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On the growth of Eden clusters in continuous time

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Abstract. Power series in the time are constructed for various versions of Eden-like clusters. The use of an Euler transform gives series with smoothly varying coefficients of positive sign, indicating that the radius of convergence of the series in the new variable is the physically interesting singularity. The growth exponent obtained from the beginning terms of the series is larger than expected from the asymptotic behaviour of large compact clusters, indicating that the accurate determination of the asymptotic form requires very long series.

1. Introduction

The Eden model (Eden 1961) is one of the simplest models for the unlimited growth of a cluster on a lattice. Here we treat the Eden model as a growth model in continuous time to see whether or not one can extract information about the asymptotic behaviour from power series in the time. The construction of time–power series has proved useful for the treatment of cooperative adsorption to lattices (Poland 1989, 1990). The main difference between adsorption models and growth models like the Eden model is that in the former one is calculating the average density of particles on the lattice, a quantity that is bounded (and usually defined to vary between zero and one), while in the latter the number of particles in the average cluster goes to infinity.

In the Eden model one starts with a single cell, species (1, 1) in figure 1(a), and allows the growth of a second cell into one of the four surrounding cells (perimeter cells), where the cell is chosen at random, giving rise to the dimer, species (2, 2) in figure 1(a). In the next state one goes from species (2, 1) to one of the species (3, 1) or (3, 2), and then on to one of the species (4, 1) to (4, 5), and so on, the process giving rise to the so-called lattice animals.

It is known that this process gives rise to compact structures (where the fractal dimension is the same as the dimension of space) and that the interior of large clusters contains very few holes, the holes being concentrated near the surface (Eden 1961, Richardson 1973, Meakin 1983). A sample cluster is shown in figure 2. Growth takes place from the surface cells (shown in light shading). While the overall cluster is compact, the surface can be ragged. The nature of the surface has been extensively studied (Meakin and Witten 1983, Plischke and Racz 1984). The number of growth sites is governed by the exponent δ (n being the number of particles in a cluster)

$$G \sim n^\delta \quad (1.1)$$

where δ is rigorously known as a function of the dimension of space (Richardson 1973)

$$\delta = (d-1)/d. \quad (1.2)$$

In two dimensions equation (1.2) gives $\delta = \frac{1}{2}$, which of course is what one expects for compact circular clusters.

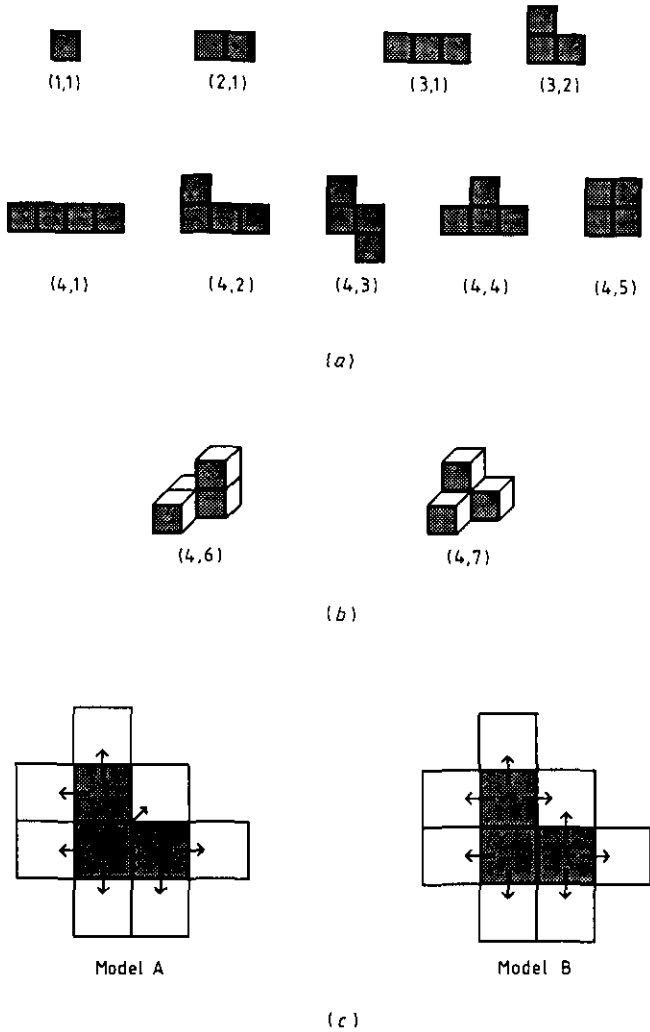


Figure 1. (a) Lattice animals for $n = 1-4$ for the plane-square lattice. (b) Three-dimensional lattice animals for $n = 4$. (c) Two modes of growth for cell clusters: in model A all perimeter cells have the same probability of turning into a cell; in model B the probability of transforming a perimeter cell is proportional to the number of neighbouring occupied faces.

