

## Isotropic model for cluster growth on a regular lattice

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There exists a plethora of mathematical models for cluster growth and/or aggregation on regular lattices. Almost all suffer from inherent anisotropy caused by the regular lattice upon which they are grown. We analyze the little-known model for stochastic cluster growth on a regular lattice first introduced by Ferreira Jr. and Alves [*J. Stat. Mech. Theo. & Exp.* (2006) P11007], which produces circular clusters with no discernible anisotropy. We demonstrate that even in the noise-reduced limit the clusters remain circular. We adapt the model by introducing a specific rearrangement algorithm so that, rather than adding elements to the cluster from the outside (corresponding to apical growth), our model uses mitosis-like cell splitting events to increase the cluster size. We analyze the surface scaling properties of our model and compare it to the behavior of more traditional models. In “1 + 1” dimensions we discover and explore a new, nonmonotonic surface thickness scaling relationship which differs significantly from the Family-Vicsek scaling relationship. This suggests that, for models whose clusters do not grow through particle additions which are solely dependent on surface considerations, the traditional classification into “universality classes” may not be appropriate.

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### I. INTRODUCTION

On-lattice models for cluster aggregation have been studied for at least the last 50 years. One of the earliest, originally designed to simulate tumor formation, is known as the Eden model [1,2] and comes in three versions, A, B, and C [3]. In each version particles are added to the surface of the cluster incrementally. On-lattice cluster aggregation models like Eden’s have been used to represent biological phenomena such as wound healing [4], slime mold growth [5], and, more recently, *in vitro* growth of tumor monolayers [6,7].

Some models of cluster aggregation can be classified into universality classes (UCs) depending on the surface scaling properties of their aggregates. For example, version C of the Eden model has scaling characteristics which are most similar to those of the Kardar-Parisi-Zhang (KPZ) UC [3,8]. The continuum equation associated with the KPZ UC predicts circular clusters [8]. However, when Eden clusters are realized on a regular lattice there is an inherent anisotropy that does not diminish as the clusters grow larger [9] (see Suppl. Fig. 1(a), in the Supplemental Material (SM) [10]); the shape of large on-lattice Eden clusters is dominated by the underlying lattice anisotropy [see Suppl. Fig. 1(b)]. Such artificial anisotropy is clearly an undesirable property for any on-lattice cluster growth model.

Several related models have attempted to reduce the effects of this inherent, regular-lattice-induced anisotropy by altering or completely revising the cluster aggregation algorithms. However, few of these attempts have been shown to produce a truly isotropic cluster aggregation model. In this paper we adapt and analyze a little-known cluster formation model, model II of Ferreira and Alves [11], so that cluster growth is driven by random elemental division and rearrangement events on a square lattice. We demonstrate the isotropy of the model in both the noisy and the noise-reduced limits by

considering both a bespoke anisotropy measure and a more standard series decomposition of the surface. The elemental division mechanism we introduce can also be thought of as being more akin to biological growth than the surface addition rules employed by many Eden-derived models of cluster aggregation. Moreover, the clusters produced have the desirable properties of being concave and hole-free. We go on to investigate the scaling properties of this aggregation model and find that the traditional techniques of classification into UCs are not sufficient. A new surface scaling relationship which may be more appropriate for this cluster aggregation model is suggested. We conclude by employing the revised model with the explicit elemental division algorithm to act as the lattice on which a position-jump model of diffusion is implemented. This model of diffusion on a growing domain is compared both qualitatively and quantitatively to a continuum model of the same process, with good agreement being found in the mean field.

### II. MEASURING ANISOTROPY

In order to accurately determine the anisotropy of a cluster it is important to have a method of measurement which is itself free of lattice artifacts. Although box-counting methods such as those employed by Meakin [12] can be useful in characterizing large-scale anisotropies, they may suffer from anisotropy themselves. As such we consider a bespoke measure, the “angular surface anisotropy”. This is given by the normalized square of the distance to the surface from the center of the cluster in a particular direction [9,13]: for each surface element,  $i$ , calculate the angle,  $\phi_i$ , subtended by the  $x$  axis and the line connecting the center of the seed particle (or center of mass, translating the cluster so that this lies at the origin) to the element’s center (see Fig. 1). Also, calculate the element’s distance from the seed or center of mass,  $r_i$  (see Fig. 1). The angular surface anisotropy in direction  $\theta_k$  is then

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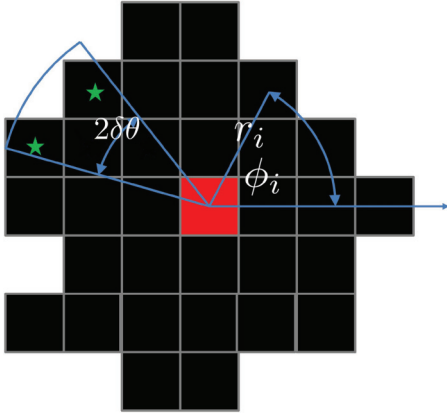


