the rescaled variable $n^\phi(z_c - z)$, where ϕ is a *crossover* exponent which describes the crossover to criticality as $z \rightarrow z_c$ with increasing n .

While it is the case that tricriticality seems to give an adequate description of collapse in a model of animals, there is also very little known about the θ -transition. In particular, there seems to be some evidence that a percolation phenomenon might provide the underlying mechanism for collapse; numerical evidence for this has been seen in the Monte Carlo simulations by Madras and Janse van Rensburg (1997), and Janse van Rensburg *et al* (1999); and this question was explored explicitly for collapsing self-avoiding walks by Nidras (1997). The data for the collapsing self-avoiding walk have been interpreted as evidence that the percolation of clusters and the collapse transition may not occur at the same critical activity by Nidras (1997). However, a re-examination of the data obtained by Nidras shows that the estimated critical activity $z_\delta = 1.325 \pm 0.012$ for percolation of contact clusters in collapsing walks is numerically indistinguishable from the best estimated critical value z_c in the θ -transition in walks ($z_c \approx 1.31$, Meirovitch and Lim 1990, Grassberger and Hegger 1995). Thus, it may be premature to claim a connection either way, and this issue remains unresolved.

It is known that percolation clusters are weighted animals, and the critical percolation point has been shown to lie on a critical line of θ -transitions (Domb 1976, Grimmet 1989, Flesia *et al* 1992). Indeed, the only point on this critical line where it is known that the limiting free energy of self-interacting animals is non-analytic is the percolation point, no proof is known to suggest the presence of other non-analyticities in the line of θ -transitions. In section 2 I address this question again. I show that there are other non-analyticities in the limiting free energy by again exploiting the connection with percolation; in effect, I slightly generalize the proof by Domb (1976) to achieve this result. In sections 3 and 4 the statistics of contact clusters in collapsing animals in the contact model is considered. The motivation for this work is the possibility that there may be an interpretation of the collapse in animals in terms of the percolation of clusters of contacts. Numerical evidence for percolation of contact clusters is produced in section 4, where I also estimate the critical activity for this, and its crossover exponent.

2. Collapsing animals

An animal is characterized by five quantities. These are n , the number of edges, the number of vertices v , the number of contacts k , the number of independent cycles c and the number of ‘solvent contacts’ (edges in the lattice with exactly one endpoint in the animal) s . There are two relations between these quantities, namely Euler’s relation $v - n + c = 1$, and $2dv = 2n + 2k + s$. Moreover, $k + s$ is also the edge perimeter (or simply the *perimeter*) of the animal. A model of self-interacting animals (the cycle–contact model) may be defined by the partition function

$$Z_n(y, z) = \sum_{c \geq 0} \sum_{k \geq 0} a_n(c, k) y^c z^k \tag{2.1}$$

where $a_n(c, k)$ is the number of animals with n edges, c independent cycles and k nearest-neighbour contacts between vertices adjacent in the lattice, but not in the animal. Note that if n , c and k are fixed in the animal, then so are v and s . There are two independent activities in this model, y is an activity conjugate to the number of cycles in the animal and z is conjugate to the number of contacts. It is known that the limiting free energy

$$\mathcal{F}(y, z) = \lim_{n \rightarrow \infty} \frac{1}{n} \log Z_n(y, z) \tag{2.2}$$

exists for all $y < \infty$ and $z < \infty$ (Janse van Rensburg and Madras 1997) in this model, and that $\mathcal{F}(y, z)$ is convex in each of its arguments follows from the Cauchy–Schwartz inequality.

It is also known that $\mathcal{F}(y, z)$ is a non-analytic function; the argument uses a connection between this model, and edge percolation in the hypercubic lattice (Domb 1976, Grimmett 1989, Flesia *et al* 1992). In particular, let $P_n(p)$ be the probability that the open cluster at the origin contains n vertices, given that each edge has probability p to be open, and $q = 1 - p$ to be closed. Then it is known that

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log P_n(p) = \begin{cases} 0 & \text{if } p > p_c \\ -\gamma(p) & \text{if } p < p_c \end{cases} \tag{2.3}$$

where $\gamma(p) > 0$ and p_c is the critical percolation probability (see, for example, Grimmett (1989), the proof was due originally to Aizenmann and Newman (1984)). Note now that if $q = 1 - p$, then

$$\begin{aligned} P_n(p) &= \sum_{c \geq 0} \sum_{k \geq 0} v a_n(c, k) p^n q^{k+s} \\ &= p^n q^{2d+2(d-1)n} \sum_{c \geq 0} \sum_{k \geq 0} v a_n(c, k) q^{-2dc} q^{-k}. \end{aligned} \tag{2.4}$$

In other words, $P_n(p)$ is a combination of $Z_n(y, z)$ and a derivative of $Z_n(y, z)$, with $y = q^{-2d}$ and $z = q^{-1}$, and multiplied by some factors of p and q . Hence $\mathcal{F}(y, z)$ is non-analytic at the points $y = (1 - p_c)^{-2d}$ and $z = (1 - p_c)^{-1}$; this follows immediately from equation (2.3). This point is the *critical percolation point* in the phase diagram of the animals with limiting free energy $\mathcal{F}(y, z)$ (see figure 1).

It is, in fact, possible to show that there are more non-analyticities in the phase diagram depicted in figure 1, *other* than the percolation point. The proof for this relies on equation (2.4), and is in theorem 1.