Our purpose here is to explore the Eden model when the growth of clusters is governed by differential equations, i.e. the growth takes place in continuous time rather than in discrete steps. We expect that for large n the rate of growth will depend on the average number of growth sites as follows:

$$d\langle n \rangle / dt \sim \langle G \rangle \sim \langle n \rangle^{\delta'} \tag{1.3}$$

where δ' measures the average amount of surface. We anticipate that for sufficiently large n we will have $\delta' = \delta = \frac{1}{2}$, that is, we will obtain the same growth exponent as in (1.2). Integrating (1.3) and changing variable via the Euler transform

$$s = t / (1 + t) \quad t = s / (1 - s) \tag{1.4}$$

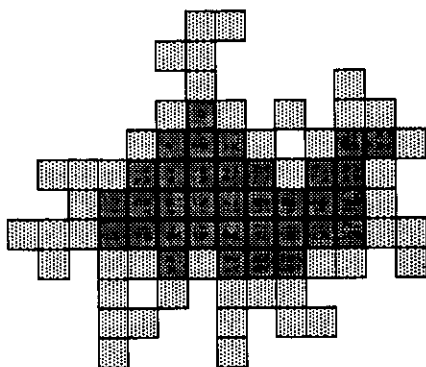


Figure 2. Illustration of a growing cluster. The interior of the cluster (dark shading) tends to be compact with few interior holes. The border (light shading) is where growth occurs and is more ragged. The exponent δ' measures the extent of the growth surface.

we obtain

$$\langle n \rangle \sim \left(\frac{1}{1-s} \right)^\gamma \tag{1.5}$$

where

$$\gamma = \frac{1}{1-\delta'}. \tag{1.6}$$

Our purpose here is to see how well behaved the s -series is for the Eden model and to determine whether this is a practical way to ascertain the asymptotic behaviour. There are precedents for determining exponents from a moderate number of exact coefficients in the appropriate series in the field of equilibrium critical phenomena. The best example is the low-temperature expansion of the coexistence curve in the two-dimensional Ising model where Padé approximants to the low-temperature series for the order parameter give the famous exponent $\beta = \frac{1}{8}$ with great accuracy. Here we explore whether or not analogous series for the time evolution of Eden clusters are similarly useful.

Julien and Botet (1985) have outlined three different modifications of the Eden model, denoted as models A, B and C; models A and B are illustrated in figure 1(b). In model A (which is the version most commonly studied) any of the perimeter sites of the given animal (in the illustration this is species (3, 2)) can be turned into a new cell with equal probability. In model B (the original model of Eden) every perimeter face of the original animal is considered to be able to give rise to a new cell with equal probability. Thus the corner cell in the illustration, which has two adjacent faces of occupied cells, will have twice the probability as the other perimeter cells of becoming the new cell. If a perimeter cell is surrounded by three existing cell faces, the probability is three times as great for growth in that cell as in a cell bordered by just a single occupied cell, and so on. In model C one first picks at random an occupied site on the surface of a cluster and then picks at random an unoccupied site adjacent to the particle just chosen. This mode of growth thus involves two steps in determining the ultimate probability of growth and cannot easily be converted into a continuous time form. The beginning terms in the animal-counting series for the plane-square lattice

are (Harary 1964)

$$\Gamma = x + x^2 + 2x^3 + 5x^4 + 12x^5 + 35x^6 + 108x^7 + \dots \quad (1.7)$$

where the coefficient of x^n gives the number (irrespective of orientation on the lattice) of distinct lattice animals containing n cells.

2. Time-power series

To construct the evolution of the clusters in continuous time one must write down the differential equations connecting the evolution of the various clusters. The hierarchy of equations begins with (where P_{nm} is the probability of species (n, m))

$$dP_{11}/dt = -4kP_{11}. \quad (2.1)$$

The factor of four arises since there are four faces in species $(1, 1)$ from which growth can occur. The parameter k is the growth rate constant; with no loss of generality we can set $k = 1$ (which is equivalent to scaling the units of time). The differential equations involving the species shown in figure 1(a) are given below (the equations given are for model A; the numbers of parentheses are the changes required to treat model B):

$$\begin{aligned} dP_{11}/dt &= -4P_{11} & dP_{21}/dt &= -6P_{21} + 4P_{11} \\ dP_{31}/dt &= -8P_{31} + 2P_{21} & dP_{32}/dt &= -7(8)P_{32} + 4P_{21} \\ dP_{41}/dt &= -10P_{41} + 2P_{31} & dP_{42}/dt &= -9(10)P_{42} + 4P_{31} + 2P_{32} \\ dP_{43}/dt &= -8(10)P_{43} + 2P_{32} & dP_{44}/dt &= -8(10)P_{44} + 2P_{31} + 2P_{32} \\ dP_{45}/dt &= -8P_{45} + 1(2)P_{32}. \end{aligned} \quad (2.2)$$

The time evolution of each species can be written as a series expansion in time,

$$\begin{aligned} P_{nm} &= \sum_{k=0}^{\infty} \alpha_k(n, m) t^k / k! \\ \alpha_k(n, m) &= \left(\frac{d^k P_{nm}}{dt^k} \right)_{t=0} \end{aligned} \quad (2.3)$$

which become recursion relations for the $\alpha_k(n, m)$. The recursion process begins with

$$\alpha_0(1, 1) = 1 \quad \alpha_0(n, m) = 0 \quad (n > 1, \text{ all } m). \quad (2.4)$$

With (2.2) one finds that

$$\alpha_k(n, m) = 0 \quad (k < (n-1), \text{ all } m). \quad (2.5)$$

The average cluster size is given by

$$\langle n \rangle = \sum_n n \sum_m P_{nm} \quad (2.6)$$

giving

$$\langle n \rangle = \sum_{k=0}^{\infty} a_k t^k / k! \quad (2.7)$$

where

$$a_k = \sum_n n \sum_m \alpha_k(n, m). \quad (2.8)$$

We have determined the series for $\langle n \rangle$ through the a_6 -term (requiring consideration of clusters through $n = 7$). We find (for model A the coefficient of the t^3 -term is zero):

$$\langle n \rangle = 1 + 4t + \frac{8}{2!} t^2 + \frac{16}{4!} t^4 - \frac{48}{5!} t^5 + \frac{176}{6!} t^6 + \dots \quad (\text{model A}) \tag{2.9}$$

$$\langle n \rangle = 1 + 4t + \frac{8}{2!} t^2 + \frac{16}{3!} t^3 - \frac{32}{4!} t^4 + \frac{192}{5!} t^5 - \frac{1408}{6!} t^6 + \dots \quad (\text{model B}).$$

If one applies the above procedure to the case of irreversible growth from a single cell in one dimension one obtains the exact result $\langle n \rangle = 1 + 2t$.