FIG. 1. (Color online) Measuring the anisotropy of particle aggregates. In this example cluster elements of the aggregate are represented by black squares. The angle to the  $x$  axis,  $\phi_i$ , and the distance from the seed particle [center (red) square],  $r_i$ , are determined for each element. In each segment of the circle the mean square distance of the centers of mass of the surface elements [(green) stars] is calculated and then normalized to find the “angular surface anisotropy”.

given by

$$P(\theta_k) = \frac{1}{N_s^{\theta_k}} \sum_{i=1}^{N_s} r_i^2 \mathbb{I}_{\theta_k - \delta\theta < \phi_i < \theta_k + \delta\theta}, \quad (1)$$

where the sum is over the  $N_s^{\theta_k} = \sum_{i=1}^{N_s} \mathbb{I}_{\theta_k - \delta\theta < \phi_i < \theta_k + \delta\theta}$  surface elements with angles in the appropriate region  $[\theta_k - \delta\theta, \theta_k + \delta\theta]$  [(green) stars in Fig. 1].  $\mathbb{I}$  represents the indicator function. The  $K$  values of  $\theta_k$  are chosen so as to cover the entire circle. This necessarily defines  $\delta\theta = \pi/K$ . We choose  $K$  to be a power of two [14] and  $\theta_1 = 0$  in order to capture the anisotropy that might be caused by the square lattice. The angular surface anisotropy is normalized by dividing  $P(\theta_k)$  by  $\sum_{k=1}^K P(\theta_k)$  for each value of  $k$ .

In order to quantitatively analyze the angular surface anisotropy,  $P(\theta)$ , we can consider a Fourier decomposition of the curve. Fourier modes with large coefficients will indicate larger contributions to the overall anisotropy from that mode. For example, for a cluster with positive axial anisotropy we would expect to see a large positive quadrupole (coefficient of the fourth Fourier mode).

### III. SOME ANISOTROPIC MODELS

In order to get a better idea of the anisotropy of small clusters, “noise reduction” can be employed [9]. Noise reduction is a useful tool for reducing finite-size effects which can sometimes obscure inherent anisotropy in small clusters. (See the SM for a detailed description.) The Eden model exhibits anisotropy in both the noisy and the noise-reduced limits (see Suppl. Figs. 1 and 2, respectively).

There have, however, been several Eden-like cluster aggregation models which purport to produce isotropic clusters. Paiva and Ferreira [15], for example, have found on-lattice versions of the Eden A and C models which are isotropic (see Fig. 2). Growth events, in these models, depend on the neighborhood of the free space into which a new element is to be positioned. Their technique for ensuring isotropy is inspired by an isotropic, on-lattice version of diffusion-limited aggregation by Bogoyavlenskii [16]. In Bogoyavlenskii’s model, growth at a selected site is implemented with probability  $P_i = i^2$ , where  $i$  is the number of occupied nearest neighbors of the growth site. However, this choice of occupancy-dependent probability was found to produce diagonal anisotropy in the diffusion-limited aggregation clusters [17]. Instead Alves and Ferreira [17] suggested growth probabilities given by

$$P_k = \left(\frac{i}{n}\right)^\nu, \quad (2)$$

where  $n$  is the lattice coordination number (i.e., number of possible neighbors of a lattice site),  $\nu$  is an adjustable parameter, and  $i$ , as before, is the number of occupied nearest neighbors of a site selected for growth. The majority of the work in this method is finding the value of the tunable parameter,  $\nu$ , which minimizes the anisotropy. Paiva and Ferreira [15] do this by recognizing that the scaling behavior of the Eden model is affected by the lattice anisotropy. They reason that if they can find an exponent  $\nu = \nu_c$ , in Eq. (2), for which the growth parameter,  $\beta$ , of the on-lattice model is as close as possible to its predicted value,  $1/3$ , then this will be the value that produces the most isotropic clusters. Using this method they find  $\nu_c \approx 1$  for version C of the Eden model and  $\nu_c \approx 1.72$  for version A of the model, although they do not provide any quantitative comparisons of the clusters’ anisotropy for these values other than visually comparing the cluster border with a circle.

