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Statistics of lattice animals

Hsiao-Ping Hsu *, Walder Nadler, Peter Grassberger

John-von-Neumann Institute for Computing, Forschungszentrum Jülich, D-52425 Jülich, Germany

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Abstract

The scaling behavior of randomly branched polymers in a good solvent is studied in two to nine dimensions, modeled by lattice animals on simple hypercubic lattices. For the simulations, we use a biased sequential sampling algorithm with re-sampling, similar to the pruned-enriched Rosenbluth method (PERM) used extensively for linear polymers. We obtain high statistics of animals with up to several thousand sites in all dimension $2 \leqslant d \leqslant 9$. The partition sum (number of different animals) and gyration radii are estimated. In all dimensions we verify the Parisi–Sourlas prediction, and we verify all exactly known critical exponents in dimensions 2, 3, 4, and $\geqslant 8$. In addition, we present the hitherto most precise estimates for growth constants in $d \geqslant 3$. For clusters with one site attached to an attractive surface, we verify the superuniversality of the cross-over exponent at the adsorption transition predicted by Janssen and Lyssy.

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1. Introduction

Site lattice animals are clusters of connected sites on a regular lattice. Such clusters play an important role in many models of statistical physics, as percolation and the Ising model. The ensemble of site animals is defined by giving the same weight to all clusters with the same number N of sites. Similarly one can define bond animals and site/bond trees. They are in the same universality class (same exponents, same scaling functions) as randomly branched polymers.

Therefore the number of animals (i.e. the microcanonical partition sum) and the gyration radius should scale for large N as

$$Z_N \sim \mu^N N^{-\theta}(1 + b_z N^{-\Delta} + \cdots), \tag{1}$$

and

$$R_N \sim N^{\nu}(1 + b_z N^{-\Delta} + \cdots). \tag{2}$$

In the present paper we verify all previous predictions [1–4] by means of a novel Monte Carlo algorithm which follows essentially the strategy used in the *pruned-enriched Rosenbluth method* (PERM) [5]. This is a recursively (depth first) implemented sequential sampling method with importance sampling (bias) and re-sampling ("population control").

* Corresponding author.
E-mail address: h.p.hsu@fz-juelich.de (H.-P. Hsu).

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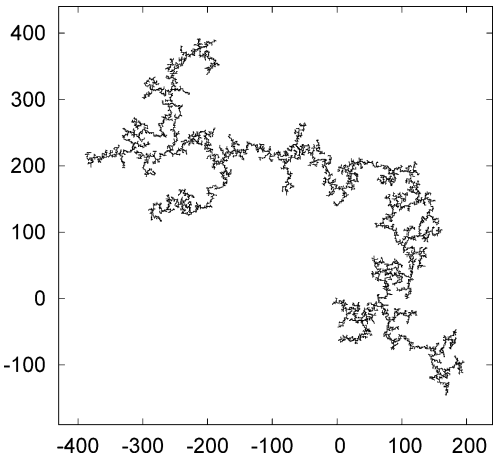

Fig. 1. A typical lattice animal with 12000 sites on the square lattice.

Essentially we start simulating site percolation clusters by a *breadth first* Leath algorithm [6] at a slightly subcritical value of the occupation probability, re-weigh them according to the animal ensemble, and prune or branch the further growth according to a heuristic fitness function. In contrast to most previous applications of PERM, this fitness function is *not* the weight with which the actual configuration would contribute to the partition sum, but is closely related to it. A typical 2-d site animal is shown in Fig. 1.

2. Numerical results

We first studied site animals in 2 to 9 dimensions. Our estimates of the growth constant μ, as well as all the exponents θ, ν, and Δ are listed in Table 1. They are all in very good agreement with previous predictions [1–4,7]. In particular, our data satisfy the Parisi and Sourlas prediction $\theta = (d-2)\nu + 1$ [3], see Fig. 2. Next, we studied site animals grafted to a planar attractive surface. The partition sum now is written as

$$Z_N^{(1)}(q) = \sum_{m=1}^{N} A_N(m) q^m, \tag{3}$$

where $A_N(m)$ is the number of configurations of lattice animals with N sites m of which are located on the walls, and $q = \mathrm{e}^{\epsilon/KT}$ is the Boltzmann factor, $\epsilon > 0$ is the attractive energy between the monomer and the wall. As $q \to 1$, there is no attraction between the monomer and the wall, i.e. $Z_N^{(1)}(1) \sim Z_N$. On the other hand it is clear that any cluster will collapse onto the wall, if q becomes sufficiently large. Therefore we expect a phase transition from a grafted but otherwise detached phase to an adsorbed phase, similar to the transition observed also for linear polymers.

