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LETTER TO THE EDITOR

# Surface structure and anisotropy of Eden clusters

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**Abstract.** The simple Eden model is simulated with clusters which are orders of magnitude larger than those of some previous work. The 'surface' (perimeter) is slightly anisotropic and feels the underlying structure of the square lattice even for 17 million cluster sites. The width of the surface layer increases with increasing cluster mass, with an effective exponent presumably larger than 1/4 for averages over the whole circumference, and perhaps equal to 1/4 for flat surfaces. Width averages over a small angle are compared with the recent prediction of Plischke and Racz. Even 17 million sites are not enough to see directly the asymptotic behaviour.

The growth and forms of clusters [1, 2], and among them those of Eden clusters [3], are of great current interest [4, 5]. In the simplest version of the Eden cluster one starts from one occupied site as a seed on a lattice, and at every time step occupies one randomly selected perimeter site. Perimeters are the empty neighbours of the already occupied growth sites and can be called growth sites because of their kinetic implications. The growth sites in percolation [6] reduce to these growth sites only in the limit $p \to 1$. Since there are no such perimeter sites deep in the cluster interior [7, 8], in the Eden model we do not have to distinguish between perimeter, surface, and growth sites, in contrast to more complicated models like crystal growth [9], percolation [10]†, or Ising domain walls [11]. We do not discuss here the possible biological implications and other applications of the Eden growth model but regard it as one of the most basic examples of clusters. For the same reason we restrict ourselves here to the aforementioned version of this model (model A of [5]) and do not consider the more complicated versions B and C of reference [5] even though they might be easier to investigate asymptotically.

Most of our effort was put into Monte Carlo simulations on the square lattice, but we will also mention surface studies on a simple cubic lattice.

The width $W$ of the surface layer is defined through

$$W^2 = \langle r^2 \rangle - \langle r \rangle^2$$

and is expected to vary asymptotically with some power of the number $s$ of sites in a cluster:

$$W \propto s^x \qquad (s \to \infty).$$

Here $r$ is the distance of a surface site from the origin (or centre of mass) of the cluster. Peters *et al* [7] claimed from simulations of full clusters containing about $10^3$ sites

† For growth surfaces see [10a].

that the width is proportional to the cluster radius, i.e. $x = 1/d$ in $d$ dimensions for $d = 2$ and 3. Instead, Plischke and Racz [4] observed in similar simulations an effective width exponent $x$ near 0.18 for $d = 2$, for clusters up to $s = 4000$, but found it to decrease with increasing $s$ and suggested an asymptotic logarithmic variation ($x = 0$). Jullien and Botet [5], and more recently Plischke and Racz [4], simulated flat surfaces in a strip geometry with lengths $R$ up to 768; they found $x$ first to decrease, then to increase with increasing $R$, and concluded $x = 1/4$ in two dimensions. That latter value would correspond to the standard behaviour of $(d-1)$-dimensional surfaces in $d$ dimensions [9-12]†: the surface width increases as the square root of the radius for $d = 2$, logarithmically for $d = 3$, and remains finite for $d$ above 3. (The Eden clusters are fully compact and have a radius $R$ increasing [7, 8] as $s^{1/d}$; thus the width increases as $R^{xd}$, and $xd = 2x$ in two dimensions can be called the fractal width dimension. The square-root law thus means $2x = 1/2$.) Simulations for much larger systems were asked for [4], and are presented here, to clarify these discrepancies between $x = 0$, $x = 1/4$, and $x = 1/2$. (If the Eden clusters would behave like self-avoiding walks we would have $x = 3/4$, and $x = 1$ were they straight lines; $x > 1$ or $x < 0$ is impossible.)