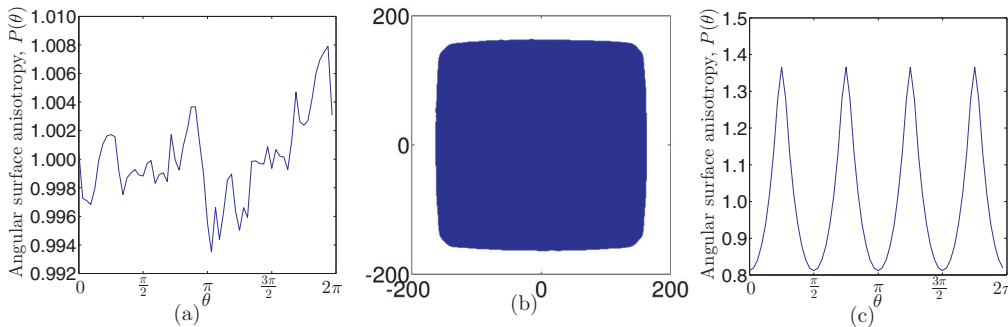


FIG. 2. (Color online) Anisotropy of the “isotropic” Eden C model of Paiva and Ferreira [15]. (a) The angular surface anisotropy,  $P(\theta)$ , of the isotropic Eden C model displays no clear periodicity. (b) A typical noise-reduced ( $m = 60$ ) isotropic Eden cluster. (c) Angular surface anisotropy,  $P(\theta)$ , of the noise-reduced clusters. A clear diagonal anisotropy is present. Clusters were grown to  $N = 10^5$  elements and anisotropy values are averaged over 200 repeats.

We have explicitly tested Eden clusters grown with the relevant  $v_c$  values for anisotropy. In the full model it is clear that the anisotropy of the model is reduced [cf. Fig. 2(a) and Suppl. Fig. 1(b)]. No periodicity is evident and the maximum anisotropy value is well below 1%, in comparison to the  $\sim 2\%$  anisotropy exhibited by the original Eden C model. However, the noise-reduced version of the model ( $m = 60$ ) shows a clear positive diagonal anisotropy [see Figs. 2(b) and 2(c)] of around 40% and a negative axial anisotropy of around 20%. These anisotropies are confirmed when considering the Fourier decomposition of  $P(\theta)$  (see Sec. IV B in the SM). Similar results are observed for the noise-reduced version of the “isotropic” Eden A model (results not shown). Clearly the randomness of the order of addition of the particles is important in the isotropic Eden models of Paiva and Ferreira [15] to maintain isotropy. In addition to these on-lattice cluster models there have also been a variety of isotropic off-lattice versions of the Eden model [18–20], with which we do not concern ourselves further in this on-lattice-focused paper.

Recently Drasdo [7] introduced an on-lattice model of cluster growth via mitosis in order to model tumor growth. An element of the cluster is chosen randomly to be a division candidate, and, providing it is within distance  $\Delta R$  of an unoccupied lattice site, it divides. Division is such that the two daughter elements are positioned adjacent to each other and the elements of the cluster are rearranged so that the empty site nearest to the original parent element is filled. Although it produces circular-looking clusters [see Fig. 3(a)], this model is also inherently anisotropic. Large clusters can show a periodic variation in anisotropy (indicative of an inherent anisotropy) and a peak anisotropy of about 1.5–2% [Fig. 3(b)]. Note that this is of a similar magnitude, but with inverse orientation, to the anisotropy found in the Eden model: in Drasdo’s model the positive bias is in the diagonal directions and the negative bias in the axial directions. The dominant nature of the axial and diagonal anisotropies in Drasdo’s model is confirmed by considering the Fourier decomposition of  $P(\theta)$  (see Sec. IV C in the SM). In the noise-reduced limit, the cluster anisotropy is even more evident [7]. It should be noted, however,

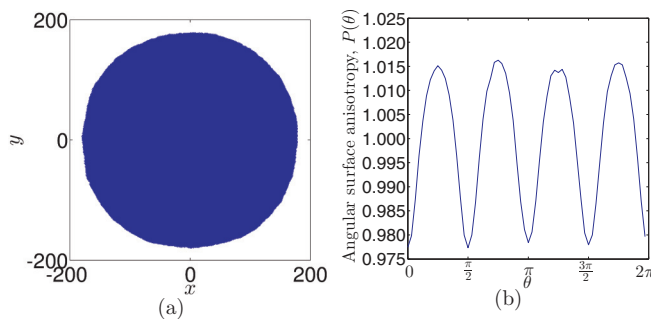


FIG. 3. (Color online) Anisotropy of clusters of the Drasdo model. (a) A typical example of a cluster grown using the algorithm of Drasdo with  $k = 10$ . The cluster displays slightly flatter edges in the axial directions. (b) Angular surface anisotropy,  $P(\theta)$ . Clear diagonal anisotropy of the clusters is evident. Clusters were grown to  $N = 10^5$  elements and anisotropy values are averaged over 200 repeats.

