Irreversible aggregation and network renormalization

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received 28 April 2011; accepted in final form 22 July 2011
published online 25 August 2011

PACS 89.75.Hc – Networks and genealogical trees
PACS 02.10.Ox – Combinatorics; graph theory
PACS 05.70.Ln – Nonequilibrium and irreversible thermodynamics

Abstract – Irreversible aggregation is revisited in view of recent work on renormalization of complex networks. Its scaling laws and phase transitions are related to percolation transitions seen in the latter. We illustrate our points by giving the complete solution for the probability to find any given state in an aggregation process \((k + 1)X \rightarrow X\), given a fixed number of unit mass particles in the initial state. Exactly the same probability distributions and scaling are found in one-dimensional systems (a trivial network) and well-mixed solutions. This reveals that scaling laws found in renormalization of complex networks do not prove that they are self-similar.

Droplets beget rain, goblets coagulate to make butter or cream, and dust particles stick together to form aggregates that can eventually coalesce into planets. At the microscopic level, irreversible aggregation of atoms and molecules creates many familiar forms of matter such as aerosols, colloids, gels, suspensions, clusters and solids [1]. Almost a century ago, Smoluchowski proposed a theory based on rate equations to describe processes governed by diffusion, collision and irreversible merging of aggregates [2]. The theory predicts how many small and large clusters exist at any given time and yields a mass distribution that depends on certain details such as the initial conditions, reactions present, relative rates, the presence or absence of spatial structure, etc. A key interest to physicists has been to derive scaling laws that characterize different universality classes ([3], and references therein).

By contrast, wide interest in complex networks [4–7] has emerged recently. Vast applications to physics, computer science, biology, and sociology ([8–10], and references therein) continue to be vigorously investigated. An important question is whether or not complex networks exhibit self-similarity at different length scales and if they can be grouped into universality classes on that basis. Renormalization schemes for networks were proposed [11–14] to address this question. Scaling of the mass or degree distribution of the renormalized nodes was used to argue that many complex networks are self-similar. The semi-sequential renormalization group (RG) flow underlying the box covering of [11–14] was studied carefully in [15,16], where it was found that scaling laws may be related to an “RG fixed point” which was observed for a wide variety of networks. A convenient, fully sequential scheme called random sequential renormalization (RSR) was introduced [17]. At each RSR step, one node is selected at random, and all nodes within a fixed distance \(\ell\) of it are replaced by a single super-node.

We point out a simple mapping between RSR and irreversible aggregation on any graph. Hence any conclusion drawn for one process holds also for the other. Indeed, a local coarse-graining step to produce a new super-node represents one aggregation event, where a “molecule” aggregates with all its neighbors within distance \(\ell\) to produce a new cluster. Exact combinatorial analysis in one dimension without diffusion reveals that even this trivial network exhibits scaling laws for the cluster mass distribution under RSR —with exponents that depend on \(\ell\). Consequently, and somewhat counter-intuitively, self-similarity observed in RSR and similar network renormalization schemes cannot be used to prove that complex networks are themselves self-similar. Instead scaling laws arise due to a percolation transition in irreversible aggregation.

The correspondence between aggregation and renormalization is relevant for any model with stochastic coarse-graining of a network. For instance, the theory of space and time “Graphity” [18,19], based on loop quantum...
gravity, involves a stochastic coarsening similar (albeit more structured) to RSR. Hence the critical point of aggregation may also be relevant in that and related cases. The breakdown of conventional universality, where critical exponents depend on the microscopic scale of coarse-graining, $\ell$, seems to present a dilemma for theories based on stochastic coarse-graining of a network to arrive at, e.g., a universal large-scale theory of gravity.

In order to demonstrate these points, here we consider irreversible aggregation $(k+1)X \rightarrow X$, where a randomly picked cluster coalesces with $k$ neighbors. For even $k = 2\ell$ this corresponds precisely to RSR on a 1-d chain with coarsening range $\ell$. The mass of the newly formed cluster is the sum of the $(k+1)$ masses. We assume that the “target” cluster is picked with uniform probability from all clusters. Other choices will be discussed elsewhere [20].