We needed a computer time of about 13 $\mu$s on an IBM 3081 (one byte per site) and CDC Cyber 176 (one bit per site) to add one site; storing each site in a full word reduced this time by a factor 3 on the CDC computer. More than 100 h were spent in total. Each site of a large lattice carried one bit of information: 'Yes' if it is occupied (or a perimeter site), and 'No' if it is empty. In addition, the coordinates of all current perimeters are stored. Once one of these perimeter sites is selected randomly as occupied we check for each of its neighbours if it is an empty site separated from the old cluster; if the answer is 'yes' we include it in the perimeter list. Typically a thousand different clusters were generated and averaged over. To find easily the variation of the effective $x$ with cluster size $s$, our $s$ values were chosen as integer powers of 2; the effective exponent was then determined as

$$x(s) = \log[W(s\sqrt{2})/W(s/\sqrt{2})]/\log 2.$$

We also looked at the anisotropies in the direction of the lattice axes and of the lattice diagonal, that means we investigated the ratio of the mean square distance (from the origin) of perimeters along these directions to the mean square distance of all perimeter sites. (The non-monotonic behaviour discussed below for $x = x(s)$ at first suggests a computing error. However, we found it in two separate calculations made with different algorithms on different computers and programmed with a time interval of one year. Moreover this unusual behaviour is consistent with the results published by Jullien and Botet [5] as well as Plischke and Racz [4].)

For clusters above $s = 2^{22} = 4$ million, we simulated only one quadrant of the cluster, which allows the study of $s = 2^{24} = 17$ million with the memory and computer time of $s = 2^{22}$. The growth laws near the lattice axes at the border of the quadrant are influenced by these boundaries; thus the anisotropies calculated along the lattice axes are unreliable and the width averaged over the whole perimeter is slightly diminished in such quadrant simulations. However, the anisotropy along the diagonal as well as the effective width exponent seem not to be affected by these boundary effects and thus are used in our study. For the strip geometry [5] we let the growth process start upward from a line of length $R$ until it reaches a height of $6R$. These results were extrapolated where

† For a recent review see also [12a].

necessary (large $R$) to infinite heights. Then the exponent $x$ is defined through $W \propto R^{2x}$ in two dimensions.

For clusters with a few thousand sites we first checked the assertion $x = 1/d$ of Peters *et al* [7] which was already criticised in reference [4]. Their complicated definition of the surface (needed for other clusters [7-11] but not for the fully compact Eden clusters) leads to difficulties with the binned density profile near the origin. There the density is basically 0/0; depending on the details of the binning procedure we recovered the conflicting results of both references [4] and [5]. Using a better evaluation of the surface width [4] or identifying [5] surface with perimeter we recovered the results of Plischke and Racz, not those of Peters *et al.* Thus the surface widths determined by Peters *et al* should be discarded, although we did confirm their cluster radii and number of perimeter sites. Clearly, the method of Jullien and Botet [5] to look at the perimeter sites only is simpler and more reliable for Eden clusters and thus is used here.

Figure 1 gives our main results on the square lattice. For the round clusters (or quadrants) the effective width exponent $x$ decreases with $s$, reaches the previous value 0.18 in the size range investigated by Plischke and Racz and continues to decrease to about 0.16. But for clusters containing millions of sites it increases again with $s$, reaching $x = 0.28 \pm 0.01$ between $s = 2^{22}$ and $s = 2^{23}$, and even $x = 0.36 \pm 0.02$ between 8 and 17 million. Clearly large scale computational efforts, as requested in reference [4], were needed to show in this way that $x$ does not continue to go to zero as suggested before [4] on the basis of much smaller clusters. It seems likely that the asymptotic exponent $x$ is larger than 1/4 for finite clusters. For our largest clusters with 23 million sites, small sections of the surface look similar to figure 3($a$) of reference [5].

For the flat surfaces of the strip geometry the same non-monotonic behaviour of $x(R)$ is seen, as found before [4, 5]. However, our simulations show the increase of

