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Random Aggregation and Random-Walking Center of Mass

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Two random aggregation models are used in demonstrating the properties of the random displacements $\mathbf{r}_i$ of the center of mass of aggregating particles. It is found that $|\mathbf{r}_i|$ is a randomly decreasing sequence that scales with the cluster size (steps) s and $\sum_{i=1}^{s} |\mathbf{r}_i| \propto s^{1/D}$, where D is the fractal dimension. The center-of-mass random walk is a consistent representation of the dynamics of aggregation.

KEY WORDS: Random aggregation; random walk; fractal dimension.

The phenomena of random aggregation can be found in most physical processes that involve phase transformation, such as in the growth or recrystalization of crystals, etc. In all of these processes, growth can be modeled by the growth of a single particle initially planted at a given site.[1-6] This particle then grows by the addition of one particle at a time, subject to some given laws which determine which of the unoccupied perimeter sites can be occupied at each stage. Thus, the shape of the consequent aggregates changes as new perimeter sites are occupied one at a time. Until now it has been assumed that the center of mass (gravity) of the growing aggregates is stationary and, if not, the deviation is probably so insignificant and the phenomenon relatively isolated as to not relate to any major properties of the aggregation, particularly if a form of symmetry is perceived in the spatial patterns of the aggregates. The phenomenon of nonstationary center of mass may lead to the understanding of the dynamics of particle-by-particle aggregation.[4]

In this paper, it is shown by means of computer simulations that, during random aggregation of particles, the center of mass of the growing

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aggregates moves randomly with a randomly decreasing sequence of step lengths $|\mathbf{r}_i|$, where $\mathbf{r}_i$ is the center-of-mass displacement vector at the ith step (cluster size). The displacement lengths $|\mathbf{r}_i|$ scale with the number of steps (cluster size) and $\sum_{i=1}^{s} |\mathbf{r}_i| \propto s^{1/D}$, where D is the fractal dimension. Random walk models[7–10] are based on either equal or random displacement lengths, but not on random decreasing sequence of step lengths, in order to arrive at a scaling relation between the net displacement of the random walker (Euclidean distance from the origin) x_n and the number of steps n, so that $x_n \propto n^{1/2}$. For an oscilating particle, the net displacement from an equilibrium position is a deterministic decreasing sequence of lengths with time. De Gennes[10] showed that the net distance x traveled by a randomly walking ant on a fractal network with equal displacement lengths at a time scales with the time t, i.e., $x \propto t^{1/D}$. If $D = 2$ in two dimensions, then the diffusion process is normal; and $D < 2$ corresponds to anomalous diffusion.[11] In either case, the dynamics and hence kinetics of the diffusion process are characterised: in the present case, the fractal

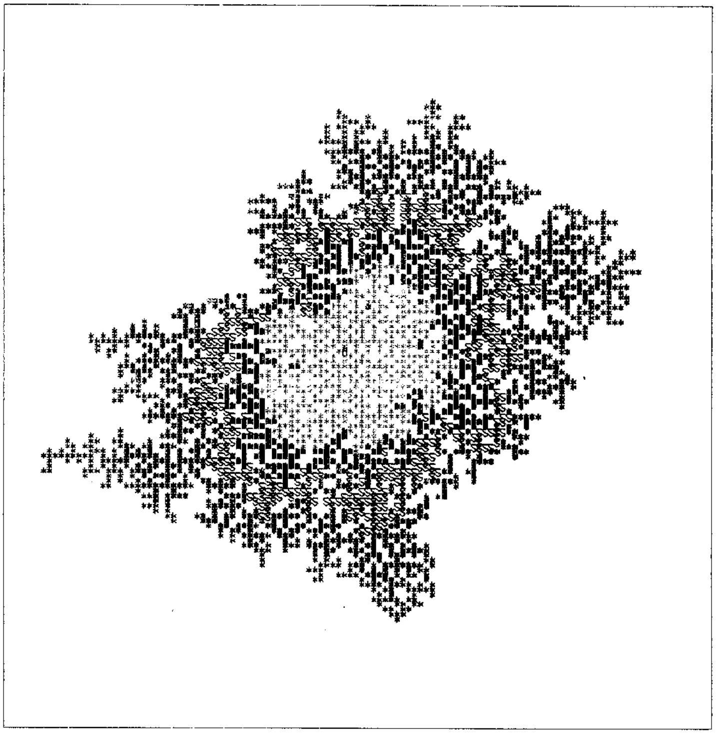

Fig. 1. Random aggregates of 3000 particles on a square lattice with the initial particle planted at the center (Eden growth model).

trajectory of the center of mass of the growing aggregates is generated as a consequence of the growth process. They have a common random and kinetic ancestory.

