Off-lattice Noise Reduced Diffusion-limited Aggregation in Three Dimensions

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Using off-lattice noise reduction it is possible to estimate the asymptotic properties of diffusion-limited aggregation clusters grown in three dimensions with greater accuracy than would otherwise be possible. The fractal dimension of these aggregates is found to be 2.50 ± 0.01, in agreement with earlier studies, and the asymptotic value of the relative penetration depth is $\frac{\xi}{R_{dep}} = 0.122 \pm 0.002$. The multipole powers of the growth measure also exhibit universal asymptotes. The fixed point noise reduction is estimated to be $\epsilon^f \sim 0.0035$ meaning that large clusters can be identified with a low noise regime. The slowest correction to scaling exponents are measured for a number of properties of the clusters, and the exponent for the relative penetration depth and quadrupole moment are found to be significantly different from each other. The relative penetration depth exhibits the slowest correction to scaling of all quantities, which is consistent with a theoretical result derived in two dimensions.

Diffusion-limited aggregation (DLA) [1] is an extensively studied model of diffusion limited growth which appears to capture the essential features of many different physical growth phenomena [2, 3, 4, 5]. However, the fractals generated have evaded a complete understanding for many years and there has recently been controversy over whether diffusion-limited aggregates are truly fractal [6].

DLA is modelled [1] by allowing particles to randomly walk from a sphere surrounding the cluster, one at a time, until they contact the cluster, at which point they are irreversibly stuck. Detailed study [7] has shown that DLA growth in two dimensions does approach true fractal scaling, but with slowly decaying corrections to scaling of the form

$$Q_N = Q_\infty + CN^{-\nu} \tag{1}$$

where Q_N is some property of the cluster, tending towards the value Q_∞ as the number of particles in the cluster, N, tends to infinity. Here the correction to scaling exponent ν is expected to exhibit some universality whilst the constant C will not. For aggregates grown in two dimensions, it has been argued [7] that there should be no quantity whose correction to scaling is slower than that of the relative penetration depth, $\frac{\xi}{R_{dep}}$, where R_{dep} is the average radius at which new particles are deposited and ξ is the standard deviation of the same. Here and below we take as origin the centroid of the depositing particles.

When studying DLA grown on a lattice, reducing the shot noise associated with the growth being by discrete particles [8] has proved valuable in understanding the asymptotic properties of clusters, complicated by their sensitivity to lattice anisotropy [9, 10]. Using a conformal map from the unit circle to the boundary of a growing cluster, Hastings & Levitov [11] introduced a technique for implementing a noise reduction scheme for DLA clusters grown off-lattice. Rather than adding particles to the cluster, bumps were added to the conformal map. Ball *et al.* [12] built on this work, allowing crescent-shaped bumps to be added to DLA clusters without the need for a conformal map. In this approach, the particles are allowed to diffuse normally until they contact the cluster. At this point the new particle is touching the cluster, and the distance between the centre of the new particle and the centre of the particle it contacted in the cluster is equal to the diameter of one particle. To implement noise reduction, this distance is reduced by a factor $A < 1$, so that the new particle is deposited partially inside the cluster: the effect is to protrude a shallow bump of height A on the cluster perimeter. Since this method does not rely on a conformal map it allows the growth of noise reduced DLA clusters off-lattice in any dimension.

Most of the work on DLA has been restricted to two dimensions. Meakin pioneered work on DLA in higher dimensions, growing clusters in dimensions up to $d = 8$ [13]. Much of that work has focused on estimating the fractal dimension of DLA clusters and the scaling of the relative penetration depth [14, 15, 16], yet firm conclusions have proved difficult. There has also been some progress measuring the multifractal spectrum of DLA in three dimensions [17, 18, 19]. However, Davidovitch *et al.* [20] recently claimed that all previous attempts to measure $f(\alpha)$ in two dimensions are poorly converged, so the early three dimensional measurements should be taken with caution. Other work has also examined DLA on a cubic lattice in the limit of zero noise [21], and the extension of the fixed scale transformation to 3 dimensions [22].