For most models in which one calculates some type of lattice density as a function of time, the time-power series strictly alternate in sign (Poland 1989, 1990). Here, where we are describing a single cluster, the signs have an erratic behaviour. Converting to the s -variable defined in (1.4), we have

$$\langle n \rangle = 1 + 4s + 8s^2 + 12s^3 + 16\frac{2}{3}s^4 + 22\frac{4}{15}s^5 + 28\frac{41}{45}s^6 + \dots \quad (\text{model A}) \tag{2.10}$$

$$\langle n \rangle = 1 + 4s + 8s^2 + 14\frac{2}{3}s^3 + 22\frac{2}{3}s^4 + 32\frac{4}{15}s^5 + 43\frac{17}{35}s^6 + \dots \quad (\text{model B}).$$

In contrast to the behaviour of the t -series in (2.9), the coefficients in the s -series given in (2.10) are very well behaved.

We define the ratio of successive coefficients in the s -series in the standard manner

$$\langle n \rangle = \sum_{k=0}^{\infty} b_k s^k \tag{2.11}$$

$$r_k = \frac{b_k}{b_{k-1}}.$$

If the singularity of (1.3) is the closest singularity in $\langle n(s) \rangle$ to the origin, then the ratios of coefficients should be asymptotic to the following linear relation (Stanley 1971):

$$r_k = \frac{1}{s_r} \left(1 + \frac{1}{k} (\gamma - 1) \right). \tag{2.12}$$

Taking $s_r = 1$ (corresponding to $t = \infty$), each value of r_k , with (1.6), gives an estimate of the exponent δ' . These estimates are shown in table 1 for model A and model B. The values for δ' so obtained all cluster in the neighbourhood of $\delta' \approx \frac{2}{3}$. The data for model B are particularly well behaved. The ratios r_k plotted as a function of $1/k$ for the model B system are shown in figure 3. The straight line is (2.12) using $s_r = 1$ and $\delta' = \frac{2}{3}$ ($\gamma = 3$). Thus while the ratios are very smooth, for small clusters one does not find the expected limiting behaviour of $\delta' = \frac{1}{2}$.

Table 1. Estimate of the exponent δ' from ratios of the coefficients in the appropriate s -series

k	Two dimensions:		Three dimensions:
	Model A	Model B	Model B
1	0.750	0.750	0.833
2	0.667	0.667	0.800
3	0.600	0.714	0.824
4	0.609	0.686	0.819
5	0.630	0.679	0.827
6	0.642	0.674	

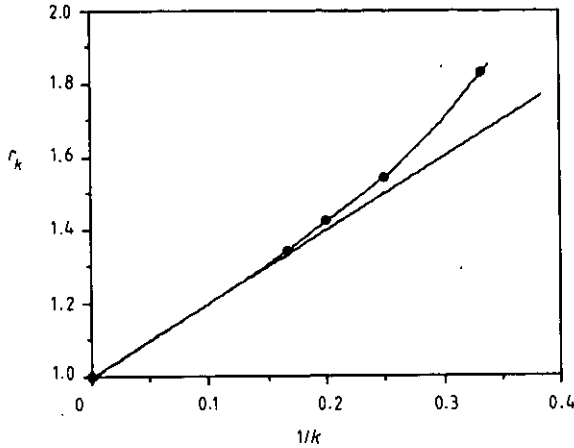


Figure 3. The ratios r_k as a function of $1/k$ for the model B case in two dimensions. The straight line is equation (2.12) with $s_v = 1$ and $\delta' = \frac{2}{3}$ ($\gamma = 3$).

An alternative analysis of the data involves the use of the Dlog/Padé technique (Baker 1975). We form the function $f(s) = \langle n \rangle - 1$ and construct the series $d \ln f / d \ln s = 1 + 2s + 3.333s^2 + 2.711s^4 + 2.777s^5 + \dots$ which, if the singularity in (1.5) dominates the behaviour of the function, should be a simple pole (all coefficients equal). Removing the simple pole by multiplying $d \ln f / d \ln s$ by $(1 - s)$ we then form the (2, 3) and (3, 2) Padé' approximants to the resulting series. When the Padé' approximants are evaluated at $s = 1$ they give estimates of the exponent γ (the residue of the pole). For the two approximants indicated we find (converting to δ') $\delta' = 0.747$ and $\delta' = 0.649$, with an average value close to the value obtained by the ratio method.

To see if the behaviour of the series is similar for the model in three dimensions we have calculated the analogous series for $\langle n \rangle$ through the t^5 -term for cells on the cubic lattice. The three-dimensional clusters of cubes for $n = 4$ are shown in figure 1(b) (species (4, 6) is chiral). The species shown in figure 1(a) are the same in the three-dimensional case, one simply interprets the squares as cubes. The counting series for animals in three dimensions begins

$$\Gamma = x + x^2 + 7x^4 + 23x^5 + \dots \tag{2.13}$$

We will use model B kinetics, i.e. we assume that each occupied face bordering a perimeter cell can give rise to the formation of a new cell. The differential equations for the species shown in figure 1 are

$$\begin{aligned} dP_{11}/dt &= -6P_{11} & dP_{21}/dt &= -10P_{21} + 6P_{11} \\ dP_{31}/dt &= -14P_{31} + 2P_{21} & dP_{32}/dt &= -14P_{32} + 8P_{21} \\ dP_{41}/dt &= -18P_{41} + 2P_{31} & dP_{42}/dt &= -18P_{42} + 8P_{31} + 2P_{32} \\ dP_{43}/dt &= -18P_{43} + 2P_{32} & dP_{44}/dt &= -18P_{44} + 4P_{31} + 2P_{32} \\ dP_{45}/dt &= -16P_{45} + 2P_{32} & dP_{46}/dt &= -18P_{46} + 4P_{32} \\ dP_{47}/dt &= -18P_{47} + 2P_{32} \end{aligned} \tag{2.14}$$