Let us start with the model defined on a ring, i.e., with periodic boundary conditions. Initially, $N_0$ sites labelled by $i \in [1, \ldots, N_0]$ are each occupied by a particle of mass $m = 1$. Time can be either discrete or continuous, but we demand that two events never happen simultaneously. Hence events, ranked by increasing time, are denoted by positive integer values $t$. For each event, particles coagulate to form clusters of mass $m > 1$. More precisely, an event consists of picking a random cluster with uniform probability and joining it with $k$ clusters to its immediate right, using periodic boundary conditions. We note that no diffusion procedure is involved here. For $k$ even, the same results are found if we aggregate clusters symmetrically. After $t$ events, $N_t = N_0 - kt$ clusters exist. Our main result is the probability to find any sequence of adjacent cluster masses $p_{N_0}^N(m_1, m_2, \ldots, m_{N_t})$ —where a cluster of mass $m_1$ is followed by a cluster of mass $m_2$, etc., moving clockwise (see fig. 1). We start with the single-cluster mass probability.

Cluster masses are restricted to any $m \equiv 1 \pmod{k}$. Defining $m-1 = ks$, the integer $s$ is the number of events needed to make the cluster of mass $m$. As depicted in fig. 1, we can represent any realization of the process by a forest of $N_t$ rooted trees with $N_0$ leaves and $t$ internal nodes. Each tree $\alpha$ has $s_\alpha$ internal nodes, with $\sum_\alpha s_\alpha = t$. We simplify the notation by $N$ for $N_t$.

Let $p_{N_0}^N(m)$ denote, for fixed $k$ (the dependence on $k$ is not written explicitly in the following), the probability that a cluster of mass $m$ has its leftmost member at site $i \in [1, \ldots, N_0]$ after $t$ events. The probability that any of the $N$ clusters picked at random has mass $m$ is then

$$p_{N_0}^N(m) = \frac{N_0}{N} \pi_{N_0}^N(m), \quad (1)$$

because there are $N_0$ choices for $i$ and the chance to pick that particular cluster, given that it exists, is $1/N$. Since events occur completely at random, each history occurs with equal probability. The term “history” refers to a fixed forest, which includes a fixed temporal order of events. Thus $\pi_N^N(m)$ is equal to the number of histories leading to a final configuration with a cluster of mass $m$ starting at position $i$, divided by all possible histories leading to $N$ clusters. The latter is equal to

$$n_{\text{hist, tot}} = N_0 \times (N_0 - k) \times \cdots \times (N + k), \quad (2)$$

where each of the $t$ factors equals the number of choices for the next event. Using Pochhammer $k$-symbols or, equivalently, generalized rising factorials [21–24], this can be written as $n_{\text{hist, tot}} = (N + k)_{t,k}$. Similarly, the number of histories leading to a cluster of size $m$ starting at a fixed position $i$ is

$$n_{\text{hist, cluster}} = (m - k)(m - 2k) \times \cdots \times 1 = (1)_{s,k}, \quad (3)$$

and the number of histories for the remaining $N - 1$ clusters is

$$n_{\text{hist, rest}} = (N_0 - m - k)(N_0 - m - 2k) \times \cdots \times (N - 1) = (N - 1)_{t - s, k}. \quad (4)$$

So far we have not included the number of choices associated with different time orderings for the $s$ events in the cluster and $(t - s)$ events in the rest of the forest. The number of different time orderings is given by

$$n_{\text{orderings}} = \binom{t}{s}. \quad (5)$$

Combining eqs. (1)–(5), we obtain

$$P_{N_0}^N(m) = \frac{N_0}{N} \binom{t}{s} \frac{(N - 1)_{t - s, k} (1)_{s, k}}{(N + k)_{t,k}} = \binom{t}{s} \frac{(N - 1)_{t - s, k} (1)_{s, k}}{(N)_{t,k}}. \quad (6)$$

Fig. 1: (Color online) Illustration of aggregation on a ring with $k = 1$, $N_0 = 24$, and $N = 5$. The tree in color corresponds to a cluster of mass $m = 5$. It has five leaves (blue) and four internal nodes (red). Its leaves start at site $i$ and end at site $i + m - 1$. The numbers beside internal nodes correspond to the time order when coalescence occurs.
This result can be further simplified into beta functions or, more conveniently, k-beta functions (see, e.g., [22]),

\[ B_k(x, y) = \frac{1}{k} B \left( \frac{x}{k}, \frac{y}{k} \right), \]

giving a remarkably simple final result

\[ p_N^{N_0}(m) = \left( \frac{t}{s} \right) B_k(N_0 - m, m) \frac{B_k(N - 1, 1)}{B_k(N, 1)}. \]  