In this paper we exploit the new noise reduction techniques to explore the convergence to scaling of DLA in

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three dimensions. We grew 1000 DLA clusters off-lattice in three dimensions spanning five different values of the noise reduction $A = 1$, 0.3, 0.1, 0.03, 0.01, and an example cluster with $N = 10^4$ particles and $A = 0.1$ is shown in figure 1. At regular intervals, the growth of the clusters was suspended and 10^5 probe particles were "fired at" the cluster: these probe particles were allowed to diffuse freely, one at a time, until they contacted the cluster, at which point their location was recorded and the particle was deleted. In this way the growing properties of the clusters (such as the penetration depth and multipole moments) were estimated. The code used is a direct descendent of that of Meakin [14], which in turn builds on the computational tricks of Ball & Brady [23] to speed up computation. Whilst the code is truly lattice free, the smallest step size that a particle was allowed to take was set equal to one particle radius. Comparisons in 2 dimensions between this and an algorithm which uses a much smaller minimum step size have shown that any effect that this has on the results is the same order as the noise in the measurements attributable to inter-cluster variability [24].

I. FRACTAL DIMENSION AND CORRECTION TO SCALING EXPONENTS

We calculate the effective value of fractal dimension from the local slope of the average radius of deposition vs number of particles N according to

$$D = \frac{\ln(N_2) - \ln(N_1)}{\ln(R_{dep}(N_2)) - \ln(R_{dep}(N_1))} \tag{2}$$

where the properties are measured at two different cluster sizes N_1 and N_2. For the clusters grown, the value of the fractal dimension is shown in figure 2. The dimensions estimated for each value of A appear to be converging to a common value of $D = 2.50 \pm 0.01$ which is consistent with previous computational estimates [13]. The data for $A = 0.03$ and $A = 0.01$ are less well converged, and the results could be made more accurate with data for larger N.

We now consider the correction to scaling exponents for DLA in three dimensions. In two dimensions it has been shown that no property of the cluster has a slower correction to scaling than the relative penetration depth and suggested that all properties should show influence of this slowest correction [7]. To measure the slowest correction to scaling exponent of a quantity, we used differential plots which proved effective for DLA in two dimensions [12]. For some converging quantity Q_N, which displays a single correction to scaling (eq. 1), then

$$\frac{dQ_N}{d\ln(N)} = -\nu(Q_N - Q_\infty). \tag{3}$$

so a plot of $\frac{dQ}{d\ln(N)}$ against Q should exhibit a straight line with slope $-\nu$, intercepting the x-axis at the asymptotic value Q_∞. The differential is approximated by

$$\frac{dQ}{d\ln(N)} \simeq \frac{Q_{N_2} - Q_{N_1}}{\ln\left(\frac{N_2}{N_1}\right)} \tag{4}$$

and the error in the differential by

$$\sigma\left(\frac{dQ}{d\ln(N)}\right) \simeq \frac{\sqrt{\sigma^2(Q_{N_2}) + \sigma^2(Q_{N_1})}}{\ln\left(\frac{N_2}{N_1}\right)}. \tag{5}$$

where $\sigma(Q_N)$ is the standard error in Q_N.

To characterise the DLA clusters we measured the multipole powers, since the corresponding multipole moments provide an orthogonal set which may be used to totally describe the growing properties of the clusters. In three dimensions the multipole moments are estimated by (see [25], chapter 4)

$$q_{l,m} = \frac{1}{n}\sum_{i=1,n} r_i^l Y_{l,m}(\theta_i, \phi_i) \tag{6}$$

using n probe particles which contact the cluster at (r_i, θ_i, ϕ_i) for $i = 1$ to n. We normalised the multipole power as

$$P_l = \frac{\sum_{m=-l}^{l} |q_{l,m}|^2}{(2l+1)R_{\text{eff}}^{2l}} \tag{7}$$

where the effective radius is in turn given by

$$\frac{1}{R_{\text{eff}}} = \frac{1}{n}\sum_i \frac{1}{r_i}. \tag{8}$$

The definition of R_{eff} is such that it gives the radius of spherical target of equivalent absorption strength to the cluster. Note that for each measurement we used the centre of charge as origin, meaning zero dipole moments and hence $P_1 = 0$; otherwise there is confusion between cluster shape and drift of the cluster centre (albeit the latter is rather negligible).