Theorem 1. *There are non-analyticities in the free energy of animals in the cycle–contact model at points other than the critical percolation point.*

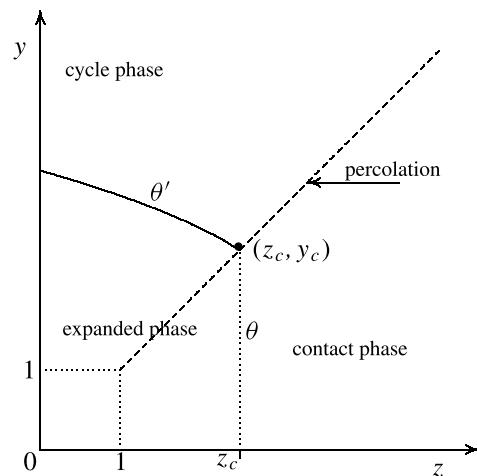


Figure 1. The phase diagram of lattice animals with a contact and a cycle fugacity. Critical percolation occurs at (z_c, y_c) and is marked with \bullet . It is on the intersection of a curve of θ -transitions (collapsed transitions) and the broken line along which animals are weighted as percolation clusters. The critical percolation point is a multicritical point which separates the critical line of θ -transitions into a line of tricritical collapse to a phase rich in contacts (the θ -line), and into a line of tricritical collapse into a phase rich in cycles (the θ' -line). Presumably the phases marked ‘cycle phase’ and ‘contact phase’ are not different, but together form a phase of collapsed animals.

Proof. Define the following function:

$$R_n(u, p) = p^n q^{2d+2(d-1)n} \sum_{c \geq 0} \sum_{k \geq 0} v a_n(c, k) q^{-2dc} (u/q)^k$$

by introducing a parameter u which takes values in $(0, 1]$ in equation (2.4). It is the case that

$$R_n(u, p) \leq P_n(p). \tag{†}$$

This shows that

$$\limsup_{n \rightarrow \infty} [R_n(u, p)]^{1/n} \leq \lim_{n \rightarrow \infty} [P_n(p)]^{1/n} \leq e^{-\gamma(p)}$$

from equation (2.3), where $\gamma(p) > 0$ if $p < p_c$, and $\gamma(p) = 0$ if $p > p_c$. On the other hand, use $2dv = 2n + 2k + s$ to see that

$$\begin{aligned} R_n(u, p) &= \sum_{c \geq 0} \sum_{k \geq 0} v a_n(c, k) p^n q^{s+k} u^k \\ &= \sum_{c \geq 0} \sum_{k \geq 0} v a_n(c, k) (p/u^2)^n (q/u)^{s+k} (u^{2d})^v. \end{aligned}$$

Observe that $1 - p/u^2 = q/u$ if $p = -u \leq 0$, and that if $p = 0$, then $1 - p/u^2 \leq q/u$. This shows that $1 - p/u^2 \leq q/u$ for all values of $p \in [0, 1]$, as long as $u \in (0, 1]$. Thus,

$$R_n(u, p) \geq \sum_{c \geq 0} \sum_{k \geq 0} v a_n(c, k) (p/u^2)^n (1 - p/u^2)^{s+k} (u^{2d})^v = Q_n(p/u^2, u^{2d}).$$

$Q_n(p/u^2, u^{2d})$ is the probability that the open cluster at the origin has size n in a combined edge–site percolation model where edges are open with probability p/u^2 , and sites are occupied

with probability u^{2d} , provided that $p \leq u^2$ (and where every vertex in the cluster is occupied). If u is close enough to 1, then p can be picked as large enough that the open cluster at the origin is infinite with positive probability (this follows from the fundamental theorem of percolation). Thus, there is a $u_c < 1$ so that if $u > u_c$, then $\lim_{n \rightarrow \infty} [Q_n(p/u^2, u^{2d})]^{1/n} = 1$, provided that p/u^2 is large enough. Comparing this with equation (†) above, and using equation (2.3), this shows that

$$\lim_{n \rightarrow \infty} [R_n(u, p)]^{1/n} = 1$$

if $u > u_c$ and p is large enough. Thus, there is a non-analyticity at a critical value of p (say p_u) for every $u > u_c$.

$R_n(u, p)$ is a combination of $Z_n(q^{-2d}, u/q)$ and its derivative, and since $\lim_{n \rightarrow \infty} [R_n(u, p)]^{1/n}$ is non-analytic, so will $\mathcal{F}(q^{-2d}, u/q)$ be for each value of $u \in (u_c, 1]$ and at a critical value of q . Since the critical percolation point is not on the line $(z, y) = (u/q, 1/q^{2d})$ if $u < 1$, this non-analyticity is not the critical percolation point, and presumably corresponds to a collapse into the cycle phase. \square

The usual finite-size tricritical assumptions indicate that the finite-size free energy, $F_n(\sigma, \tau) = [\log Z_n(y, z)]/n$, is a function of two scaling fields σ and τ (these are appropriate combinations of y and z , and both σ or τ approaches zero as the animals approaches a critical point). It is expected from equation (2.2) that if $\sigma \rightarrow 0$, then

$$F_n \sim \frac{1}{n} \hat{f}(n^{\phi_k} \sigma) \tag{2.5}$$

along the θ -line in figure 1, and

$$F_n \sim \frac{1}{n} \hat{f}(n^{\phi_c} \tau) \tag{2.6}$$

along the θ' -line in figure 1. The exponents ϕ_k and ϕ_c are *crossover exponents* describing the crossover behaviour in the model to criticality with increasing n , with respect to contact and cycle collapse, respectively. Numerical simulations indicate that $\phi_k = 0.62 \pm 0.03$ and $\phi_c = 0.62 \pm 0.04$ (Janse van Rensburg *et al* 1999). It is unclear that the cycle- and contact-driven collapse transitions in figure 1 are in different universality classes, and claims exist for both cases (see Janse van Rensburg *et al* 1999 for a discussion).