We make a number of observations: i) For \( k = 1 \) the process simply maps to bond percolation on a 1-d ring. For \( N = 2 \), the mass distribution is uniform over the entire range \( m \in [1, N_0 - 1] \). For \( N > 2 \), the distribution is proportional to the \( (N - 2)^{nd} \) factorial power \((N_0 - m - 1)(N_0 - m - 2) \cdots (N - m - N + 2)\). ii) For \( N = 2 \) and any \( k \geq 1 \), \( p_N^{N_0}(m) \) is symmetric under the exchange \( m \leftrightarrow N_0 - m \). iii) For \( N = 2 \) and \( k = 2 \) we obtain an equation formally identical to Spitzer’s discrete arc sine law for fluctuations of random walks [25]. iv) Asymptotic power laws for \( N_0 \to \infty \) can be determined using Stirling’s formula. If \( N \) is fixed and both \( m \) and \( (N_0 - m) \to \infty \),

\[ p_N^{N_0}(m) \sim \frac{(t - s)^{N_0 - 1}}{s^k}. \]  

For small masses, this gives a decreasing power law with exponent \(-1 + 1/k\). For \( N = k + 1 \), the power law \( p_N^{N_0}(m) \sim s^{-1+1/k} \) holds up to the largest possible value, \( m = N_0 - N + 1 \), and the cutoff is a step function. For \( m/N_0 \to 1 \) different power laws appear if \( N \neq k + 1 \), and the sign of the exponent changes at \( N = k + 1 \). For \( N < k + 1 \), the distribution has a peak at \( m/N_0 \to 1 \), while it goes to zero for \( N > k + 1 \). These scaling laws are illustrated for \( k = 2 \) in fig. 2. v) The scaling laws found for \( m \ll N_0 \) are identical to those obtained by Krapivsky [26] for the well-mixed case, even no diffusion is considered. However, the behavior for \( m/N_0 \to 1 \) given in [26] does not agree with our result. vi) The probability \( p_N^{N_0}(m) \) satisfies a number of recursion relations:

\[ p_N^{N_0}(m + k) = \frac{m(N_0 - m - N + 1)}{(m + k - 1)(N_0 - m - k)} p_N^{N_0}(m), \]

\[ p_N^{N_0+k}(m) = \frac{N(N_0 - m - N + 1)}{(N - 1)(N_0 - N)} p_N^{N_0}(m). \]

A third nonlinear recursion relation is given later.

Joint distributions for masses of adjacent clusters can also be found. We denote by \( p_N^{N_0}(m_1, m_2) \) the probability to find a cluster of mass \( m_1 \) followed immediately to the right by a cluster of mass \( m_2 \). This is nonzero only if \( m_1 = 1 + s_1 k \) and \( m_2 = 1 + s_2 k \), where \( s_\alpha \) is the number of events needed to form a cluster of mass \( m_\alpha \). By the same arguments that led to eq. (6) we get

\[ p_N^{N_0}(m_1, m_2) = \frac{t}{s_0, s_1, s_2} \frac{(N_0 - 2)(1)(s_1, k)(1)(s_2, k)}{(N)_t, k}, \]

where \( s_0 = t - \sum_{\beta=1}^{\infty} \beta s_\beta \) and the first factor is the multinomial coefficient instead of the binomial coefficient. When \( \alpha = 2 \), it is a trinomial coefficient that counts the number of ways in which the three sequences of events—for the two clusters considered, and for all \( (N - 2) \) other clusters—can be interleaved in a single history.