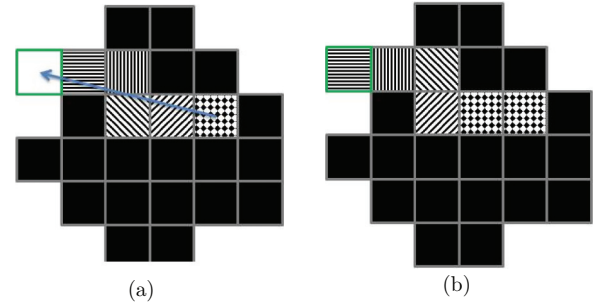


FIG. 4. (Color online) Rearrangement protocol for division in a random direction from a random parent interval. (a) An element of the cluster is chosen randomly to divide (checked pattern), and a uniformly distributed random angle is used to determine the direction in which the element will divide. A line [(blue) arrow] is drawn from the parent interval in this direction until the first free site is encountered [white square with (green) boundary]. (b) Elements (various patterns) are pushed in this direction in such a way that one of them occupies the free lattice site. The daughter interval (also checked) is placed on the lattice site adjacent to the original parent interval in the direction of division.

that [7] also gives an analog of his model on a “Dirichlet lattice” [6]. In this case there is no observable anisotropy to the clusters [6,7].

#### IV. A MORE ISOTROPIC MODEL OF CLUSTER AGGREGATION

We adapt the model of Ferreira and Alves [11] to include a specific particle rearrangement algorithm. This rearrangement algorithm mimics the reorganization of cells in a biological cluster upon mitosis of an internal cell. The revised algorithm proceeds as follows: an element of the cluster is randomly selected to divide. A uniformly distributed random number (representing a clockwise angle with the  $x$  axis) between 0 and  $2\pi$  (the “direction of division”) is then generated [see Fig. 4(a)]. Upon division a daughter element is placed on a lattice site neighboring the parent interval in the direction of division and other elements are displaced sequentially to make room. Displaced elements follow the direction of an arrow, drawn from the center of the parent element in the direction of division to a neighboring lattice site. Elements are sequentially displaced in this way until a free lattice site is encountered [see Fig. 4(b)]. The resulting model is similar to Drasdo’s but is less anisotropic, even in the noise-reduced limit. In addition, the specific rearrangement algorithm engenders a biological realism in the model. In particular, the algorithm can now be used to represent a discrete underlying growing domain for an on-lattice position-jump model of a reaction-diffusion process (see Sec. VI).

Figure 5 demonstrates the values of the anisotropy metric,  $P(\theta)$ , produced by this model in both the noisy and the noise-reduced regimes. For a strongly anisotropic cluster we might expect to see a periodic variation in the anisotropy metric as a result of the strong contribution of a single multipole. Since, for the noisy cluster [Fig. 5(a)], there is no clear periodicity to the values of the angular surface anisotropy metric,  $P(\theta)$ , we suggest that the model is more isotropic than previously

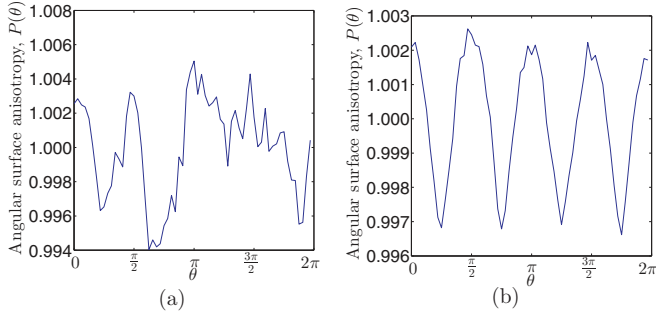


FIG. 5. (Color online) Anisotropy of clusters grown by elements dividing in random directions. (a) Angular surface anisotropy,  $P(\theta)$ . (b) Angular surface anisotropy for the noise-reduced variant of the model with  $m = 60$ . Clusters were grown to  $N = 10^5$  elements and anisotropy values are averaged over 200 repeats.

proposed models of on-lattice cluster growth. We employ a Fourier decomposition of  $P(\theta)$ , in Sec. IV D of the SM, in order to investigate this suggestion further. Furthermore, for the noise-reduced variant of the model with parameter  $m = 60$  [see Fig. 6(b) for a sample cluster], we find that the clusters appear even more isotropic than their random counterparts with a lower overall anisotropy of maximum absolute value around 0.3%. There do appear to be periodic variations in the anisotropy values, however, we found variations of comparable magnitude for a truly circular cluster [see Suppl. Fig. 3(d)]. The anisotropy of the noise-reduced clusters is also analyzed further in Sec. IV D in the SM.

This model has the added benefit that it is more computationally efficient than Drasdo's since every element selected to divide produces a daughter element, which increases the size of the cluster rapidly. In Drasdo's model (especially for large cluster sizes) a large amount of time is spent selecting sites that are unable to divide because of their distance from the surface. Hence growth is retarded at long times. The slowing of growth in the model is related to saturation of the surface, which allows the classification of the Drasdo model into a UC.