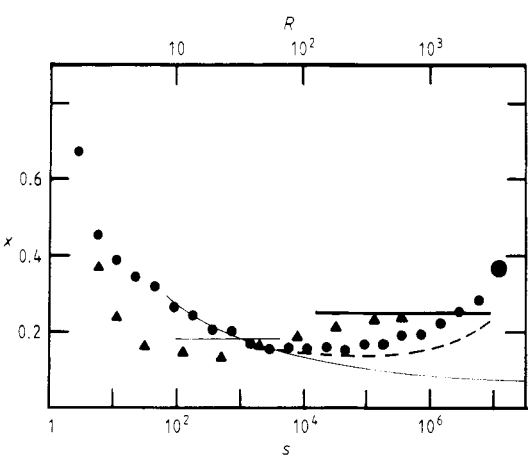


**Figure 1.** The effective exponent $x$ for surface width $\xi \propto s^x \propto R^{2x}$ for two-dimensional Eden clusters and strips. The bold full line indicates the suggestion $x = 1/4$ of Jullien and Botet. The light horizontal line gives the size range and effective exponent of Plischke and Racz and the full decaying curve their suggested asymptotic law (logarithmic increase). The circles show our Monte Carlo results for clusters as function of number $s$ of sites (lower scale), triangles our data for strips of linear dimension $R$ (upper scale). The statistical error is of the order of the symbol size. The broken curve gives $x$ for the width in a small sector near the lattice diagonal.

$x$ after the minimum to be less steep than for round clusters. It seems possible that the asymptotic exponent is 1/4 as for usual surface roughening; between $R = 512$ and $R = 724$ our last exponent is 0.24 with an error of the order of 0.02. (Our height was typically $6R$; for large $R$ we had to extrapolate to infinite heights.)

(Even for these flat surfaces the spatial distribution of surface sites is unsymmetric: it is possible to find isolated holes rather far behind the growth front but impossible to have isolated occupied sites ahead of the surface. This asymmetry, however, seems to go to zero for $R \to \infty$, as a comparison of density profiles shows. The symmetric section seems to follow a Gaussian law, as found in reference [4].)

How can we explain this highly complex behaviour of the surface width? Figure 2 indicates qualitatively that Eden clusters are not completely round, the underlying lattice structure forces them to deviate from circles towards diamond shape. Figure 3 shows that even the largest Eden clusters are slighly anisotropic, with the degree of

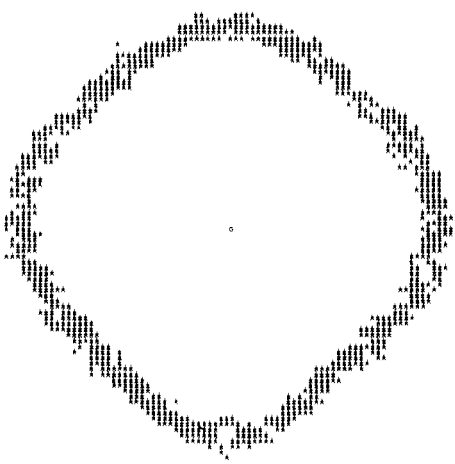

**Figure 2.** The centre of perimeter region, averaged over nine clusters with 4 million sites each. To make the very slight anisotropy more visible, most of the inner space is omitted; actually the radius is two orders of magnitude larger than the width of the ring.

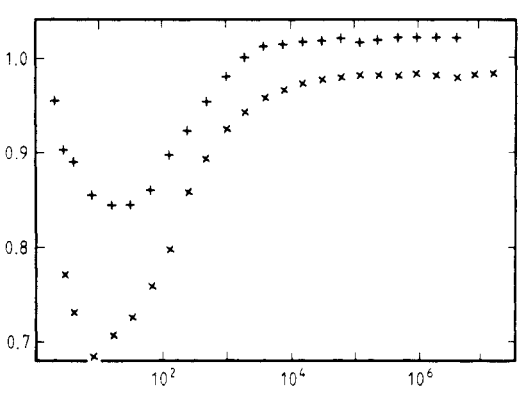


**Figure 3.** Asymmetry of two-dimensional Eden clusters, as measured by the ratio of the mean square distance along the lattice axes (+) or lattice diagonal (×) to the overall mean square distance of surface sites. Note the logarithmic scale for the cluster size $s$.

anisotropy not going to zero for $s \to \infty$. Clusters seem to grow slightly faster along a lattice axis than in the diagonal direction. Such anisotropies were predicted by Dhar [13] at least for much higher dimensionalities $d$. The anisotropy we found seems more 'serious' than that found by Family *et al* [14] for other cases. They look at each cluster separately and determine for each the axes of largest and smallest moment of inertia; thus their anisotropy might vanish in the average if the width is determined with respect to fixed lattice axes. (We thank F Leyvraz for explaining this point to us.) Our figure 3, on the other hand, already gives this anisotropy with respect to a fixed coordinate system and shows that it does not vanish.