The collapse transition is best characterized by a change in metric behaviour. Two-dimensional expanded animals have metric exponent $\nu = 0.644 \pm 0.002$ (Janse van Rensburg and Madras 1997), but generally $\nu \approx 0.53$ along the critical curve (Janse van Rensburg *et al* 1999). This value is also the metric exponent for critical percolation clusters (Stauffer 1979, Essam 1980, Grimmett 1989), and if percolation is interpreted as a tricritical θ -point, then the metric exponent of critical percolation clusters can be shown to be $\nu = \frac{48}{91} = 0.5275 \dots$. In view of this, it seems tempting to attempt to interpret collapse in animals as a percolation phenomenon along the entire critical curve in figure 1.

3. Clusters in collapsing animals

The discussion in this section will be limited to animals undergoing contact-collapse (with $y = 1$ in equation (2.1)). This is the ‘contact’ model of collapsing animals (Flesia and Gaunt (1992); see also equations (1.2) and (1.3)). It is known that the free energy in this model exists, and it is given by equation (1.3). Moreover, a number of bounds on $\mathcal{F}(z)$ have been derived (Flesia *et al* 1994). It does not follow from theorem 1 that $\mathcal{F}(z)$ is non-analytic; observe that

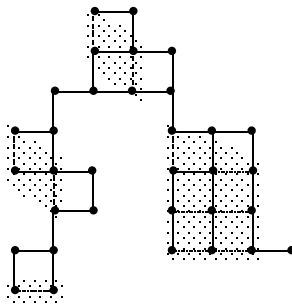


Figure 2. Clusters of contacts in an animal. This animal has one cluster of size 6, two clusters of size 2 each, and one cluster of size 1.

$\mathcal{F}(z) = \mathcal{F}(1, z)$, see equation (2.2). A ‘cluster’ in an animal will be a group of contacts which are near to one another in the animal. With increasing densities of contacts, these clusters of contacts will grow, and they should percolate at a high enough density. Moreover, it also seems not unlikely that a change in the distribution of clusters at the critical point of contact collapse may be expected. This possibility was explored in self-avoiding walks by Nidras (1997), who studied the percolation of clusters as a critical phenomenon.

Two contacts are said to be *adjacent* if they contain two vertices (one in each) which are a unit distance apart, or if they contain the same vertex. A *cluster* in an animal is a maximal set of pairwise-adjacent contacts (maximal with respect to adjacency; there are no more contacts which can be added to enlarge the cluster). An animal with a number of clusters is illustrated in figure 2. Observe that any edge in the animal with both endpoints in a cluster is considered to be part of the cluster. Edges with exactly one endpoint in a cluster are *perimeter edges* of the cluster (if the cluster is part of an animal, then at least some of the perimeter edges will be animal edges as well). Note that an edge cannot be in the perimeter of two clusters simultaneously. In this sense, the clusters are independent; the event that a cluster occurs in an animal is predicated only on the occurrence of its perimeter in the animal, and it is otherwise independent of what occurs elsewhere in the animal.

The *size* of a cluster is the number of contacts it contains (as opposed to the number of edges it contains). Suppose that there are $D(k)$ clusters with k contacts (and any number of animal edges), and with one vertex rooted at the origin. The number of clusters counted up to translation will be denoted by $d(k)$. Any cluster counted by $D(k)$ (or by $d(k)$) has at most $2(2d - 1)k$ animal edges (and also at most $2(2d - 1)k$ perimeter edges).

The *top vertex* and the *bottom vertex* in a cluster are the lexicographic most and lexicographic least vertices, respectively. Two clusters can be concatenated by translating the second cluster until its bottom vertex is one edge from the top vertex of the first animal. A new contact will form between these vertices. If the first cluster is rooted and has k_1 contacts, then it can be chosen in $D(k_1)$ ways. The second cluster cannot be rooted, and if it has k_2 contacts, then it can be chosen in $d(k_2)$ ways. The outcome for every pair of clusters is a unique rooted cluster with $k_1 + k_2 + 1$ contacts. Thus

$$D(k_1)d(k_2) \leq D(k_1 + k_2 + 1). \quad (3.1)$$

Since every contact and every animal edge in a cluster counted by $d(k_2)$ has both endpoints in the cluster, there are at most $2k_2$ vertices which can be chosen as a root. Thus $d(k_2) \leq D(k_2) \leq 2k_2D(k_2)$, and equation (3.1) can be manipulated into

$$D(k_1 - 1)D(k_2 - 1) \leq 2(k_1 + k_2 - 2)D(k_1 + k_2 - 1) \quad (3.2)$$

and thus $D(k - 1)$ satisfies a generalized supermultiplicative inequality discussed by Hammersley (1962). The consequence is the following theorem.

Theorem 2. *There exists a constant δ such that*

$$\lim_{k \rightarrow \infty} [D(k)]^{1/k} = \delta.$$

Proof. Note that each cluster can be changed into a lattice animal by turning all the contacts in it into edges. The resulting animal will have at most $k + 2(2d - 1)k = (4d - 1)k$ edges. On the other hand, some animals with at most $(4d - 1)k$ edges can be turned into clusters by changing some edges into contacts. Thus, $D(k) \leq \sum_{m=k}^{(4d-1)k} \binom{m}{k} A_m$, where A_m is the number of animals with m edges, rooted at the origin. It is known that $A_m \leq K^m$, for some finite constant K (Klein 1981), and thus $D(k) \leq C_0^{(4d-1)k}$ for some finite constant C_0 . Together with the supermultiplicative inequality in equation (3.2), this implies the existence of the limit as claimed (Hammersley 1962). \square