Table 1
Main results for site animals. For convenience we also give in the second column the critical p-values for site percolation

d	p_c	$a = \ln \mu$	θ	ν	Δ
2	0.5927	1.4018155(30)	1.0 (exact)	0.6412(5)	0.9(1)
3	0.3116	2.1218588(25)	3/2 (exact)	1/2 (exact)	0.75(8)
4	0.1968	2.587858(6)	1.835(6)	0.4163(30)	0.57(8)
5	0.1407	2.922318(6)	2.080(7)	0.359(4)	0.47(7)
6	0.1090	3.178520(4)	2.261(12)	0.315(4)	0.39(6)
7	0.0889	3.384080(5)	2.40(2)	0.282(5)	0.26(6)
8	0.0752	3.554827(4)	5/2 (exact)	1/4 (exact)	log(?)
9	0.0652	3.700523(10)	5/2 (exact)	1/4 (exact)	0.25(5)

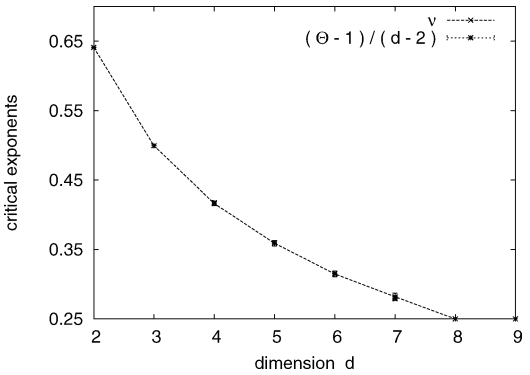

Fig. 2. The critical exponents ν and $(\theta-1)/(d-2)$ against d.

Near the critical point we expect a scaling ansatz

$$Z_N^{(1)}(q) \sim \mu^N N^{-\theta_s} \Psi\big[(q-q_c)N^{\phi}\big], \tag{4}$$

with the exponent θ_s and the crossover exponent ϕ being new exponents. Evaluating the derivative of $\ln Z_N^{(1)}(q)$ with respect to q at $q = q_c$, we obtain for the average energy $E_N(q_c) = \langle \epsilon m \rangle \sim N^{\phi}$. From the second derivative we obtain for the specific heat per monomer near (but not exactly at) the critical point $C_N(q) = \frac{1}{NKT^2}(\langle(\epsilon m)^2\rangle - \langle \epsilon m \rangle^2) \sim (q-q_c)^{-\alpha}$ with $\alpha = 2 - 1/\phi$. In principle, all three scaling laws can be used to locate the critical value q_c. With conventional (Metropolis type) Monte Carlo simulations usually the scaling law of specific heat is used since precise estimates of the partition sum are difficult to obtain. With PERM we do have very precise estimates of $Z_N^{(1)}(q)$,

Table 2
Critical Boltzmann factors, crossover exponents, and critical exponents θ_s at the adsorption transition for site animals on simple (hyper-)cubic lattices grafted to a flat attractive wall

Dimension	q_c	ϕ	θ_s
2	2.2778(8)	0.480(4)	0.870(9)
3	1.4747(6)	0.50(1)	1.476(7)
4	1.2674(6)	0.50(2)	1.91(1)
5	1.1786(5)	0.51(3)	2.18(4)

and therefore we can use Eq. (4), indeed the scaling of the average $E_N(q_c)$, which gives—together with the two others—the most precise estimate.

Taking into account the correction to scaling, the best estimates of the critical values of q_c and the cross-over exponents ϕ are listed in Table 2. Our results are in perfect agreement with the Janssen–Lyssy prediction $\phi = 1/2$ in all dimensions $d \geqslant 3$ [4].

3. Conclusions

We have shown that the basic idea of PERM can also be applied to lattice animals. High statistics of animals with up to several thousand sites are obtained in all dimension $2 \leqslant d \leqslant 9$. We verified a number of theoretical predictions. In particular, we verified the Parisi–Sourlas connection between entropic and Flory exponents, and we verified the values of these exponents whenever they are exactly known. We also verified that the cross-over exponent for branched polymer adsorption on planar walls is super-universal for $d > 2$, as predicted some time ago (but not for $d = 2$!), and we gave precise estimates of the other critical exponents at this adsorption transition. Our methods can also be applied to bond animals and lattice trees [7], and are equally efficient in these cases.

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