Using the initial conditions of (2.4) one finds

$$\langle n \rangle = 1 + 6t + \frac{24}{2!} t^2 + \frac{96}{3!} t^3 + \frac{192}{4!} t^4 + \frac{1152}{5!} t^5 + \dots$$

$$\langle n \rangle = 1 + 6s + 18s^2 + 46s^3 + 96s^4 + 191\frac{3}{5}s^5 + \dots$$
(2.15)

Again, the *s*-series is very uniform. The successive values of δ' calculated from the respective ratios are given in table 1. While the limited data we have are not as smooth as for the two-dimensional case, the values of δ' cluster around the value $\delta' \approx 0.82$. For large clusters in three dimensions one expects, from (1.2), $\delta' = \delta = \frac{2}{3}$.

We have already commented that time-power series for adsorption models, giving the average site occupation probability as a function of time, generally have coefficients that alternate in sign. When inverted to give the time as a power series in the average density, these series are often very well behaved, the coefficients all being positive with the radius of convergence determined by the physically interesting steady-state value of the density. In order to invert the time series for the Eden clusters considered here we introduce two new variables,

$$w = \frac{\langle n \rangle - 1}{\langle n \rangle} \quad t' = 4t.$$
(2.16)

For models A and B in two dimensions one then finds

$$t' = w + \frac{1}{2}w^2 + \frac{1}{2}w^3 + \frac{5}{16}w^4 + \frac{23}{64}w^5 + \frac{55}{256}w^6 + \dots \quad (\text{model A})$$

$$t' = w + \frac{1}{2}w^2 + \frac{1}{4}w^3 + \frac{3}{8}w^4 + \frac{3}{16}w^5 + \frac{9}{32}w^6 + \dots \quad (\text{model B}).$$
(2.17)

From (1.5), (1.6) and (2.16) we expect t' to have the asymptotic form

$$t' \sim \left(\frac{1}{1-w} \right)^{1-\delta'}.$$
(2.18)

The *w*-series in (2.17) are well behaved in the sense that the coefficients are all positive and are of the same order of magnitude. The ratios, at least for the beginning terms that we have in (2.17), are not however very smooth, and hence the series are not, in this case, as useful as the *s*-series of (2.10). It appears that the radius of convergence of the series in (2.17) is determined by the physically interesting singularity $w_c = 1$ (as $t' \rightarrow \infty$).

3. Linear reversible growth

To explore the nature of time series for other cluster growth models we consider the case where growth can take place only at the free end of a linear chain, giving rise to configurations on the plane square lattice such as that shown in figure 4(a). For this model we consider the possibility of reversible growth where a cell at the end of a chain can also die. We take k_b as the rate constant for the birth process and k_d for the rate constant for the death process; for simplicity we set $k_b = 1$ and $k_d = \kappa$.

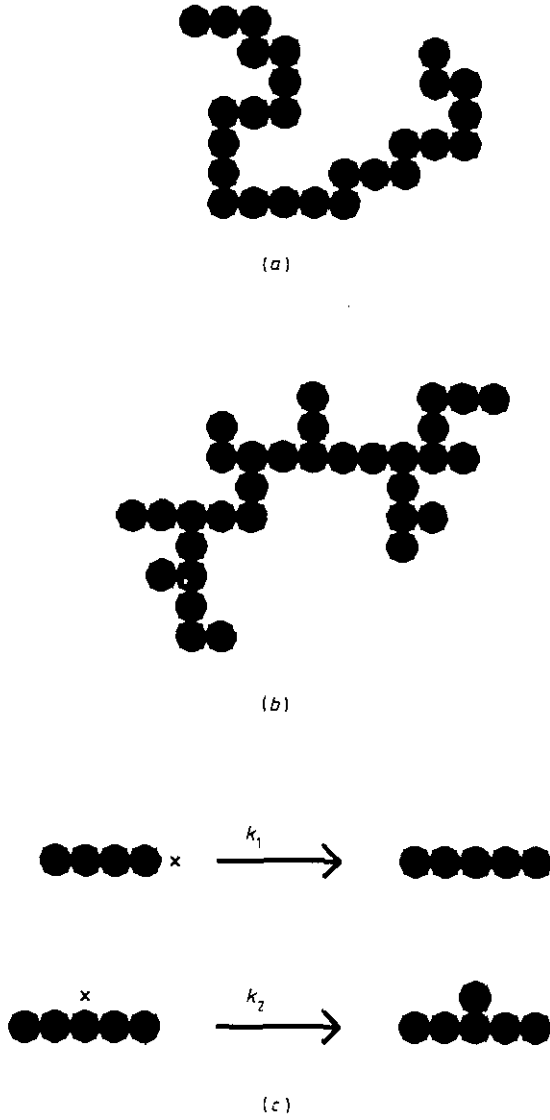


Figure 4. (a) Example of a linear cluster where the maximum coordination number of a given cell is two. (b) Example of a branched cluster where the maximum coordination number of a given cell is three. (c) Illustration of the two reactions, growth from the ends (with rate parameter k_1) and growth from the interior (with rate parameter k_2), for branched clusters.