The generating function of clusters is defined by

$$D(z) = \sum_{k=0}^{\infty} D(k) z^k. \tag{3.3}$$

An immediate consequence of theorem 2 is that $D(z) < \infty$ if $z < \delta^{-1}$, and $D(z) = \infty$ if $z > \delta^{-1}$. These results imply that there is an infinite cluster at the root with probability one in a model where clusters are generated by $D(z)$. To see this, let α be the cluster at the origin and note that theorem 2 implies that

$$D(k) = \delta^{k+o(k)}. \tag{3.4}$$

If the size of α is $|\alpha|$, then the probability that α has size m is given by

$$P_z(|\alpha| = m) = \frac{D(m) z^m}{D(z)}. \tag{3.5}$$

$P_z(|\alpha| = m)$ is a probability distribution, and moreover, if $P_z(|\alpha| \leq m)$ is the probability that a cluster of size at most m is found in a model where clusters are generated by $D(z)$, then

$$P_z(|\alpha| \leq m) = \sum_{k=0}^m P_z(|\alpha| = k) \begin{cases} > 0 & \text{if } m < \infty \text{ and } z < \delta^{-1} \\ = 0 & \text{if } z > \delta^{-1}. \end{cases} \tag{3.6}$$

In other words, if m is taken to infinity, then

$$P_z(|\alpha| < \infty) = \begin{cases} 1 & \text{if } z < \delta^{-1} \\ 0 & \text{if } z > \delta^{-1}. \end{cases} \tag{3.7}$$

Consider now the situation where α is a cluster at the origin in an animal. The probability $\theta_n(\alpha)$ that a cluster α occurs at the origin in an animal of size n is found by noting that α must occur, and that the perimeter of α must also occur. In other words, if α has $k(\alpha)$ contacts then its weight is $z^{k(\alpha)}$, and if $P_n(\text{per}(\alpha))$ is the probability that the perimeter of α occurs in an animal of size n , then

$$\theta_n(\alpha) = \frac{z^{k(\alpha)}}{D(z)} P_n(\text{per}(\alpha)) \leq \frac{z^{k(\alpha)}}{D(z)}. \tag{3.8}$$

Thus, the probability that a cluster of size exactly k appears in an animal of size n is bounded from above by

$$\theta_n(|\alpha| = k) \leq \frac{D(k) z^k}{D(z)} \tag{3.9}$$

and consequently

$$\theta_n(|\alpha| \leq k) \leq \frac{\sum_{l \leq k} D(l) z^l}{D(z)}. \tag{3.10}$$

Since the right-hand sides of equations (3.8)–(3.10) are independent of n , take $n \rightarrow \infty$, and define $\theta = \lim_{n \rightarrow \infty} \theta_n$. Then, if $z > \delta^{-1}$, it appears from equation (3.6) that $\theta(|\alpha| \leq k) = 0$, and if k is taken to infinity, $\theta(|\alpha| < \infty) = 0$. In other words, the probability of a finite cluster at the origin is zero. Otherwise, the probability that a cluster of size at least k appears is given by

$$\theta(|\alpha| \geq k) = \frac{D(k) z^k}{D(z)} \tag{3.11}$$

because if a cluster of size k appears at the origin, then it may be a subcluster of a larger cluster (if its perimeter does not occur). If $z < \delta^{-1}$, then from equation (3.4),

$$\theta(\infty) = \lim_{k \rightarrow \infty} \theta(|\alpha| \geq k) = 0 \tag{3.12}$$

and this shows that $\theta(|\alpha| < \infty) = 1 - \theta(\infty) = 1$, in other words, the cluster at the origin is finite. These arguments shows that there is a percolation phenomenon in the animal at a critical value of z .

4. Numerical study of clusters in lattice animals

Animals of fixed size n and at contact activity z were sampled by a cut-and-paste metropolis Monte Carlo algorithm (Janse van Rensburg and Madras 1999). Clusters of contacts were detected in the animals by performing breadth-first searches through the animal, and statistics were collected on the distribution of clusters, and on the density of contacts in the neighbourhood of the centre of mass of the animal. The invariant limit distribution of the algorithm is

$$\Pi_z(k) = \frac{a_n(k) z^k}{\sum_k a_n(k) z^k} \tag{4.1}$$

for animals with k contacts.

The number of clusters of size s in an animal α of size n will be denoted by $n_s(\alpha)$. Following the arguments in Nidras (1997), the average size of a cluster per animal edge is given by

$$\langle n_s \rangle_z = \frac{\sum_{\alpha} n_s(\alpha) z^{k(\alpha)}}{n Z_n(z)} \tag{4.2}$$

where $k(\alpha)$ is the number of contacts in the animal α of size n . In analogy with sub-critical percolation clusters, it should be expected that $\langle n_s \rangle_z$ decays exponentially with s (Grimmett 1989), provided that $z < z_\delta$, where z_δ is the critical activity for percolation of the clusters (and z_c will be reserved for the critical activity for contact collapse). In other words, there is a correlation size $s_\xi(z)$ (this may be viewed as a typical cluster size) such that for large n ,

$$\langle n_s \rangle_z \sim e^{-s/s_\xi(z)}. \tag{4.3}$$

The distribution of clusters in animals of size 1000 is plotted in figure 3.