In this paper, two growth models, Eden[1] and diffusion-limited aggregation (DLA),[2] that generate compact and open random structures are used to demonstrate and explore the phenomenon of random walking center of mass. Figure 1 shows a 3000-particle aggregate on a (192×192) square lattice produced using the Eden growth model, and Fig. 2 shows the consequent trajectory of the center of mass; Fig. 3 is the log–log plot of the total distance traveled $\sum_{i=1}^{s} |\mathbf{r}_i|$ versus the size of the cluster s. An approximate linear relation between log[total distance] versus log[cluster size] can be observed in Fig. 3 for cluster size greater than 100, which is less than 0.5% of the total size of the random aggregates (3000) under study, and the statistical nature of these aggregates suggests that rather than fit a straight line over the rest of the curve to obtain the expo-

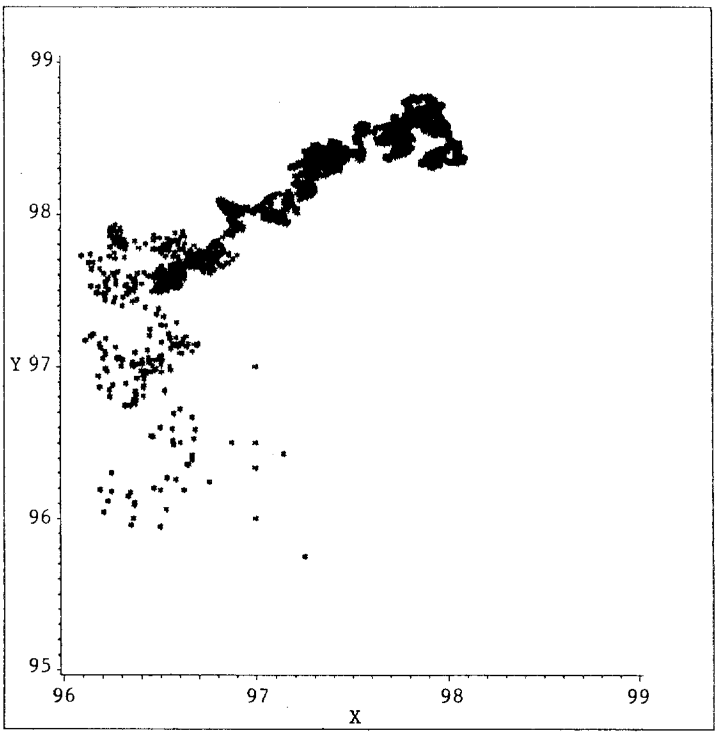

Fig. 2. Fractal trajectory of the center of mass in the course of growth of 3000 particles on a square lattice (Eden growth model).

nent α, the average sectional variation of same should be used.[15] The average values of α is 0.4891, and $D_\alpha = 2.044$. This is consistent with the expected value of the fractal dimension of aggregates generated by the Eden growth model.

Figure 4 shows a 2713-particle aggregate on a (292×292) square lattice produced using the DLA model. Figure 5 shows the log–log plot of the total distance covered by the moving center of mass and the aggregate size. The average value of the exponent is $\alpha = 0.6025$ and $D_\alpha = 1.6598$. Figure 6 shows the log–log plot of the random displacement lengths $|\mathbf{r}_i|$ versus cluster size s for DLA. The points of the graph of $\log |\mathbf{r}|$ versus $\log(s)$ in Fig. 6 are relatively considerably scattered but consistently linearly decreasing, so that linear regression lines were fitted over the last 80, 70, 60, 50, 40, 30, 20, and 10% of the entire graph in order to estimate quatitatively the variations of the exponent ξ. In the range $100 < s < 1900$, $\xi \simeq -0.4099 \pm 0.01$ and for $s > 1900$, ξ increases from -0.3819 to -0.2335 up to the last 26% of the total cluster size and beyond which the degree of scatter of the points of the graph does not justify further approximation by