Using the labelling of figure 1(a) (deleting species (4, 4) and (4, 5) since they are not linear clusters) one has the analogue of equations (2.2),

$$\begin{aligned}
 dP_{11}/dt &= -4P_{11} + 2\kappa P_{21} \\
 dP_{21}/dt &= -6P_{21} + 4P_{11} + 2\kappa P_{31} + 2\kappa P_{32} \\
 dP_{31}/dt &= -6P_{31} + 2P_{21} + 2\kappa P_{41} + \kappa P_{42} \\
 dP_{32}/dt &= -4P_{32} + 4P_{21} + \kappa P_{42} + 2\kappa P_{43} \\
 dP_{41}/dt &= -6P_{41} + 2P_{31} + 2\kappa P_{51} + \kappa P_{52} \\
 dP_{42}/dt &= -5P_{42} + 4P_{31} + 2P_{32} + \kappa P_{52} + 2\kappa P_{53} + \kappa P_{54} + 2\kappa P_{55} + 2\kappa P_{56} \\
 dP_{43}/dt &= -4P_{43} + 2P_{32} + \kappa P_{54} + 2\kappa P_{57}.
 \end{aligned}
 \tag{3.1}$$

We have determined the coefficients a_k in (2.7) through a_7 :

$$\begin{aligned}
 a_0 &= 1 & a_1 &= 4 & a_2 &= 8 - 8\kappa \\
 a_3 &= -64 + 16\kappa + 16\kappa^2 \\
 a_4 &= 448 + 224\kappa - 192\kappa^2 - 32\kappa^3 \\
 a_5 &= -2944 - 4160\kappa + 768\kappa^2 + 896\kappa^3 + 64\kappa^4 \\
 a_6 &= 18\,688 + 45\,952\kappa + 11\,904\kappa^2 - 11\,520\kappa^3 - 3200\kappa^4 - 128\kappa^5 \\
 a_7 &= -116\,224 - 407\,552\kappa - 306\,432\kappa^2 + 61\,440\kappa^3 + 71\,680\kappa^4 + 9984\kappa^5 + 526\kappa^6.
 \end{aligned}
 \tag{3.2}$$

Switching to the s -series we have:

$$\begin{aligned}
 b_0 &= 1 & b_1 &= 4 & b_2 &= 8 - 4\kappa \\
 b_3 &= 1\frac{1}{3} - 5\frac{1}{3}\kappa + 2\frac{2}{3}\kappa^2 \\
 b_4 &= 2\frac{2}{3} + 5\frac{1}{3}\kappa - 1\frac{1}{3}\kappa^3 & & \text{(no } \kappa^2 \text{ term)} \\
 b_5 &= 6\frac{2}{15} + 2\frac{2}{3}\kappa - 9\frac{3}{5}\kappa^2 + 2\frac{2}{15}\kappa^3 + \frac{8}{15}\kappa^4 \\
 b_6 &= 7\frac{13}{45} - 9\frac{23}{45}\kappa - 4\frac{4}{5}\kappa^2 + 8\kappa^3 - 1\frac{7}{9}\kappa^4 - \frac{8}{45}\kappa^5 \\
 b_7 &= 6\frac{2}{315} - 15\frac{83}{315}\kappa + 14\frac{2}{3}\kappa^2 + 1\frac{11}{21}\kappa^3 - 4\frac{4}{9}\kappa^4 + \frac{288}{315}\kappa^5 + \frac{16}{315}\kappa^6.
 \end{aligned}
 \tag{3.3}$$

For $k=0$ (irreversible growth) equations (3.3) give

$$\langle n \rangle = 1 + 4s + 8s^2 + 1\frac{1}{3}s^3 + 2\frac{2}{3}s^4 + 6\frac{2}{15}s^5 + 7\frac{13}{45}s^6 + 6\frac{2}{315}s^7 + \dots
 \tag{3.4}$$

For irreversible linear growth we expect

$$\begin{aligned}
 d\langle n \rangle / dt &= \text{constant} \\
 \langle n \rangle &\sim \text{constant} \left(\frac{1}{1-s} \right).
 \end{aligned}
 \tag{3.5}$$

The asymptotic form of (3.5) requires that the coefficients in (3.4) settle down to a constant value and this seems to be happening for the coefficients shown.

4. Branched clusters

Between the model of linear clusters discussed in the previous section and the general growth model of the first two sections is a model where a branch point can have a maximum coordination number of three, giving rise to branched or tree-like clusters as illustrated in figure 4(b). We will consider the case where growth from the ends of chains will occur with rate parameter k_1 while branching from the interior of a chain will occur with rate parameter k_2 . For simplicity we take $k_1=1$ and $k_2=\kappa$. The differential equations describing the growth for the clusters shown in figure 1(a) (deleting species (4, 5)) are

$$\begin{aligned}
 dP_{11}/dt &= -4P_{11} \\
 dP_{21}/dt &= -6P_{21} + 4P_{11} \\
 dP_{31}/dt &= -6P_{31} - 2\kappa P_{31} + 2P_{21} \\
 dP_{32}/dt &= -4P_{32} - 2\kappa P_{32} + 4P_{21} \\
 dP_{41}/dt &= -6P_{41} - 4\kappa P_{41} + 2P_{31} \\
 dP_{42}/dt &= -5P_{42} - 3\kappa P_{42} + 4P_{31} + 2P_{32} \\
 dP_{43}/dt &= -4P_{43} - 2\kappa P_{43} + 2P_{32} \\
 dP_{44}/dt &= -5P_{44} + 2\kappa P_{31} + 2\kappa P_{32}.
 \end{aligned} \tag{4.1}$$