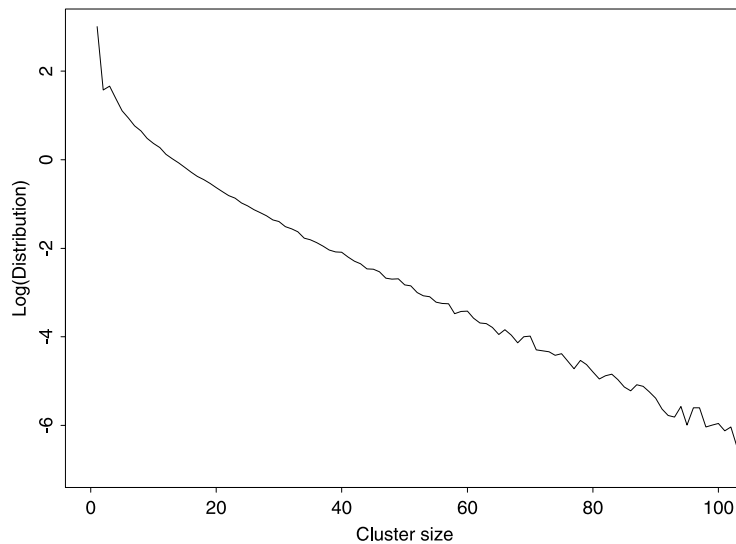


Figure 3. The distribution $\langle n_s \rangle_z$ of clusters as a function of the cluster size s . These data were collected from animals of size 1000 edges at an activity $z = 1.0$.

Table 1. $s_{\xi}(z)$ ($n = 1000$).

z	$s_{\xi}(z)$
1.0	18.9(1.2)
1.1	22.4(1.0)
1.2	32(2)
1.3	58(4)
1.4	84(6)
1.5	108(16)
1.6	162(22)
1.7	570(150)

As z approaches its critical value, $s_{\xi}(z)$ should diverge, this will be consistent with the view that the size of clusters diverge as the critical point is approached. In fact, the divergence should occur as

$$s_{\xi}(z) \sim |z_{\delta} - z|^{-1/\phi_p} \quad (4.4)$$

where ϕ_p is the *crossover* exponent associated with percolation of clusters (Nidras 1997). The correlation size $s_{\xi}(z)$ can be estimated by linear fits from data such as in figure 3, as long as $z < z_{\delta}$. This was done by assuming a normal dispersion of the data points about the best-fitted least-squares line (while discarding data at small values of s), and the results are listed in table 1. Once an estimate of z_{δ} has been made, then these data can be used to estimate ϕ_p from equation (4.4).

If z is large enough, then the cluster of contacts should have percolated, and this shows itself in the appearance of large clusters in the distribution $\langle n_s \rangle_z$. For example, in figure 4 the distribution of clusters $\langle n_s \rangle_z$ is plotted for $n = 1000$ at $z = 2.5$, and a peak appears for clusters of size around 1500 contacts. Similar effects are seen in data for percolation in a finite square (Stauffer 1979, Essam 1980).

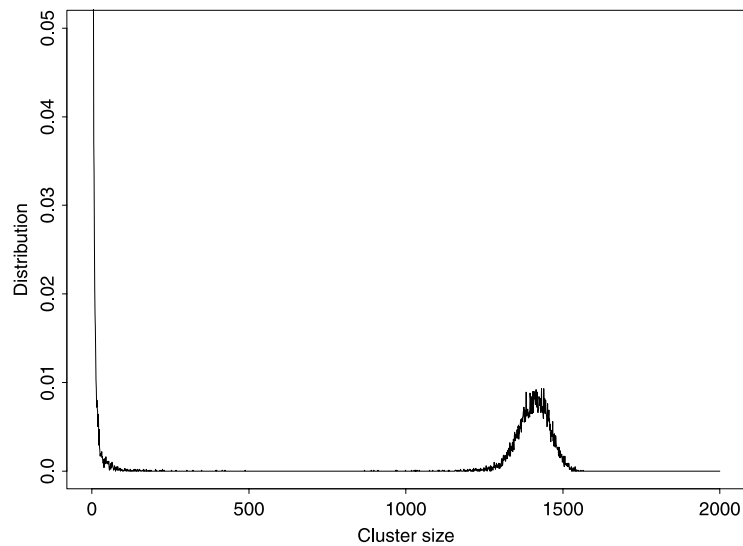


Figure 4. The distribution of clusters in an animal of size 1000 and with $z = 2.5$. The new peak around 1500 contacts is due to the appearance of a largest cluster of size comparable to that of the animal. This is an indication that percolation of the contacts occurred.

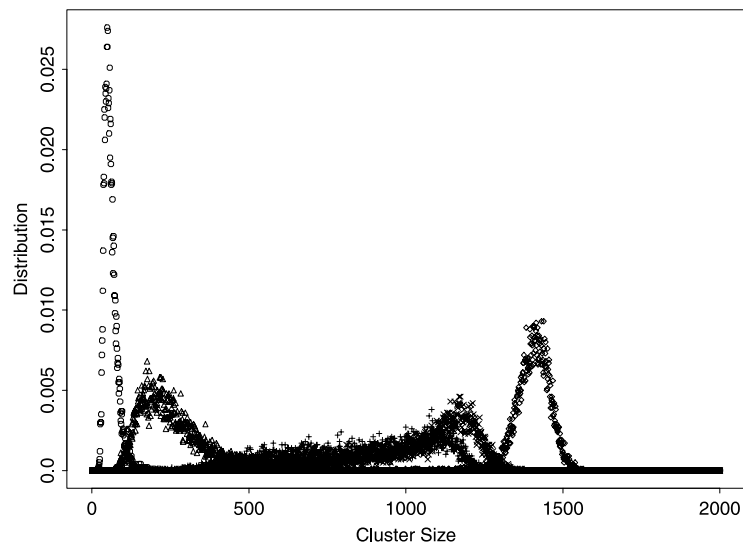


Figure 5. The distribution of the largest cluster in animals of size 1000 for $z = 1.0$ (\circ), $z = 1.5$ (Δ), $z = 1.9$ ($+$), $z = 2.0$ (\times) and $z = 2.5$ (\diamond).