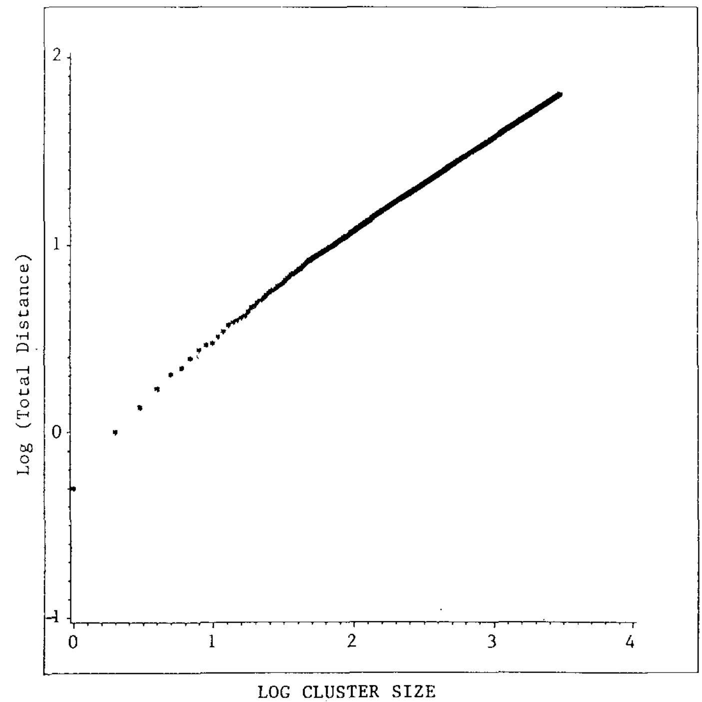

Fig. 3. Log–log graph of total distance traveled by the center of mass versus cluster size (Eden).

a linear regression fit. This is contrary to the behavior of the "total distance" exponent α of Fig. 5, which does not vary significantly over all the range of s in this study. For the Eden model, ξ is approximately a constant at -0.5091 ± 0.01 up to the last 20% of the total cluster in this study. Also, the α exponent for the Eden model did not vary significantly over the entire range of s studied. This relatively detailed analysis suggests representations of the form $[\xi^2 + \alpha^2]^{1/2} \simeq 0.707$ for the Eden growth model and for the DLA model, $[\xi^2 + \alpha^2]^{1/2} \simeq 0.729$ in the range $100 < s < 1900$. Figure 7 shows the log–log plot of the net displacement length x versus cluster size for DLA and the Eden growth model. Figure 8 shows the log–log plots of the ratio of the net and the total displacement length L versus the cluster size for the DLA and the Eden growth models.

Analogously, the random-walking process of the center of mass during aggregation provides the basis of the equilibrium dynamics of the system so