The exact series through a_6 for this model are given below, where the a_k are finite series in powers of the branching parameter κ :

$$\begin{aligned}
 a_0 &= 1 & a_1 &= 4 & a_2 &= 8 \\
 a_3 &= -64 + 48\kappa \\
 a_4 &= 448 - 1168\kappa + 144\kappa^2 \\
 a_5 &= -2944 + 21\,744\kappa - 768\kappa^2 + 240\kappa^3 \\
 a_6 &= 18\,688 - 304\,384\kappa - 43\,328\kappa^2 - 10\,576\kappa^3 + 48\kappa^4.
 \end{aligned} \tag{4.2}$$

Switching to the s -series one has

$$\begin{aligned}
 b_0 &= 1 & b_1 &= 4 & b_2 &= 8 \\
 b_3 &= 1\frac{1}{3} + 8\kappa \\
 b_4 &= 2\frac{2}{3} - 24\frac{2}{3}\kappa + 6\kappa^2 \\
 b_5 &= 6\frac{2}{15} + 34\frac{8}{15}\kappa + 17\frac{3}{5}\kappa^2 + 2\kappa^3 \\
 b_6 &= 7\frac{13}{45} + 76\frac{26}{45}\kappa - 32\frac{8}{45}\kappa^2 - 4\frac{31}{45}\kappa^3 + \frac{3}{45}\kappa^3.
 \end{aligned} \tag{4.3}$$

At $\kappa=1$ the t - and s -series are

$$\langle n \rangle = 1 + 4t + 8t^2/2! - 16t^3/3! - 576t^4/4! + 18\,272t^5/5! - 365\,664t^6/6! + \dots \tag{4.4}$$

$$\langle n \rangle = 1 + 4s + 8s^2 + 9\frac{1}{3}s^3 - 16s^4 + 60\frac{4}{15}s^5 + 47\frac{1}{15}s^6 + \dots \tag{4.5}$$

Unlike the s -series for compact clusters in (2.10), the above series for branching clusters do not give well-behaved ratios. Of course, when $\kappa = 0$ the series of (4.2) and (4.3) revert to the results for the linear model treated in the previous section.

5. Irreversible filling of a lattice

In the previous sections we have considered the growth of a single cluster from a single seed cell. The growth of the cluster was not restricted by any boundary conditions and the cluster size became infinite as $t \rightarrow \infty$. If one instead begins with a finite density of randomly distributed seed cells, as shown in figure 5(a), then the growth, as illustrated in figure 5(b) (the new cells are shaded light; the original seed cells, the same configuration as given in figure 5(a), are shown shaded dark) will eventually fill the lattice and thus have a limit as $t \rightarrow \infty$. The clusters clearly merge until finally there is one large cluster; the average cluster size at close packing is simply $1/\rho_0$, where ρ_0 is the original concentration of seed cells.

To treat the kinetics of this lattice-filling process (using model B kinetics) we consider the different possible configurations of cells surrounding an empty site that we take as the locus for growth. These configurations are designated as species B_0 to B_5 in figure 6. We let B_k represent the probability of species B_k for one species orientation (thus there are four orientations of species B_1 and the net density of this

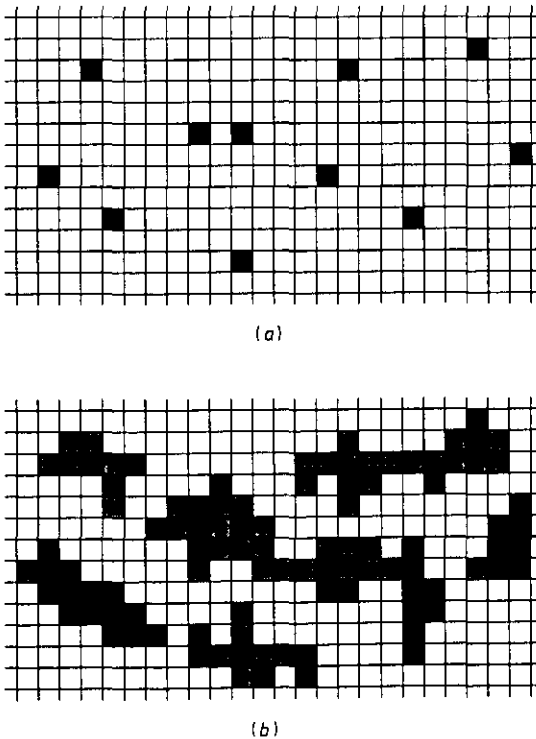


Figure 5. Irreversible filling of a lattice. (a) One begins with seed cells distributed at random. (b) Growth (shown by shading) from the original seed cells (shown as dark cells) eventually fills the lattice.