The distribution of the largest cluster in the animal can also be used to detect a percolation phenomenon. In figure 4 the peak appearing for large clusters at around 1500 contacts must be entirely due to the largest clusters, since there is no room in an animal of size 1000 for a second largest cluster containing a significant number of contacts. In figure 5 the distributions of only the largest clusters are plotted for a variety of values of z . At $z = 1$ the largest clusters are distributed around a small number of contacts, this peak diminishes with increasing z (and

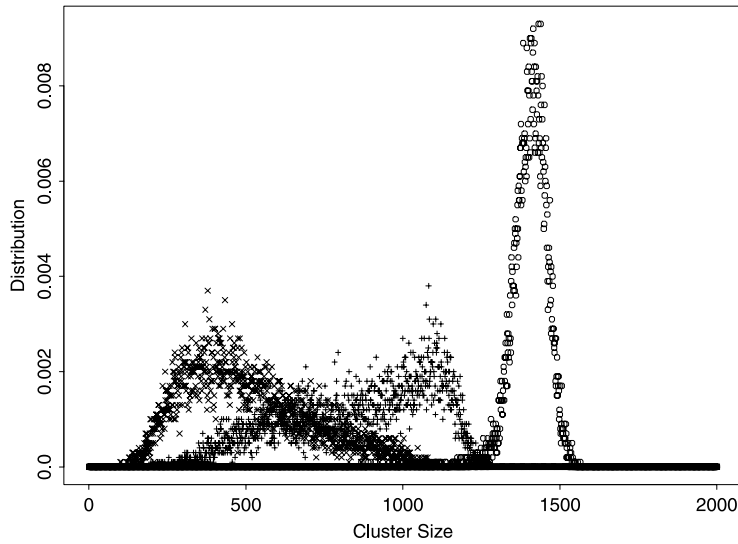


Figure 6. The distribution of the largest cluster in animals of size 1000 for $z = 1.7$ (\times), $z = 1.9$ ($+$) and $z = 2.5$ (\circ).

shift towards slightly larger clusters) with increasing z . At around $z = 1.8$ the distribution is flattish, and for larger values of z a peak appears at cluster sizes of over 1000. This appearance can be interpreted as the appearance of a percolated cluster. In figure 6 the distributions are plotted for $z = 1.7, 1.9$ and 2.5 , again suggesting a percolation phenomenon around $z = 1.8$. A double peak was not observed in any simulation; this suggests that the percolation of clusters is a continuous transition.

The average size of the largest cluster could be used to determine the critical value of z . If the distribution of largest clusters is given by $\Delta_z(k)$, then the mean size of the largest cluster is

$$\langle k \rangle_z = \frac{\sum_k k \Delta_z(k)}{\sum_k \Delta_z(k)}. \tag{4.5}$$

Since the percolated cluster will have size $O(n)$, it is necessary to compute $\langle k \rangle_z/n$, and in the limit that $n \rightarrow \infty$ it should not be unreasonable to expect that

$$\lim_{n \rightarrow \infty} \frac{\langle k \rangle_z}{n} \begin{cases} = 0 & \text{if } z < z_\delta \\ > 0 & \text{if } z > z_\delta \end{cases} \tag{4.6}$$

where z_δ is the critical value of the activity. The data in figures 5 and 6 can be used to estimate the ratio $\langle k \rangle_z/n$ as a function of z . This was done for a number of different values of n ; the results are plotted in figure 7. The curves are interpolations of the data, and the values of n were in $\{200, 400, 600, 800, 1000\}$.

The curves in figure 7 almost all intersect at about the same point. For values of z less than that of the intersection the curves decrease with increasing n , and for larger values of z , the curves increase. If it is assumed that the curves approach a limiting curve with mean largest cluster size equal to zero for values of z less than the common point of intersection, then one may take the value of z at the point of intersection as an estimate of the critical value of z at which percolation of contacts occur. This approach gives

$$z_\delta = 1.93 \pm 0.05. \tag{4.7}$$

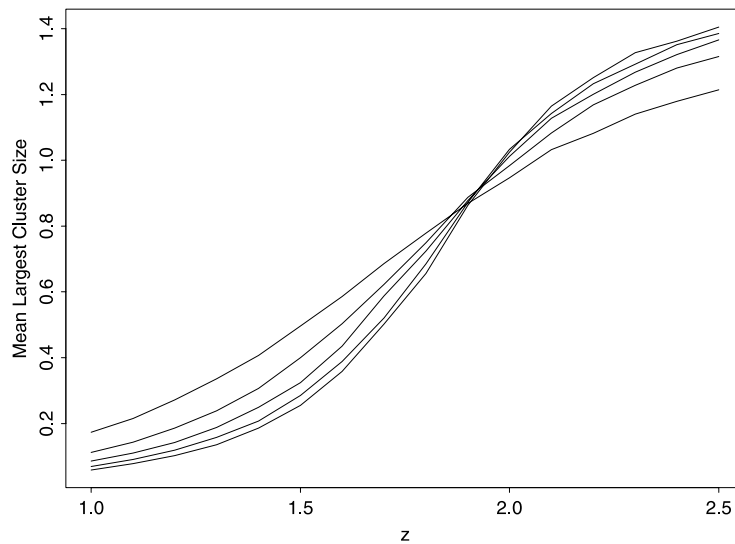


Figure 7. The mean largest cluster size per edge in collapsing animals as a function of z . The common point of intersection may be taken as an estimate of the critical percolation point of clusters. The size of the animals considered were {200, 400, 600, 800, 1000}.