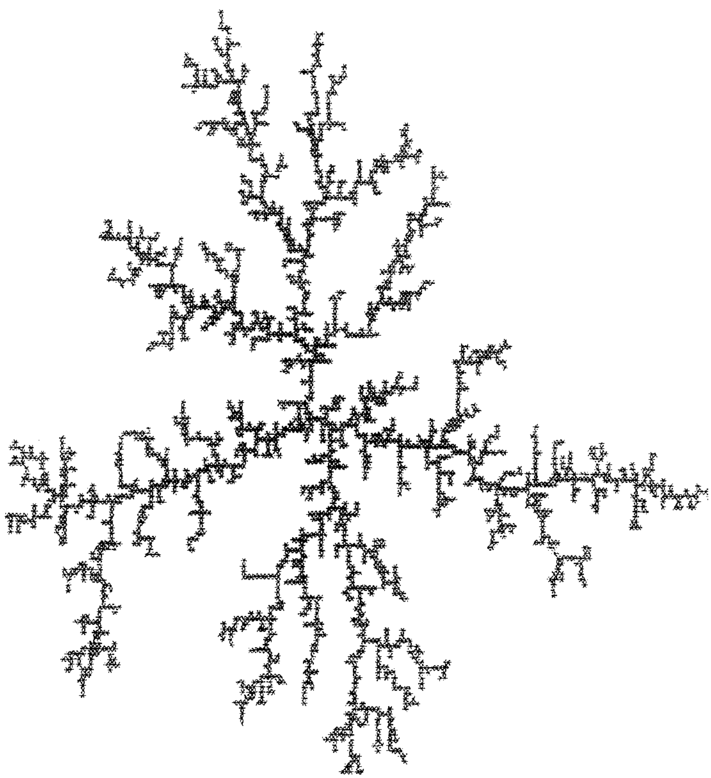

Fig. 4. Random aggregates of 2713 particles on a square lattice with the initial particle planted at the center (DLA).

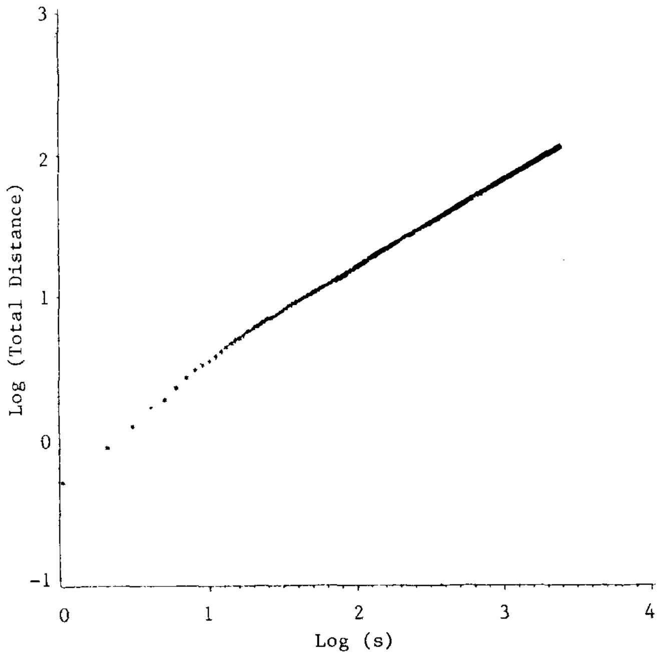

Fig. 5. Log–log graph of total distance traveled by the center of mass versus cluster size s (DLA).

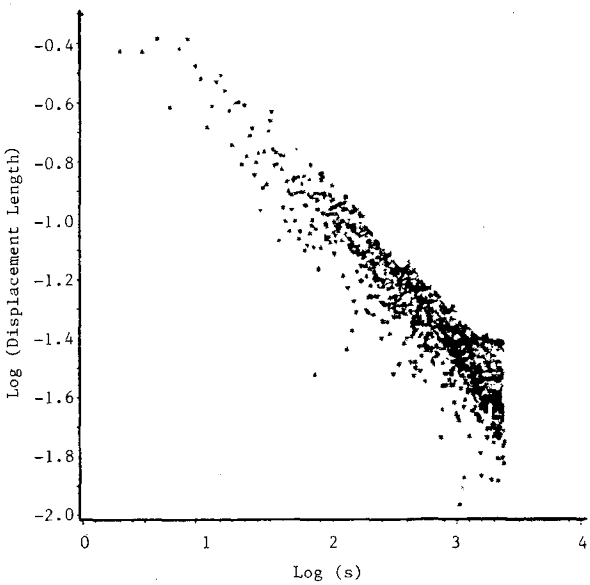

Fig. 6. Log–log graph of the center-of-mass displacement length $|\mathbf{r}|$ versus cluster size s (DLA).