## V. SURFACE SCALING AND UNIVERSALITY CLASSES

The UC of an aggregate has traditionally been determined by considering the surface scaling properties of aggregates

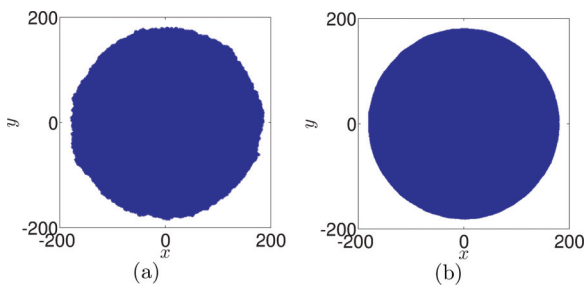


FIG. 6. (Color online) Examples of clusters grown using the algorithm of Ferreira and Alves [11]. (a) A typical example of such a cluster which looks relatively circular, displaying no obvious anisotropy. (b) A typical example of a cluster grown with the noise-reduced variant of the model with  $m = 60$ . Clusters were grown to  $N = 10^5$ .

grown in a “1 + 1”-dimensional strip geometry. In the strip geometry clusters are grown from a base layer of 1 seed particles incorporating periodic boundary conditions on the vertical boundaries. The width of an aggregate,  $w$ , is defined to be some measure of the standard deviation of the height of the surface particles. For a large class of models the width is found to increase initially as a power law in the effective height,  $\hat{h} = N/l$  (where  $N$  is the number of particles), and then to level off to a value which is dependent on the length of the substrate upon which the aggregate is grown. The effective height at which the surface levels off can also be shown to depend, as a power law, on the length of the substrate,  $l$ . These relationships are summarized by the Family-Vicsek scaling relation [21]:

$$w(l, \hat{h}) \sim l^\alpha f\left(\frac{\hat{h}}{l^z}\right), \quad f(x) \sim \begin{cases} x^\beta, & x \ll 1, \\ \text{const}, & x \gg 1. \end{cases} \quad (3)$$

The growth exponent,  $\beta$ , characterizes the initial increase in surface width, while the roughness exponent,  $\alpha$ , captures the dependence of surface roughness at saturation on substrate length. The dynamic exponent  $z$  determines the relationship between saturation height and substrate length. The three scaling exponents are related by  $z = \alpha/\beta$ . Determining these exponents enables us to classify models into UCs. Each class has its own characteristic stochastic partial differential equation of the form

$$\frac{\partial \hat{h}(x, t)}{\partial t} = F + \eta(x, t), \quad (4)$$

where  $F$  is the average rate of particle arrival at site  $x$  and  $\eta(x, t)$  is zero-mean, uncorrelated noise which models random fluctuations in the deposition process [22]. Implicitly, by searching for the scaling coefficients which characterize a model into a particular UC, we are assuming that the surface width will eventually saturate, which, as we discover, is not necessarily a valid assumption.

Upon analyzing the model of Ferreira and Alves [11] using traditional scaling techniques, it appears to exhibit a classic power-law dependence of surface width on domain length,  $l$  [Fig. 7(a)], and effective height,  $\hat{h}$  [Fig. 7(b)], in the appropriate limits. This might lead us to conclude that the model follows the classic Family-Vicsek scaling relationship,

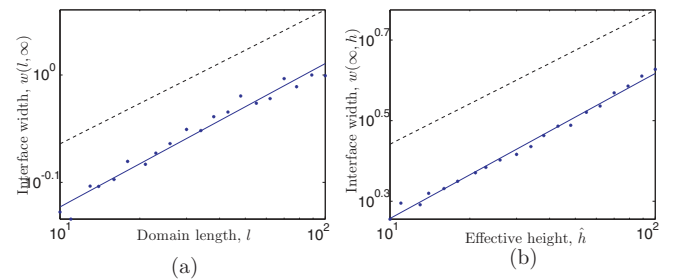


FIG. 7. (Color online) Scaling of the surface width of random direction mitosis clusters in “1 + 1” dimensions. (a) Variation of  $w(l, \infty)$  (i.e.,  $\hat{h} \gg l$ ) with domain length,  $l$ , for the random directional mitosis model. The dashed (black) line plotted for comparison has gradient 1/8. (b) Variation of  $w(\infty, \hat{h})$  (i.e.,  $l \gg \hat{h}$ ) with effective height,  $\hat{h}$ . Descriptions as for 7(a). The dashed (black) line plotted for comparison has gradient 1/3.