The collapse transition in animals has been estimated to occur at $z_c = 2.05 \pm 0.16$ (Janse van Rensburg *et al* 1999), with the error bar a 95% confidence interval. This is not inconsistent with the result in equation (4.7), but more precise measurements of both the percolation point of contacts, and of collapse in animals will be necessary before one could separate these two values, or say with some confidence that they are the same.

The estimated value of z_δ in equation (4.7) makes it possible to estimate the exponent in equation (4.4) by using the data in table 1. A log–log weighted least-squares fit to the data gives

$$\phi_p = 0.406 \pm 0.026 \quad (4.8)$$

with a 95% confidence interval. The exponent ϕ_p has also been estimated for percolation of contact-clusters in a model of collapsing self-avoiding walks (Nidras 1997). The value found there is 0.55 ± 0.15 (and note that this includes the estimate in equation (4.8) in its error bar so that one may not draw any conclusions as to the nature of the relation between contact percolation in animals and in walks).

More evidence for percolation of contact clusters can be obtained by studying the density profile of contacts. Two more simulations with animals of sizes 2000 and 3000 were performed to gain more data on this. The density of contacts in spheres of radii R centred at the centre of mass is defined by

$$\rho_n(z, R) = \frac{\sum_{\alpha} m(\alpha, R) z^{\alpha}}{R^2 Z_n(z)}. \quad (4.9)$$

$\rho_n(z, R)$ was computed for $R \geq 1$ in increments of one lattice step up to a distance of five times the root mean square radius of gyration of the animal. In figure 8 the density of clusters is plotted as a function of R for $n = 2000$ and for values of z in {1, 1.5, 1.8, 2.0, 2.5}. For $z = 1$ the density of contacts is low for all values of R , and it goes to zero as R increases. The non-zero density at small values of R is a consequence of a pattern theorem for animals (Madras 1999).

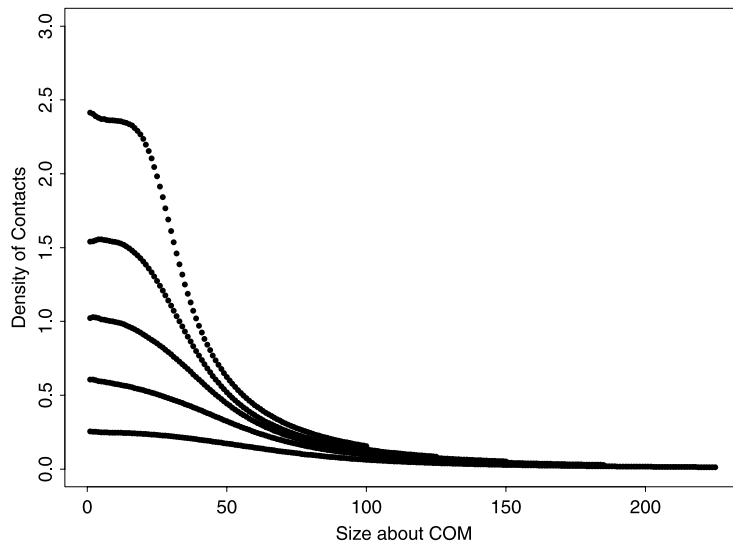


Figure 8. The profiles of contact densities about spheres centred at the centre of mass of animals of size 2000 edges. The radius R of the spheres in lattice steps along the horizontal axis, while the density $\rho_n(z, R)$ is expressed as a number density (number of contacts times π per unit volume). The profile is flattest for $z = 1$ (bottom points) but shows a sharp increase with z increasing in $\{1, 1.5, 1.8, 2.0, 2.5\}$. In the collapsed phase the profile shows a sharp boundary, but this is not the case in the expanded phase.

The density $\rho_n(z, R)$ is more interesting in the limits that first $n \rightarrow \infty$ followed by $R \rightarrow \infty$. In the case that n is large, it seems not unreasonable to expect that the number of contacts in a sphere of radius R is proportional to $R^{1/v}$, since the number of contacts should be proportional to the number of edges in the animal. Thus, the density should scale as

$$\rho_n(z, R) \sim R^{1/v-d} \quad \text{if } R \ll n^v. \tag{4.10}$$

In the expanded phase then, $\rho_n(z, R) \rightarrow 0$ if $n \rightarrow \infty$ and then $R \rightarrow \infty$, but if $z > z_\delta$, then this should approach a constant greater than zero, since $v = 1/d$ in the collapsed phase:

$$\lim_{R \rightarrow \infty} \lim_{n \rightarrow \infty} \rho_n(z, R) \begin{cases} = 0 & \text{if } z < z_\delta \\ > 0 & \text{if } z > z_\delta. \end{cases} \tag{4.11}$$

An estimate for $\lim_{R \rightarrow \infty} \lim_{n \rightarrow \infty} \rho_n(z, R)$ by choosing R to be one-half the root mean square radius of gyration can be made: in this case R is small enough compared to n to avoid surface effects, but it is also big enough to include a sizeable number of contacts. The dependence of this density on z is plotted in figure 9 for values of n ranging from 100 (the points indicated by \circ) to $n = 3000$, the points denoted by $*$.

The data in figure 9 seems to approach a limiting curve defined by equation (4.11) with increasing n , and this is reminiscent of a similar situation in percolation where the probability that there is an infinite cluster at the origin, $P_\infty(p)$ is expected to be $P_\infty(p) = 0$ if $p < p_c$ and $P_\infty(p) > 0$ if $p > p_c$. A rough extrapolation of the data in figure 9 shows that the critical point (the inflection point in the data could be taken as an estimate of the critical point) should occur at a value not inconsistent with the value taken from figure 7.