For any \( 1 \leq \alpha < N - 1 \) the joint probability distribution for \( \alpha \) consecutive, adjacent clusters is a product of a multinomial coefficient and \((\alpha + 1)\) Pochhammer k-symbols, divided by the Pochhammer k-symbol related to the total number of possible histories given \( N_0 \) initial particles. Defining again \( s_\alpha \) as the number of events in all clusters except the first \( \alpha \) ones, we can write the result compactly as

\[ p_N^{N_0}(m_1, \ldots, m_\alpha) = \frac{t}{s_0, \ldots, s_\alpha} \frac{(N_0 - \alpha)(s_0, k) \prod_{\beta=1}^{\alpha} (s_\beta, k)}{(N)_t, k}. \]  

In particular, this can also be done for the joint distribution for all \( N \) masses by setting \( \alpha = N - 1 \). The resulting expression is then manifestly invariant under any permutations of \( N \) numbers \((m_1, \ldots, m_N)\). Hence the \( N \)-cluster probability is independent of the spatial ordering of the clusters. While there are obvious correlations between the mass values (the sum of all cluster masses must be \( N_0 \)), there are no spatial correlations.

We now consider a line of \( N_0 \) particles with open boundaries. Again, aggregation events consist of a random choice of a cluster, followed by its amalgamation with its \( k \) nearest neighbors to the right. The target cluster must be at least \( k \) steps away from the rightmost boundary. Following the same arguments leads immediately to eq. (9) for \( \alpha = N - 1 \), showing that the two models lead to precisely the same statistics.
The absence of spatial correlations indicates that the same dynamics might result for the well-mixed case. Now we start with a bucket containing \( N_0 \) balls, each of unit mass. An event consists of taking \( k + 1 \) balls out of the bucket, merging them together, and returning the new ball to the bucket. The \( k + 1 \) balls are chosen completely at random, independently of their masses.

The single-cluster mass distribution for the well-mixed model can be obtained using the same strategy as before, but the details are quite different. Consider the total number of histories. Since events now correspond to choosing any \( k + 1 \) balls out of \( N_0 - kt \) balls, we have, instead of the Pochhammer Pochhammer symbol, a product of binomial coefficients,

\[
\binom{N_0}{k+1} \binom{N_0 - m - jk}{k+1} \binom{N + k}{k+1}. \tag{10}
\]

The expressions for \( \binom{N_0}{k} \) and \( \binom{N_0 - m - jk}{k} \) are analogous, with the factors \( (m - jk) \) (respectively, \( (N_0 - m - jk) \)) in eq. (3) (respectively, (4)) replaced by binomial coefficients. The number of time orderings \( n_{\text{ord}} \) is exactly the same as before, but the first factor \( N_0 / N \) in eq. (6) has to be replaced by \( \frac{1}{N} (N_0 - m) \). Putting all these things together, many cancellations take place, leading exactly to eq. (7).

The argument can be similarly extended to get the full \( N \)-particle distribution function, obtaining exactly the same result as before, for any \( k \).

The time-reversed process of aggregation is fragmentation. When considering the fragmentation process associated with any of these models, we have to carefully evaluate fragmentation rates. Assuming uniform rates would not lead to all time-reversed histories having the same probability. Indeed the fraction of all mergers arising with a cluster of mass \( m' \) is \( (s'/l) = (m' - 1)/(N_0 - N) \), which must equal the probability that an existing cluster of mass \( m \) will fragment at the next step in the time-reversed process. If it does, then for consistency its fragmentation products must have a mass distribution given by \( p_{m+1}(m) \). A quadratic recursion relation for \( p_{N+k}^{N_0}(m) \) can then be obtained by considering the likelihood of all fragmentation events in a configuration of \( N \) clusters, with \( m \) being the mass of one of the resulting \( k + 1 \) fragmentation products. The relation is

\[
p_{N+k}^{N_0}(m) = \sum_{m' = m+k}^{N_0 - N + 1} \frac{N(m' - 1)p_N^{N_0}(m')p_{m+1}(m)}{N_0 - N},
\]

where the prime on the summation symbol indicates that \( m' \) must increase in steps of \( k \).

In summary, we derived complete solutions for the probability to find any given state in three models—well-mixed solutions, particles on a ring reacting with their \( k \) nearest neighbors, and the same reaction for particles on a line with open boundaries—and that these solutions are precisely the same. The fact that we could solve exactly a one-dimensional model without detailed balance might seem surprising since such models are in general not solvable. It stems from the fact that spatial correlations, although \textit{a priori} not excluded, are in fact absent. Related to this is our finding that the well-mixed models have exactly the same solutions. Our method can be used to solve the model where the target cluster is picked with a probability proportional to its mass [20]. Perhaps generalizations of these observations hold true for more complicated models, in which case weighted path integrals would replace sums over histories.