If, therefore, the perimeter ring surrounding the Eden cluster is not exactly circular, this small anisotropy will eventually influence the surface width if it is averaged over the whole ring. This total width might approach the cluster radius, multiplied with a small constant factor accounting for the anisotropy. Then asymptotically we have $x = 1/d = 1/2$, compatible with our data in figure 1 and in agreement with the incorrectly derived claim of Peters *et al* [7].

A more 'intrinsic' surface-width definition would be to look only at perimeters exactly along the lattice diagonal. Then the statistics is very bad, but our data suggest this restricted average to give slightly smaller $x$ values for very large clusters than the unrestricted average. Thus finally we looked at the somewhat larger number of perimeter sites in a narrow sector near the lattice diagonal. The effective exponents, with error bars of the order of 0.03, follow the broken line in figure 1 and seem to be compatible with $x = 1/4$ as for the flat surface. The recent theory of Plischke and Racz [4] predicts this exponent to be $1/4z = 0.16 \pm 0.02$, which is in excellent agreement with our *effective* exponent up to $s = 2^{22}$ but not with the upward trend for our largest clusters. This prediction thus still remains doubtful though not excluded.

To give some absolute numbers besides exponents: for $s = 2^{24}$ we found from nearly 20 000 clusters (quadrant simulation only) a surface width $12.25 \pm 0.02$ and an anisotropy in the diagonal direction of $0.9838 \pm 0.0002$; the RMS distance from the origin for the about 15 600 sites on the perimeter ring was about 1154, the largest distance about 1225.

(On the simple cubic lattice we went up to $s = 2^{18}$ sites and again found results for smaller clusters in conflict with those of Peters *et al* [7] and consistent with those of Plischke and Racz [4]. The thickness increases much weaker than the radius, possibly logarithmically as figure 4 suggests: $x = 0$. Of course, we do not know what happens for larger clusters not investigated here.)

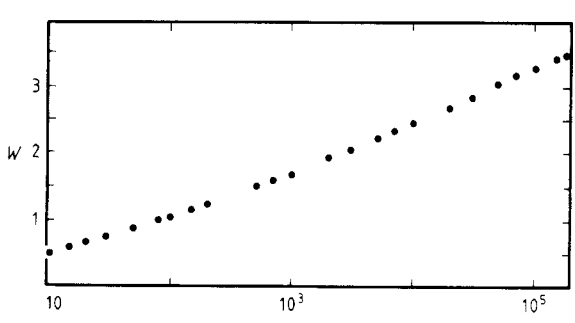


**Figure 4.** Overall surface width as function of cluster size $s$ for simple cubic lattice. The data for large $s$ follow a straight line suggesting a logarithmic increase with cluster size.

The simplest interpretation of our results therefore is a surface width increasing, as usual in two dimensions, with the square root of the radius, $x = 1/2$. Then we would not be forced to introduce a completely new width exponent for the simple Eden clusters. The anisotropy of the clusters makes it meaningless to define the surface width by a simple average over the whole circumference of the Eden cluster. In summary, with great computational effort a qualitatively clearer picture was found, or at least suggested. Nevertheless the approach towards the asymptotic properties of the seemingly simple Eden model is quite complex. An application of vector computers to this problem is planned [15], as well as simulation of flat surfaces in other than the lattice direction [16].

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*Note added in proof.* Meanwhile the anisotropy of 3D Eden clusters has been confirmed for clusters up to 6 million sites by Hirsch. Wolf has shown that for 2D Eden clusters the intrinsic surface width as well as the number of growth sites per unit length depend on the global orientation of the surface.

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