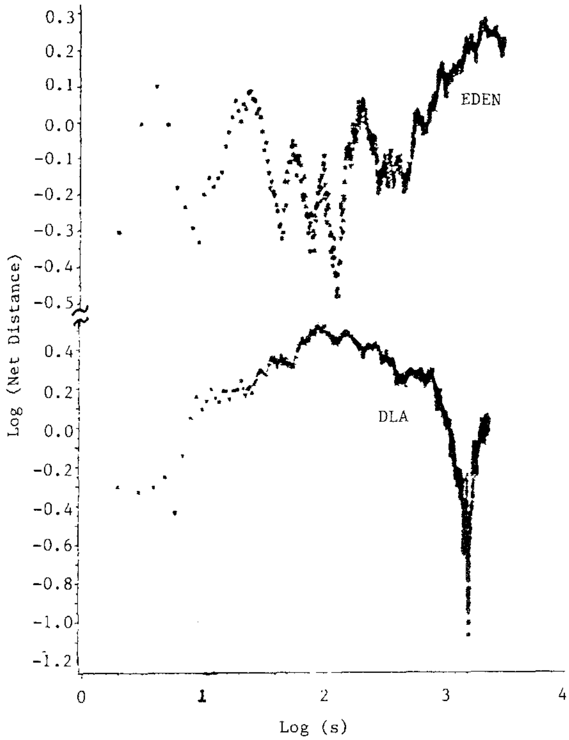

Fig. 7. Log–log graphs of the center-of-mass net distance from the origin versus cluster size s (DLA and Eden).

that one is apt to argue, for instance, that the random-walking process (hence the time scale) of the particles prior to sticking in the case of the DLA may not be uniquely associated with the equilibrium dynamics of the aggregation. In the steady state, the flux of walkers from far away is constant[13] and growth proceeds by the addition of new particles so that the equilibrium dynamics of aggregation is determined by the relationships between the cluster size and the decreasing sequence of displacement lengths analogous to the displacement versus time relations encountered in oscillators,[14] so that the exponent associated with Fig. 6 is proportional to the damping. The random displacement $|\mathbf{r}_i|$ of the center of mass with each addition of new particle is related to the change in the energy of the system so that the net distance is proportional to net energy change or flow. Thus, Figs. 6–8 are consistent representations of the dynamics of the systems.

The ratio L can be used to characterise the dynamics of random aggregation (Fig. 8): For the Eden growth model, the log–log plot of L versus s is an oscillating decreasing sequence whose local maxima or

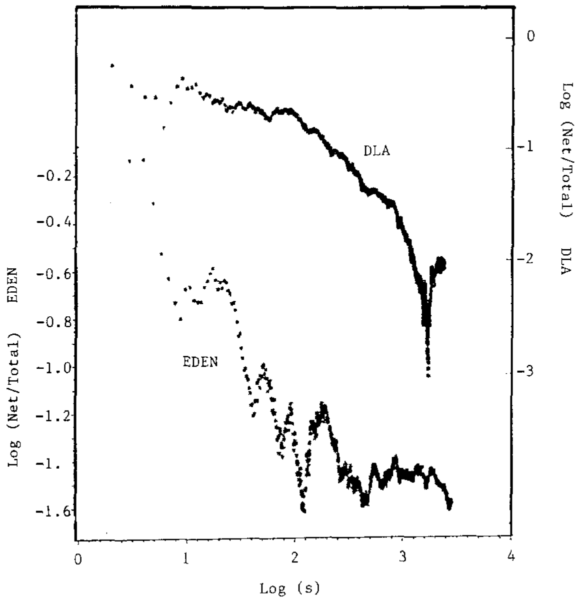

Fig. 8. Log–log graphs of the ratio of the net distance and the total distance of the center of mass versus the cluster size s (DLA and Eden).