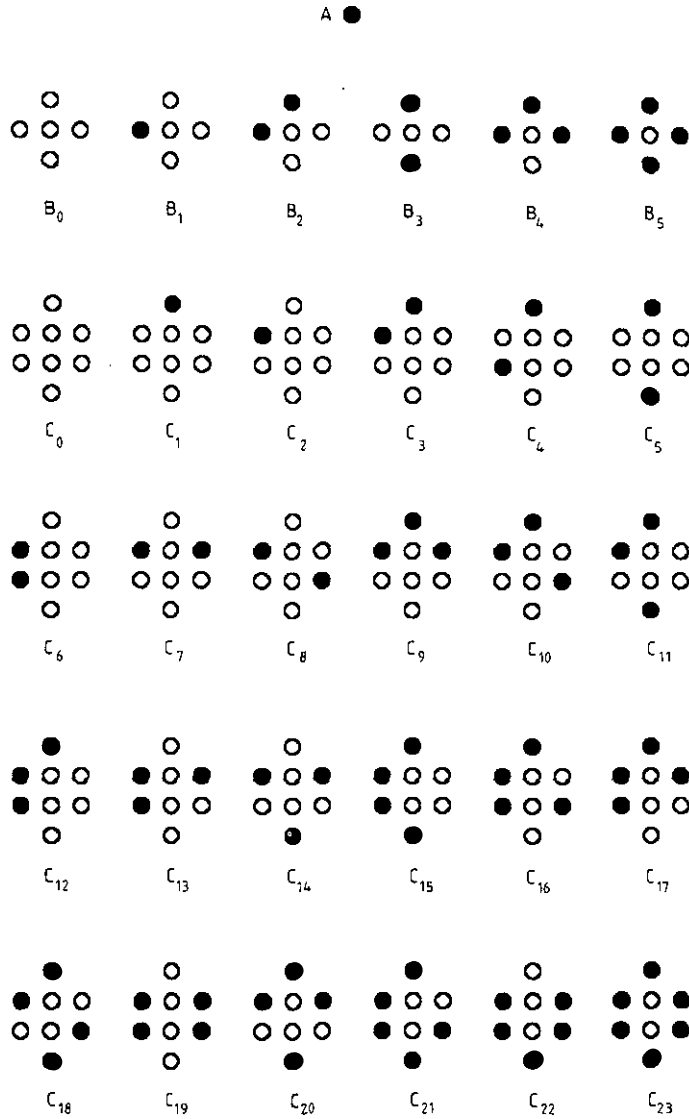


Figure 6. Lattice configurations required to treat the irreversible filling of a lattice from randomly placed seed cells.

species is $4B_k$). Then the rate of increase of occupied cells, species A in figure 6, is given by

$$d\rho/dt = dA/dt = 4B_1 + 8B_2 + 4B_3 + 12B_4 + 4B_5. \tag{5.1}$$

The factors multiplying the B_k indicate the number of orientations of species B_k and the number of faces from which growth can take place into the central site. Thus the 8 in the $8B_2$ -term reflects the fact that there are four orientations of species B_2 and that there are two cell faces from which growth can occur into the central site.

In order to obtain a time series for A (or ρ) given in (2.7) we require the differential equations for the B_k . We note that

$$\langle n \rangle = \rho/\rho_0. \tag{5.2}$$

These equations require consideration of the species C_k shown in figure 6. The differential equations are

$$\begin{aligned}
 dB_0/dt &= -4f_1 \\
 dB_1/dt &= -B_1 - 2f_2 - f_3 + f_1 \\
 dB_2/dt &= -2B_2 - 2f_4 + 2f_2 \\
 dB_3/dt &= -2B_3 - 2f_5 + 2f_3 \\
 dB_4/dt &= -3B_4 - f_6 + f_5 + 2f_4 \\
 dB_5/dt &= -4B_5 + 4f_6.
 \end{aligned}
 \tag{5.3}$$

where

$$\begin{aligned}
 f_1 &= C_1 + 2C_2 + 4C_3 + 2C_7 + 3C_9 \\
 f_2 &= C_4 + C_8 + C_6 + 2C_{10} + 2C_{12} + 2C_{13} + 3C_{17} \\
 f_3 &= 2C_4 + C_5 + 4C_{11} + 2C_{14} + 3C_{20} \\
 f_4 &= C_{10} + C_{11} + C_{12} + 2C_{15} + 2C_{16} + 2C_{18} + 3C_{21} \\
 f_5 &= 2C_{13} + C_{14} + 4C_{16} + 2C_{19} + 3C_{22} \\
 f_6 &= 2C_{17} + C_{20} + 4C_{21} + 2C_{22} + 3C_{23}.
 \end{aligned}
 \tag{5.4}$$

One then requires equations for dC_k/dt , etc., requiring eventually an infinite hierarchy of coupled equations.

The differential equations are recursion relations for the coefficients in the time series, e.g. the a_k in (2.7). The recursion process is begun with the probabilities of the clusters shown in figure at $t = 0$. For random clusters one has (where ρ_0 is the original density of seed cells):

$$\begin{aligned}
 P_0(A) &= \rho_0 & P_0(B_0) &= (1 - \rho_0)^5 \\
 P_0(B_1) &= \rho_0(1 - \rho_0)^4 & P_0(B_2) &= P_0(B_3) = \rho_0^2(1 - \rho_0)^3 \\
 P_0(B_4) &= \rho_0^3(1 - \rho_0)^2 & P_0(B_5) &= \rho_0(1 - \rho_0)^4 \\
 P_0(C_0) &= (1 - \rho_0)^8 & P_0(C_1) &= \rho_0(1 - \rho_0)^7 \quad \text{etc.}
 \end{aligned}
 \tag{5.5}$$

If the clusters were not originally distributed at random one would require a more complicated description of the probabilities of the clusters, for example a density expansion derived from the equilibrium statistical mechanics of a lattice gas with attractive interactions (Ising model).

We have derived the exact ρ_0 dependence of the a_k through a_3 which requires the construction of the differential equations (not shown) for the C_k . We obtain

$$\begin{aligned}
 a_0 &= \rho_0 \\
 a_1 &= 4\rho_0(1 - \rho_0) \\
 a_2 &= 8\rho_0(1 - 4\rho_0 + 3\rho_0^2) \\
 a_3 &= 16\rho_0(1 - 10\rho_0 + 21\rho_0^2 - 12\rho_0^3).
 \end{aligned}
 \tag{5.6}$$

The use of (5.6) in (5.2) gives the behaviour near $t=0$ of the filling in of the lattice from randomly placed seed cells. The final stages of the process can be determined from the particle configurations shown in figure 7. One has

$$\begin{aligned}
 dA/dt &= 4B + 6C + 8D_1 + 8D_2 \dots \\
 dB/dt &= -4b + 6C + 2D_1 + 4D_2 \dots \\
 dC/dt &= -6C + 6D_1 + 6D_2 \dots \\
 dD_1/dt &= -8D_1 + \dots \\
 dD_2/dt &= -8D_2 + \dots
 \end{aligned}
 \tag{5.7}$$