The first and important feature of our differential plots is the indication of limiting asymptotic values Q_∞(corresponding to $\frac{dQ}{d\ln(N)} = 0$) which are universal, independent of the level of noise reduction. This is shown for the relative penetration depth in fig. 3, multipole powers, P_2 - P_5 being shown in fig. 4, and the relative variability of extremal cluster radius in fig. 5. The universality of the asymptotic values of all these plots is strong indication that the limiting distribution of cluster shape is universal.

The slopes of these same plots indicate the correction to scaling exponents, which also appear to be universal with respect to the noise reduction. Figure 6 shows the measured values of the correction to scaling exponents for each of the quantities plotted (and all multipole moments measured). The exponent for the quadrupole power P_2 is significantly different from the exponents for $\frac{\xi}{R_{dep}}$ and

P_3. There is no quantity which shows a slower correction to scaling than $\frac{\xi}{R_{dep}}$, which suggests that the result found by Somfai *et al.* [7] in some sense also applies to clusters grown in three dimensions.

The values of the correction to scaling exponents are least precise for the highest multipole moments, as these are most sensitive to the fine structure of the cluster. Intriguingly, the asymptotic value of the relative penetration depth for DLA clusters in three dimensions is equal within measurement error to that of the two dimensional case: see figure 3 here and figure 3 in [12]. The correction to scaling exponent for $\frac{\xi}{R_{dep}}$ is around $\frac{2}{3}$ the value of the exponent for clusters grown in two dimensions, indicating that DLA clusters in three dimensions are considerably slower to mature.

II. FIXED POINT NOISE REDUCTION

It is clear from differential plots such as figure 3 that the noise reduction "controls" the slowest correction to scaling. For low values of A this correction to scaling is strongly reduced, and we may write the behaviour of this correction as follows

$$Q_N = Q_\infty + C(A)N^{-\nu}. \tag{9}$$

Other corrections to scaling need not depend on A, but it is quite evident that the amplitude of the slowest correction to scaling is strongly affected by it. If there is some value of A for which $C(A)$ is zero, then this value of the noise reduction would correspond to the fixed point of a renormalisation scheme (see [10]). The plots for $P_2 - P_4$ suggest that the fixed point noise reduction is $A^f < 0.01$ and plots of $\frac{\xi}{R_{dep}}, P_5$ are unclear as to the value of the fixed point noise reduction. Hence, one estimates that

$$A^f \leq 0.01. \tag{10}$$

The noise reduction of the fixed point can also be estimated from the asymptotic properties of DLA clusters using the Barker & Ball [10] formula

$$\epsilon^* = D^2 \left(\frac{\delta R_{ext}}{R_{ext}}\right)^2 \tag{11}$$

where R_{ext} is the extremal cluster radius (the radius of the furthest cluster particle from the seed particle) and δR_{ext} is the cluster to cluster variability of R_{ext}. From figure 5, the asymptotic value of the relative variability of extremal cluster radius is $\left.\frac{\delta R_{ext}}{R_{ext}}\right|_\infty = 0.032 \pm 0.004$. This leads to

$$\epsilon^* = 0.0064 \pm 0.0016, \tag{12}$$

which is close to the estimated value of A^f.