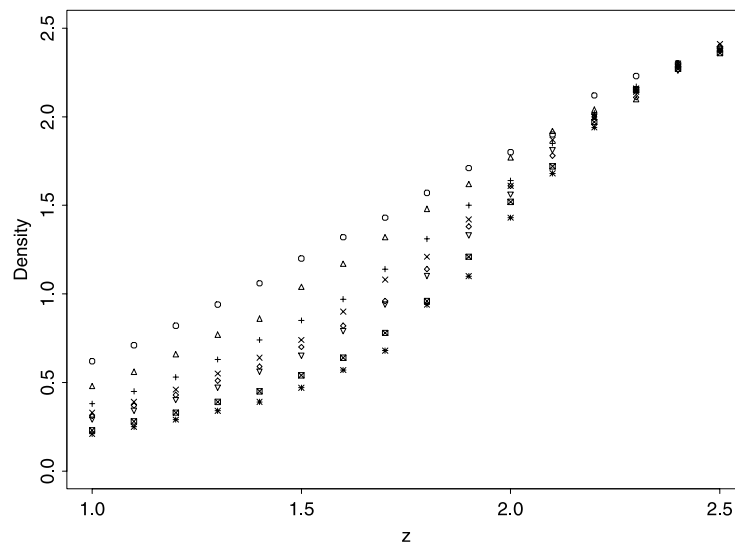


Figure 9. The density of contacts as a function of z in a sphere of radius one-half of the radius of gyration of the animals. The data denoted by \circ corresponds to animals of size 100, and the remaining data corresponds to animals of sizes $\{200, 400, 600, 800, 1000, 2000, 3000\}$ with decreasing densities as n increases in the graph from \circ for $n = 100$ to $*$ for $n = 3000$. The data seems to approach a limiting curve defined by equation (4.11).

5. Conclusions

In this paper the θ -transition in a model of self-interacting animals were considered. In the first instance, a model of animals in the cycle-contact ensemble was considered, and I proved that there is a non-analyticity in its free energy at points which include the critical percolation point. In this case the connection between self-interacting lattice animals and percolation was exploited.

In the second instance a model of animals in the contact ensemble was considered. It is not known that there is a non-analyticity in the free energy in this model, but in section 3 the percolation of clusters of contacts in this model is considered. A numerical study of the clusters in this model is reported in section 4; in particular, the data shows that there is a percolation of clusters of contacts at a critical value $z_\delta = \delta^{-1}$, where δ is the growth constant of clusters of contacts whose existence was established in section 3. It is not known that the percolation of clusters are associated with the collapse of animals, but the data on the density profile of contacts in figures 8 and 9 strongly suggest this.

Acknowledgment

The author is supported by a grant from NSERC (Canada).

References

- Aizenman M and Newman C M 1984 *J. Stat. Phys.* **36** 107
- de Gennes P-G 1975 *J. Physique Lett.* **36** L55
- Derrida B and Hermann H J 1983 *J. Physique* **46** 1365
- Domb C 1976 *J. Phys. A: Math. Gen.* **9** L141

- Essam J W 1980 *Rep. Prog. Phys.* **43** 833
- Flesia S and Gaunt D S 1992 *J. Phys. A: Math. Gen.* **25** 2127
- Flesia S, Gaunt D S, Soteris C E and Whittington S G 1992 *J. Phys. A: Math. Gen.* **25** 3515
- 1993 *J. Phys. A: Math. Gen.* **26** L993
- 1994 *J. Phys. A: Math. Gen.* **27** 5831
- Gaunt D S and Flesia S 1990 *Physica A* **168** 602
- 1991 *J. Phys. A: Math. Gen.* **24** 3655
- Grassberger P and Hegger R 1995 *J. Physique I* **5** 597
- Grimmett G 1989 *Percolation* (Berlin: Springer)
- Hammersley J M 1962 *Math. Proc. Camb. Phil. Soc.* **58** 235
- Hara T and Slade G 1990 *J. Stat. Phys.* **59** 1469
- 1995 *Comb. Theor. Comput.* **4** 197
- Harary F 1960 *MagyarTud. Akad. Mat. Kutató Intezetének Közleményei* **5** 63
- Janse van Rensburg E J and Madras N 1997 *J. Phys. A: Math. Gen.* **30** 8035
- Janse van Rensburg E J, Orlandini E and Tesi M C 1999 *J. Phys. A: Math. Gen.* **32** 1567
- Klarner D 1967 *Can. J. Math.* **19** 851
- Klein D J 1981 *J. Chem. Phys.* **75** 5186
- Lubensky T C and Isaacson J 1979 *Phys. Rev.* **20** 2130
- Madras N 1999 *Ann. Comb.* **3** 357
- Madras N and Janse van Rensburg E J 1997 *J. Stat. Phys.* **86** 1
- Mazur J and McCrackin F L 1968 *J. Chem. Phys.* **49** 648
- Mazur J and McIntyre D 1975 *Macromolecules* **8** 464
- Meirovitch H and Lim H A 1990 *J. Chem. Phys.* **92** 5144
- Nidras P P 1997 Critical behaviour of geometric cluster models *PhD Thesis* Department Mathematics and Statistics, University of Melbourne
- Park I H, Kim J H and Chang T 1992 *Macromolecules* **25** 7300
- Stauffer D 1979 *Phys. Rep.* **54** 1
- Sun S T, Nishio I, Swislow G and Tanaka T 1980 *J. Chem. Phys.* **73** 5971
- Tesi M C, Janse van Rensburg E J, Orlandini O and Whittington S G 1996 *J. Stat. Phys.* **82** 155
- Whittington S G, Torrie G M and Gaunt D S 1983 *J. Phys. A: Math. Gen.* **16** 1695