minima are linear functions of the cluster size over a limited range $s \leqslant 129$; the scaling exponent is about -0.7061. Beyond $s = 129$, L asymptotically approaches a constant value rather like a randomly decaying noise signal[14] up to the range of cluster size investigated in this study, $s \simeq 3000$. The critical cluster size, $s \simeq 129$, corresponds to the least net displacement length x of the center of mass, i.e., the least minima of the net change in energy of the system (Fig. 7). It will be interesting to investigate quantitatively the large-cluster-size ($s \simeq 10^6$) behavior of L in the Eden model, but the disk storage space available to us at present cannot accommodate large quantities of data from such a large-scale simulation experiment [present work was performed on a multi-user-shared IBM-4341 computer model 2 (1 Mips)]. For the DLA, the log–log graph of L versus s can be approximated by three linear regions (or nonlinear oscillatory behavior) up to the critical cluster size of about 1585, beyond which the limited cluster size generated in this study does not allow for larger cluster description and future independent study would be useful, but from the point of view of minimization of energy, it will not be unlikely that L may not change very significantly from a statistical constant at large s. In general, the net change in the energy of an aggregating system is at the least minima at the critical cluster size. The work of Meakin *et al.*[15] on a large DLA cluster, $s \simeq 10^6$, suggests that beyond a cluster size of 1000, the exponent describing the length and width of the four major arms vary continuously with s, so that more useful information can be derived from the physics of the phenomenon of random walking center of mass. Finally, as in diffusion processes where $D_\alpha = 2$ corresponds to normal diffusion and $D_\alpha < 2$ corresponds to anomalous diffusion, the exponent ξ also describes the damping process wherein $|\xi| = 0.5$ corresponds to normal (linear) damping and $|\xi| < 0.5$ corresponds to anomalous (nonlinear) damping.

In summary, the random walking process of the center of mass of aggregating particles consists of randomly decreasing sequence of steps $|\mathbf{r}_i|$ that scale with the aggregate size s and $\sum_{i=1}^{s} |\mathbf{r}_i| \propto s^{1/D}$, where D is the fractal dimension; $|\mathbf{r}_i| \to 0$ as $s \to \infty$ and $\sum_{i=1}^{s} |\mathbf{r}_i| \to$ constant value. The least net displacement length occurs at a critical cluster size which corresponds to the least minima of the net change in the energy of the system. The random-walking process of the center of mass during aggregation provides consistent quantitative representations of the dynamics of the system.

Finally, the result $\sum_{i=1}^{s} |\mathbf{r}_i| \propto s^{1/D}$ can be derived on the basis of what is already known about the growth of fractal aggregates. The mean deposition distance measured from the center of mass is given by $|R_i| \sim s^{1/D}$, and from this it follows that the mean displacement of the center of mass is given by $|\mathbf{r}_i| \sim s^{(1/D-1)}$ (for sufficiently large s values); and from this, it follows immediately that $\sum_{i=1}^{s} |\mathbf{r}_i| \propto s^{1/D}$.

Above all, the present method of determining the fractal dimension of random aggregates is significant because it demonstrates unambiguously that the fractal dimension is not merely a geometric parameter, but, like the diffusion coefficient, it is also a kinetic parameter.

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REFERENCES

1. M. Eden, in *Proceedings of the Fourth Berkeley Symposium on Mathematical Statistics and Probability, Berkeley, Los Angeles, 1960*, J. Neyman, ed. (University of California, Berkeley, 1961), Vol. IV, p. 223.
2. T. A. Witten and L. M. Sander, *Phys. Rev. Lett.* **47**:1400 (1981).
3. Per Arne Rikvold, *Phys. Rev. A* **26**:647–650 (1982).
4. T. A. Witten and M. E. Cates, *Science* **232**:1607 (1986).
5. L. Niemeyer, L. Pietronero, and H. J. Wiesmann, *Phys. Rev. Lett.* **52**:1033–1036 (1984).

6. J. Nittman and H. E. Stanley, *Nature* **321**:663 (1986).
7. B. B. Mandelbrot, *The Fractal Geometry of Nature* (Freeman, San Francisco, 1982).
8. B. D. Hughes, E. W. Montroll, and M. F. Shlesinger, *J. Stat. Phys.* **28**:111–125 (1982).
9. P. G. Shewmon, *Diffusion in Solids* (McGraw-Hill, New York, 1963).
10. P. G. de Gennes, *C. R. Acad. Sci. Ser. B* **296**:88 (1983).
11. R. Orbach, *Science* **231**:814–819 (1986).
12. P. Meakin, *Phys. Rev. A* **27**:1495–1507 (1983).
13. L. Peterson, *Phys. Rev. Lett.* **52**:1621 (1984).
14. M. C. Potter, *Mathematical Methods in the Physical Sciences* (Prentice Hall, London, 1978).
15. P. Meakin, R. C. Ball, P. Ramanlal, and L. M. Sander, *Phys. Rev. A* **35**:5233 (1987).