For a noise reduction of A, one would naively assume that it would require of order N/A particles to grow a cluster with the same radius as a non-noise reduced cluster of N particles. Our data below show that this is a systematic underestimate, so that each value of A corresponds to a more severe noise reduction than expected. Figure 7 shows the two point correlation function for DLA clusters grown at different noise reductions. The graphs have been shifted vertically so that all the curves collapse to a single line. From the shift factors used, we estimate the effective noise reductions to be

$$\begin{array}{ll} A = 1 & \epsilon^{\text{eff}} = 1 \\ A = 0.3 & \epsilon^{\text{eff}} = 0.19 \\ A = 0.1 & \epsilon^{\text{eff}} = 0.05 \\ A = 0.03 & \epsilon^{\text{eff}} = 0.012 \\ A = 0.01 & \epsilon^{\text{eff}} = 0.0034. \end{array} \tag{13}$$

Hence one concludes that the fixed point noise reduction in equation 10 should be adjusted to

$$\epsilon^f \leq 0.0035. \tag{14}$$

The values for ϵ_f and ϵ^* differ by a factor of 2, demonstrating that the identification process is open to some errors. If, as indicated by the results in figure 6, a single slowest correction to scaling exponent does not control the scaling of all parameters, then a renormalisation scheme which is based on a single parameter (the noise reduction) may be inaccurate and agreement between ϵ^f and ϵ^* is not expected to be perfect.

III. CONCLUSION

The growth off-lattice of noise-reduced diffusion-limited aggregates in three dimensions has been considered and shown to exhibit universality with respect to noise reduction. The fractal dimension is found to be $D = 2.50 \pm 0.01$ which agrees with previous computational [13] and mean field [26] estimates. The penetration depth scales with the radius, and the asymptotic value of the relative penetration depth is $\frac{\xi}{R_{dep}} = 0.122 \pm 0.002$ which overlaps the value found for clusters grown in two dimensions [12]. The convergence of the multipole powers provides a very strong indication that DLA cluster growth, in three dimensions and off-lattice, converges to a universal distribution of cluster shapes.

The relative penetration depth exhibited the slowest correction to scaling, $N^{0.22\pm0.03}$, and some multipole powers and also the relative fluctuations in extremal radius exhibited correction to scaling exponents which could be consistent with the same. However not all quantities exhibit the influence of the slowest correction to scaling and in particular the convergence to scaling of the dipole power, P_2, is significantly faster than that of either $\frac{\xi}{R_{dep}}$ or P_3.

Reducing the input noise by factors up to 100, by growing clusters in shallow bumps, clearly reduces the amplitude of the leading correction to scaling. This supports in three dimensions the idea of Barker & Ball [10] that the intrinsic fluctuation level is the physical origin of that slowest correction to scaling. We estimated the fixed point noise reduction to be $\epsilon^f \sim 0.0035$ and this is close to the value estimated using the Barker & Ball [10] formula in terms of relative fluctuation in extremal radius.

Taken together our results support the hypothesis that isotropic DLA in three dimensions approaches a simple ensemble of statistically self-similar clusters, with a rather slow approach to scaling which is associated with the level of local geometric fluctuation. From this point of view, a quantitative model of the convergence of that fluctuation level appears to be the outstanding challenge in understanding isotropic DLA (in any dimension). Another important challenge for three dimensions, for which work is in progress, is the role which material anisotropy can play [27].

The authors wish to thank Paul Meakin & Thomas Rage for supplying code used for growing clusters in this study, and Leonard Sander and Ellak Somfai for their enlightening discussions.

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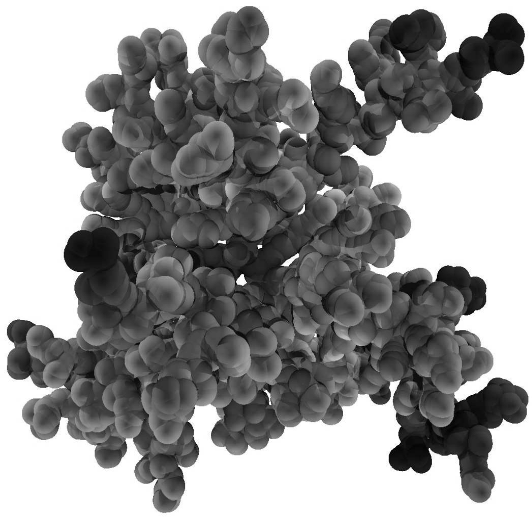

FIG. 1: A DLA cluster grown in three dimensions with $N = 10^4$ particles and noise reduction factor $A = 0.1$, where the different shading indicates a different time of deposition on the cluster.