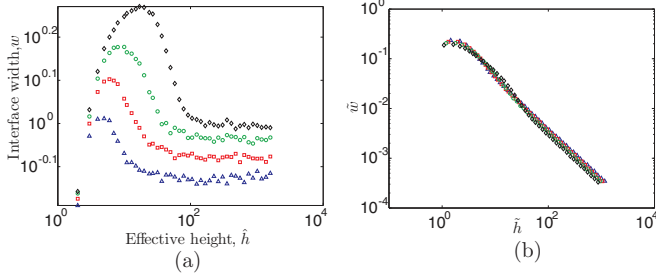


FIG. 8. (Color online) Evolution of the surface width for model II of Ferreira and Alves [11] for different system sizes. (a) The surface exhibits an initial power-law dependence on effective height but quickly peaks, then falls, and, finally, plateaus at the saturation value,  $w_{\text{cap}}(l)$ . (b) Evolution of the surface width rescaled according to Eq. (5). Axis labels are shorthand where  $\tilde{w} = w(\hat{h}, l)/l^\alpha \hat{h}^\beta$  and  $\tilde{h} = \hat{h}/l^\gamma$ . A tight collapse of the data points can be seen. In (a) and (b), (blue) triangles correspond to system size  $l = 10$ ; (red) squares, to  $l = 20$ ; (green) circles, to  $l = 40$ ; and (black) diamonds, to  $l = 80$ .

Eq. (3). However, by studying the scaling behavior of the surface we can see that the surface width exhibits a much more complicated, nonmonotonic dependence on the effective height. Figure 8(a) shows the variation of interface width with effective height for four values of domain length. We calculate critical exponents  $\alpha = 0.15 \pm 0.07$  and  $\beta = 0.35 \pm 0.07$ . When the surface width is rescaled (using the Family-Vicsek scaling relationship) by the critical exponents, derived from the scaling relationships displayed in Fig. 7, the data do not collapse onto themselves as they do for the Eden model (Suppl. Fig. 8). This suggests a different functional form for the scaling relationship for this model.

The fact that the surface width saturates at all is an artifact of the periodic boundary conditions of the strip geometry. Division events with shallow division angles displace large numbers of elements and effectively explore the surface in search of the lowest empty lattice site to occupy. This effect introduces the surface correlations required to reduce surface width, while division events with steep division angles effectively increase the surface width. When the average

surface height is low, particles chosen for division are at or near the surface a large proportion of the time. This reduces the effect of shallow division events since the surface cannot be explored fully and hence the surface width grows beyond its saturation value. As the effective height increases, a higher proportion of division events is initiated sufficiently far below the surface for shallow angle division events to allow surface exploration. This explains the nonmonotonic behavior of the surface width displayed in Fig. 8(a). In a similar division model where only elements on the bottom-most layer are allowed to divide (in analogy to model I of Ferreira and Alves [11]), this nonmonotonicity is not observed since the surface width cannot grow beyond its saturation value (data not shown).

The surface thickness of these aggregates no longer obeys the Family-Vicsek scaling relationship. Instead we propose that the thickness obeys a new scaling relationship:

$$w(l, \hat{h}) \sim l^\alpha \hat{h}^\beta f\left(\frac{\hat{h}}{l^\gamma}\right). \quad (5)$$

In order for the scaling of the saturation thickness,  $w_{\text{cap}}$ , to be correct we must choose  $\alpha = 0.15$ , the value of the roughness exponent found previously. In this case we also choose  $\gamma = \alpha$  and  $\beta = 1$  in order to achieve a tight collapse of the data points [see Fig. 8(b)].

We also investigated the surface scaling properties of this model in a full two-dimensional geometry. The findings of this investigation are presented in Fig. 9. The width is found to grow with critical exponent  $\beta = 0.22 \pm 0.07$  (which is in approximate agreement with the value found by Ferreira and Alves [11]). The small oscillations of the local slopes about the average value of  $\beta$  in Fig. 9(c) demonstrate that the value we have found for  $\beta$  is a reliable one. This value of  $\beta$  differs from the value of the growth exponent in the strip geometry,  $\beta = 0.35 \pm 0.07$ .

An even more stark difference between the strip geometry and the full two-dimensional geometry is the saturation behavior of the surface. In the strip geometry the surface was found to saturate with roughness coefficient  $\alpha \sim 0.15$ , but in the two-dimensional geometry the surface width does not appear to saturate. Figure 9(a) demonstrates unbounded