Truncating the species considered at D_1 and D_2 , the equations can then be successively integrated giving

$$\rho = A = a + b e^{-4t} + c e^{-6t} + d e^{-8t} + \dots
 \tag{5.8}$$

The coefficients a, b, c, \dots , in (5.8) will be influenced by the truncation, but the exponents will not. Constructing the function

$$\Delta = \frac{1 - \rho}{1 - \rho_0}
 \tag{5.9}$$

one has

$$\Delta \sim e^{-4t}
 \tag{5.10}$$

We recast (5.2) in the form (using the variable s defined in (1.4))

$$\Delta = \exp \left[-4 \left(\frac{s}{1-s} \right) k(s) \right]
 \tag{5.11}$$

where

$$k(s) = b_0 + b_1 s + b_2 s^2 + \dots
 \tag{5.12}$$

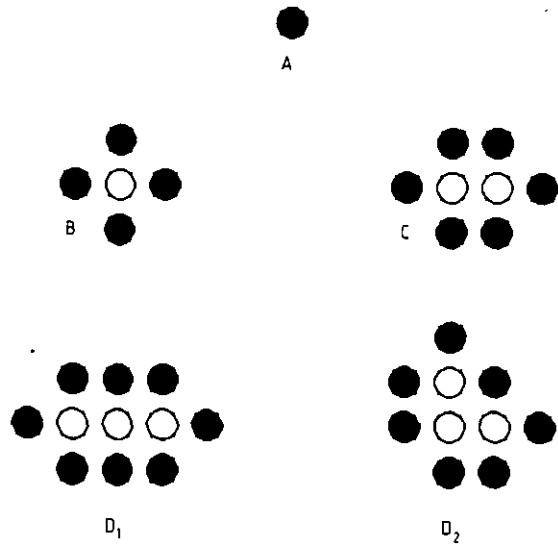


Figure 7. The most probable lattice configurations at high density of occupied cells.

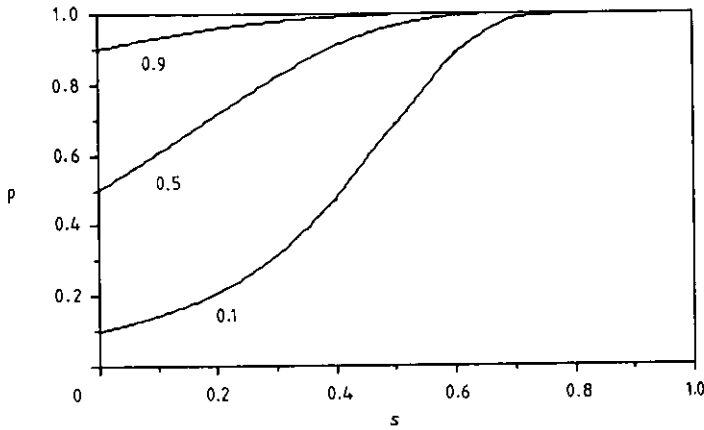


Figure 8. The time course (in terms of the variable s) for the irreversible filling of a lattice from randomly placed seed cells. The numbers refer to the original density of seed cells. The curves were calculated using equation (5.11) with equation (5.15) for $k(s)$.

With (5.6), the coefficients in (5.11) are given as

$$\begin{aligned}
 b_0 &= \rho_0 \\
 b_1 &= 2\rho_0^2 + \rho_0(1 - 4\rho_0 + 3\rho_0^2)/(1 - \rho_0) \\
 b_2 &= (4\rho_0 + 1)b_1 - 8\rho_0^3/3 + 2\rho_0(1 - 10\rho_0 + 21\rho_0^2 - 12\rho_0^3)/[3(1 - \rho_0)].
 \end{aligned}
 \tag{5.13}$$

The quantity $k(s)^{-1}$ defined in (5.11) is a kind of time-dependent relaxation time. From (5.13) and (5.10) we have

$$\begin{aligned}
 k(s=0) &= \rho_0 \\
 k(s=1) &= 1.
 \end{aligned}
 \tag{5.14}$$

Thus the filling process is faster than simple exponential decay, i.e. the effective $k(s)$ increases from ρ_0 to one over the course of the relaxation.

We can construct a function that has the correct beginning terms of (5.13) and the correct long-time limit of (5.14) by the following device. We add an additional term to the truncated form for $k(s)$ as follows

$$k(s) = b_0 + b_1s + b_2s^2 + c_0s^3
 \tag{5.15}$$

such that

$$c_0 = 1 - (b_0 + b_1 + b_2).
 \tag{5.16}$$

This function gives an approximation for the whole time course of the relaxation with the first three derivatives exact and the correct limiting behaviour (and of course the correct limiting value of $\rho = 1$ at $t = \infty$). The behaviour of $\rho(s)$ for various values of ρ_0 according to the use of (5.15) in (5.11) is shown in figure 8.

6. Discussion

We have shown that time-power series are a useful way to describe the growth of clusters in the Eden model and modifications thereon. In particular the conversion via

an Euler transform to the variable s of (1.4) gives series for the two variants of the Eden model studied that give smoothly varying ratios. For the series we studied the exponents calculated from the series have not yet settled down to their expected asymptotic values. Thus in two dimensions we obtain $\delta' \approx \frac{2}{3}$ rather than the expected asymptotic limit $\delta = \frac{1}{2}$. However, the series method appears to be a very useful way to describe the unbounded growth of clusters. In addition we have seen that time-power series are useful in the description of branching models and models for the filling of the lattice as a function of the number of original seed cells.

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