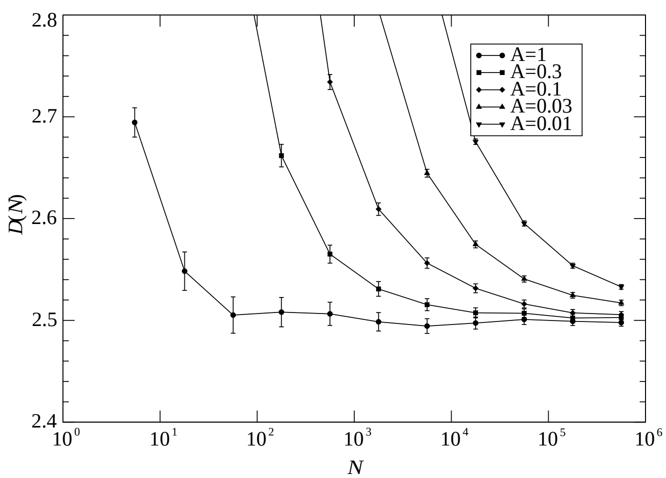

FIG. 2: The measured fractal dimension of DLA clusters, estimated by taking the local slope of R_{dep}. The dimension appears to be converging to a dimension of $D = 2.50 \pm 0.01$, universal with respect to value of noise reduction A.

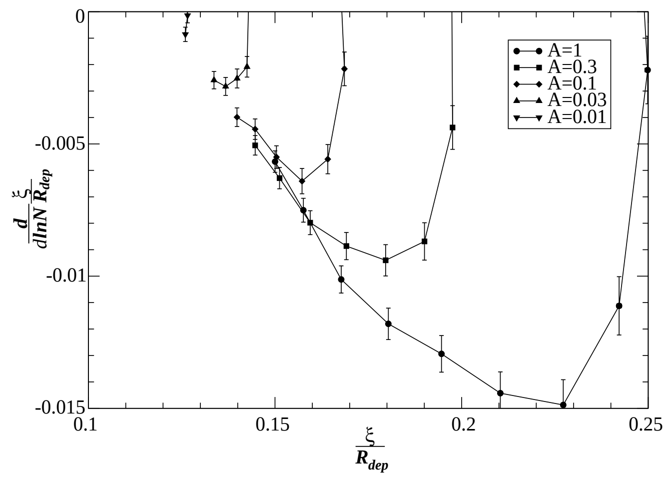

FIG. 3: Differential plot of Relative Penetration Depth $\frac{\xi}{R_{dep}}$ against its own derivative with respect to $\ln N$. The intercept with zero derivative indicates the asymptotic value of $\frac{\xi}{R_{dep}}$ for infinite N is given by $\left.\frac{\xi}{R_{dep}}\right|_{\infty} = 0.122 \pm 0.002$ and the common limiting slope of the plots indicates a correction to scaling exponent of $\nu = 0.22 \pm 0.03$. Growth at different levels of noise reduction $A \geq 0.03$ is consistent with universal values of asymptote and exponent, whilst $A = 0.01$ appears to start and remain close to the 'fixed point' value of $\frac{\xi}{R_{dep}}$.