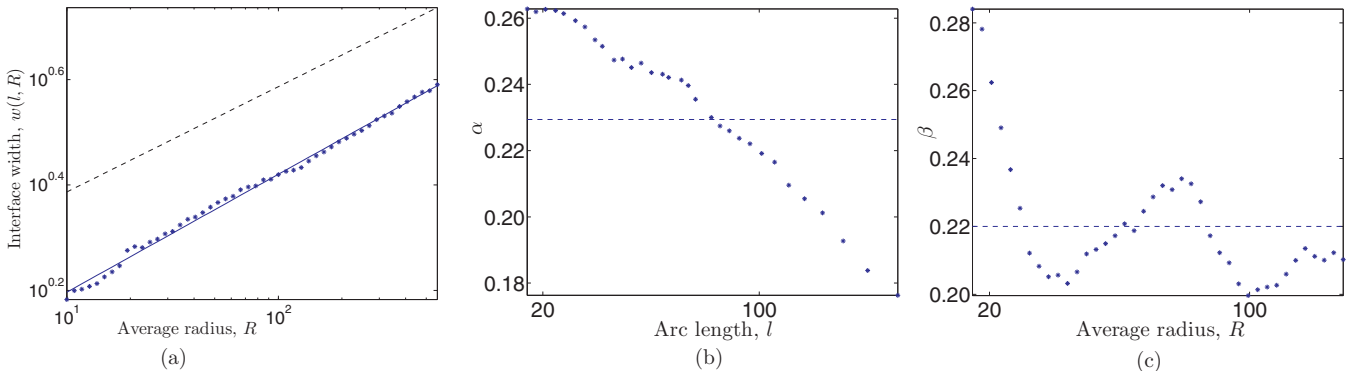


FIG. 9. (Color online) Scaling of the surface width for model II of Ferreira and Alves [11] in two dimensions. (a) Variation of surface width,  $w(l, R)$ , with average cluster radius,  $R$ , for clusters up to  $N = 10^6$  particles. Simulations are averaged over 20 repeats. Saturation of the surface width is not evident. The dashed (black) line is plotted for comparison and has gradient  $1/5$ . (b) Evaluation of the roughness exponent,  $\alpha$ , using the method of local gradients [22]. The mean value is plotted as the horizontal dashed (blue) line. (c) Evaluation of the growth exponent,  $\beta$ , using the method of local gradients. The mean value is plotted as the horizontal dashed (blue) line. Note the log scale on each of the  $x$  axes.

growth of the surface width for clusters of up to  $N = 10^6$  particles. We should expect the surface width not to saturate since additions to the surface are completely uncorrelated. A consistent value for the roughness exponent,  $\alpha$ , is unobtainable [see Fig. 9(b)]. Since the critical exponent describes the scaling of the surface thickness with a local length scale at saturation,  $w_{\text{cap}} \sim l^\alpha$ , the inability to determine  $\alpha$  is consistent with our hypothesis that the surface width does not saturate.

## VI. COMPARISON OF REACTION-DIFFUSION MODELS ON A GROWING LATTICE

Although the traditional methods of analyzing and classifying surface scaling are not sufficient for the model of Ferreira and Alves [11], this does not prevent us from utilizing the isotropic properties of the model. After the introduction of a specific element rearrangement algorithm in Sec. IV we can now employ the domain cluster aggregation model of Ferreira and Alves [11] in order to simulate discrete, stochastic reaction-diffusion processes on a radially growing domain in two dimensions. This can be quantitatively compared to an equivalent continuum model for the same process on a deterministically growing domain. This is a natural extension of the work, in one dimension, of Baker *et al.* [23] and Yates *et al.* [24] into higher dimensions. The simulations might mimic a biological tissue (a tumor, for example) which is growing radially and upon which a reaction-diffusion process is taking place [25].

For demonstrative purposes we consider a purely diffusive process in the current work, but note that the incorporation of reactions or an external signaling profile to which particles can respond would be straightforward [23,26,27]. We allow particles to diffuse on an initially (approximately) circular domain tessellated with a square lattice. The domain grows as described in Sec. IV, with an element being chosen to divide from all the currently available elements with equal probability at each time step [28]. In addition, when an element divides,

the particles that originally resided in the parent element are split symmetrically between the two daughter elements using the binomial distribution with parameter  $p = 1/2$  [23]. The elements that move in order to make room for the daughter elements do so according to the cluster rearrangement algorithm outlined in Sec. IV and take the particles at their lattice site with them, causing an advective flow of particles due to the domain growth. We restrict particles in the discrete model to remain in the domain. This corresponds to a zero-flux boundary condition.

Given the constant rate of element splitting,  $\varrho$ , in the discrete model, we can write down a probability master equation for the evolution of the number of domain elements at time  $t$ . This master equation determines that the number of domain elements grows exponentially. This, coupled with the fact that each element is equally likely to split and that the growth model is isotropic, leads us to assume uniformly exponential domain growth in the continuum model. The growth occurs at a rate,  $\rho$ , which we can easily relate to the splitting rate,  $\varrho$ , in the discrete model: the increase in area due to a division event must produce a corresponding increase in area in the continuum model and (since growth occurs isotropically) this corresponds to an increase in radius in the continuum model.