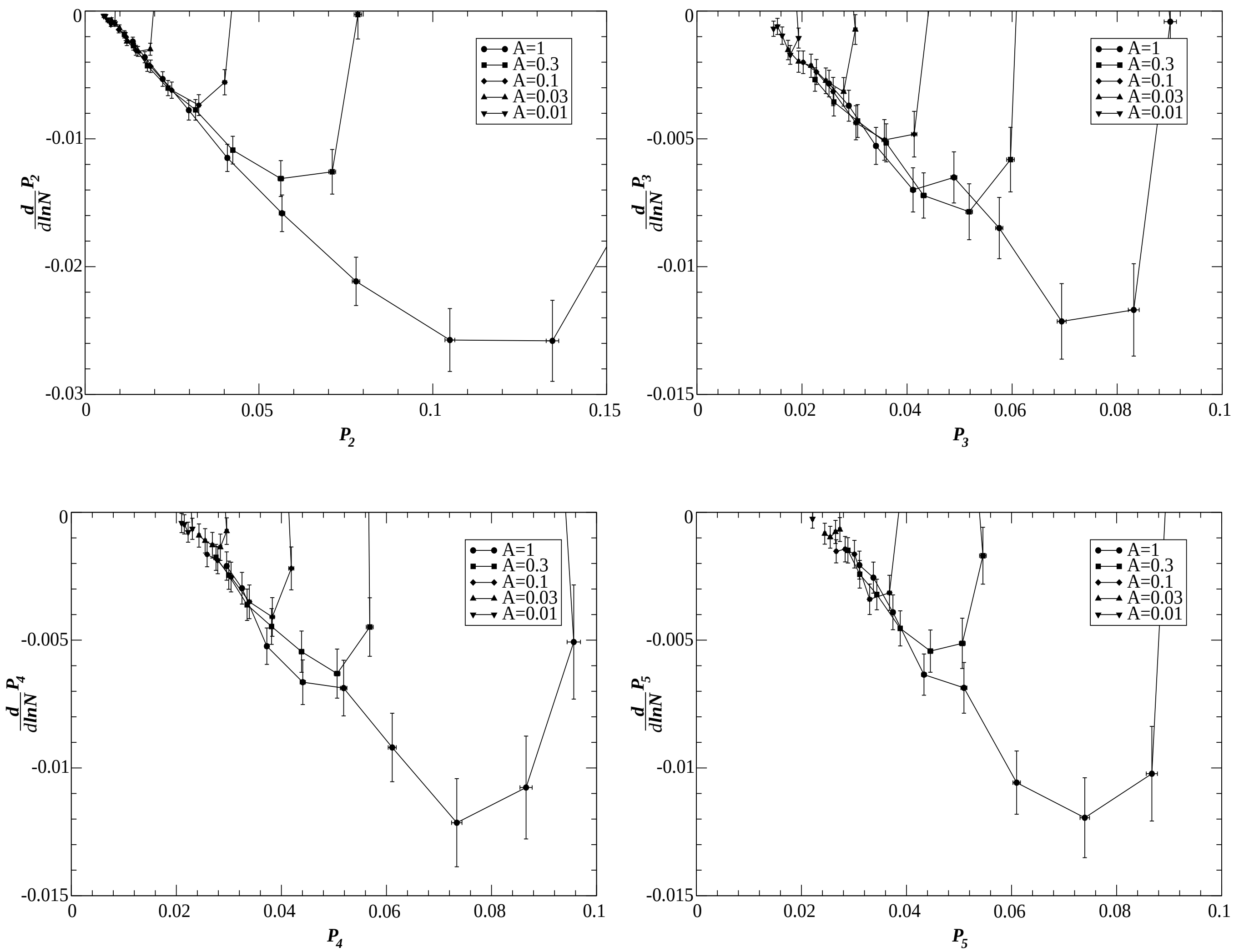

FIG. 4: Differential plots for the first four (non-trivial) multipole moments $P_2 - P_5$. All of the plots exhibit universal asymptotic values, corresponding to the extrapolation to zero derivative, and universal limiting slope corresponding to their correction to scaling exponent. The correction to scaling exponents were estimated by eye as: $\nu(P_2) = 0.32 \pm 0.02$, $\nu(P_3) = 0.24 \pm 0.03$, $\nu(P_4) = 0.26 \pm 0.06$, and $\nu(P_5) = 0.29 \pm 0.05$, where the errors represent the maximum believable error.

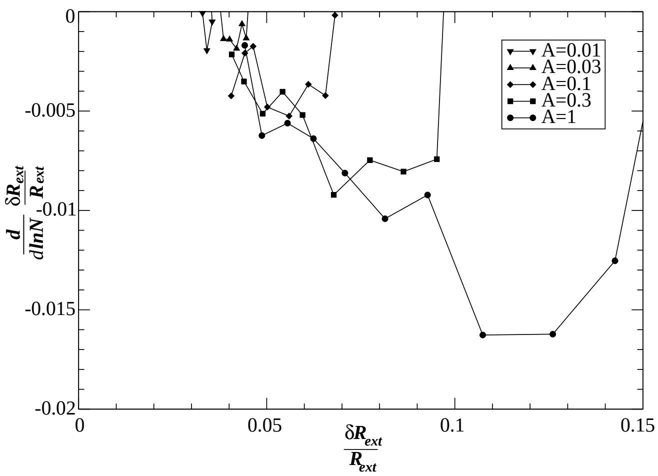

FIG. 5: Differential plot of the relative fluctuation in extremal radius, $\frac{\delta R_{ext}}{R_{ext}}$. The asymptotic value is $\left.\frac{\delta R_{ext}}{R_{ext}}\right|_{\infty} = 0.032 \pm 0.004$ which leads to an estimate of the fixed point noise reduction of $\epsilon^* = 0.0064 \pm 0.0016$.

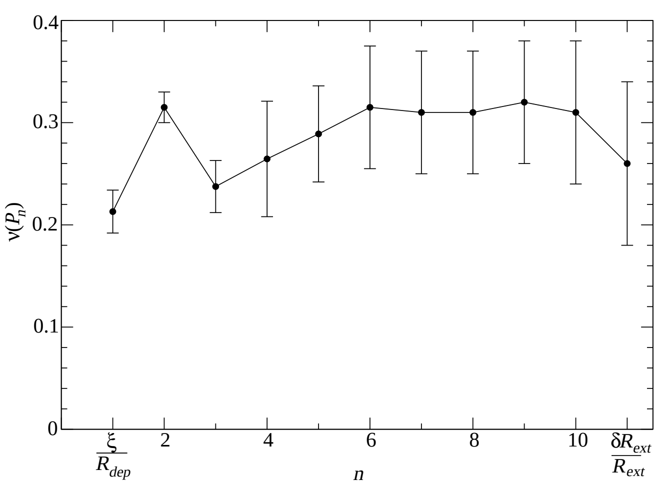

FIG. 6: The correction to scaling exponents obtained from differential plots of different multipole powers, and the two other quantities marked. The exponent for the dipole power P_2 is significantly different from the exponents measured for $\frac{\xi}{R_{dep}}$ and P_3.

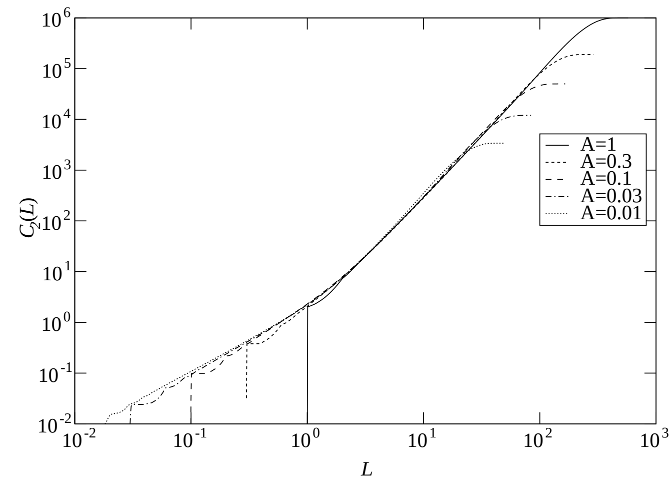

FIG. 7: The two point correlation function for clusters grown in three dimensions, scaled by effective noise reduction factors, ϵ^{eff}. This noise reduction is chosen so that a data collapse is seen for small L.