Since the PDE, boundary, and initial conditions are circularly symmetric the population-level solution will be circularly symmetric for all time. This means we need only solve a one-dimensional PDE for population density,  $u(r,t)$ , in the continuum model:

$$\frac{\partial u}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (rvu) = D \left( \frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} \right) \quad (6)$$

for  $r \in [0, \exp(\rho t)/2]$ ,  $t \in [0, \infty)$ .

The flow due to domain growth is given by  $v = dr/dt = \rho r$ , where  $\rho$  is the strain, which is determined from the element splitting rate,  $\varrho$ , in the individual-level model. We chose the

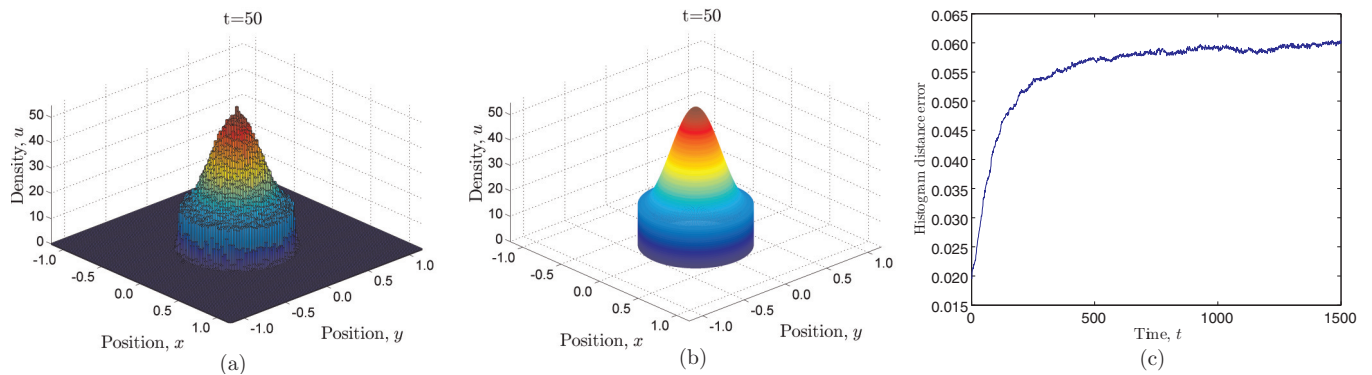


FIG. 10. (Color online) Comparison of the individual-level (with square domain tessellation) and population-level models of diffusion on a growing circular domain. In the individual-level model 50 000 particles are initialized with a density profile which decays approximately exponentially from the center to the edge of the domain. The continuum model is initialized similarly with a profile  $u = A \exp(-10r)$ , where  $A$ , the normalizing factor, ensures that the area under the continuum initial condition corresponds to the correct number of particles in the individual-level simulation. There are initially 1885 elements in the circular domain of the individual-level model. Over a simulation time of 1500 time units, with an element splitting rate of  $\varrho = 0.001$ , this number grows to  $\sim 8448$ . (a) Histograms represent the density of particles in each square of the domain tessellation. (b) The surface represents the radially symmetric solution of the PDE, (6), with  $D = h^2$ , where  $h = 1/49$  is the length of an element in the individual-level model. (c) Evolution of the histogram distance error (HDE) (see Sec. VI in the SM for a definition of the HDE metric).

initial domain to have radius  $1/2$ , which, therefore, determines the size of each lattice element in the individual-based model. We solve Eq. (6) using the NAG solver D03PE [29].

A snapshot comparison of the densities of the two models is given in Fig. 10. The models appear to give qualitatively similar results. We also plot the evolution of the histogram distance error (HDE) in Fig. 10(c). The HDE, which gives an indication of how closely the two models correspond (see Sec. VI in the SM for a definition of the HDE metric), is low, indicating a good quantitative comparison between the individual-level and the population-level domain growth models of diffusion on a radially growing domain.

## VII. DISCUSSION

In summary, we demonstrated that the model of Ferreira and Alves [11] is capable of growing circular clusters free of the inherent anisotropy of the underlying square lattice. Our revised model description also includes an explicit algorithm for rearrangement of the cluster upon division of an element. Such an isotropic model will be essential when modeling domain growth in biological contexts where no anisotropy is present. As a representative example we have presented a

comparison between a discrete position-jump model of particle diffusion on a radially growing domain and a continuum counterpart.

Our investigation into the surface scaling properties of clusters generated by the domain growth model suggests that the traditional mechanisms for classifying growing aggregates into UCs, based on the saturation behavior of their surface widths (often in a strip geometry), may be inadequate for partitioning models, such as that of Ferreira and Alves [11], whose clusters do not grow through particle additions whose probabilities are based purely on surface considerations. In particular, the model for isotropic cluster growth analyzed in this paper does not exhibit Family-Vicsek scaling behavior and, as such, cannot be placed in a traditional UC. Further work is required to determine whether the inability to be classified into UCs is common to other aggregation models whose particles are added using more global considerations.

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