We have pointed out a direct mapping between irreversible aggregation and RSR. The latter was motivated by claims that one can define finite fractal dimensions for real networks [11], using similar but more complicated and ambiguous schemes. Results for RSR with \( \ell = 1 \) on various graphs (critical trees [17], Erdős–Rényi and Barabási–Albert networks [27], and regular lattices [28]) concur with our present conclusions for \( k = 2 \). Apart from studying a system that is sufficiently simple to be exactly solvable and that is obviously not fractal, here we presented results for \( \ell > 1 \), showing that scaling laws depend in a nontrivial way on \( \ell (k) \). Results for the elementary network (a one-dimensional line) examined analytically here proves that scaling under stochastic network renormalization arises from an underlying percolation transition in aggregation and does not prove fractality or self-similarity of the underlying graph.

Our mapping suggests that the critical behavior of aggregation may also turn up in “Graphity” [18,19] or related models, where geometry, gravity, and matter emerge through an aggregation process of an underlying graph. “Geometrogenesis” is the complementary process of infinite cluster formation in irreversible aggregation. In that case, we expect that a valid microscopic model (unlike the one-dimensional lattice studied here) exhibits large-scale scaling properties that are invariant with respect to the coarse-graining scale of renormalization. This would provide a test to select physically reasonable theories [29].

REFERENCES

[1] Zangwill A., Nature, 411 (2001) 651.
[2] von Smoluchowski M., Z. Phys. Chem., 92 (1917) 129.
[3] Leyvraz F., Phys. Rep., 383 (2003) 95.
[4] Strogatz S. H., Nature, 410 (2001) 268.
[5] Albert R. and Barabási A.-L., Rev. Mod. Phys., 74 (2002) 47.
[6] Dorogovtsev S. N. and Mendes J. F. F., Adv. Phys., 51 (2002) 1079.
[7] Newman M. E. J., SIAM Rev., 45 (2003) 167.
[8] Dorogovtsev S. N., Goltsev A. V. and Mendes J. F. F., Rev. Mod. Phys., 80 (2008) 1275.
[9] Barabási A.-L., Science, 24 (2009) 412.
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[10] Barabási A.-L., Gulbahce N. and Loscalzo J., Nat. Rev. Genet., 12 (2011) 56.
[11] Song C., Havlin S. and Makse H., Nature, 433 (2005) 392.
[12] Goh K.-I., Salvi G., Kahng B. and Kim D., Phys. Rev. Lett., 96 (2006) 018701.
[13] Kim J. S. et al., Phys. Rev. E, 75 (2007) 16110.
[14] Rozenfeld H., Song C. and Makse H., Phys. Rev. Lett., 104 (2010) 25701.
[15] Radicchi F., Ramasco J. J., Barrat A. and Fortunato S., Phys. Rev. Lett., 101 (2008) 148701.
[16] Radicchi F., Barrat A., Fortunato S. and Ramasco J. J., Phys. Rev. E, 79 (2009) 26104.
[17] Bizhani G., Sood V., Paczuski M. and Grassberger P., Phys. Rev. E, 83 (2011) 036110.
[18] Konopka T., Markopoulou F. and Smolin L., e-print arXiv:hep-th/0611197v1 (2006).
[19] Hamma A. et al., Phys. Rev. D, 81 (2010) 104032.
[20] Son S.-W. et al., in preparation (2011).
[21] Normand J., J. Phys. A., 37 (2004) 5737.
[22] Díaz R. and Paríguan E., Divulg. Mat., 15 (2007) 179.
[23] Pitman J. and Picard J., Combinatorial Stochastic Processes (Springer) 2006.
[24] Kingman J., J. Appl. Probab., 19 (1982) 27.
[25] Spitzer F., Principles of Random Walk (Springer Verlag) 2001.
[26] Krapivsky P., J. Phys. A, 24 (1991) 4697.
[27] Bizhani G. et al., in preparation (2011).
[28] Christensen C. et al., e-print arXiv:1012.1070 (2010).
[29] Paczuski M. et al., in preparation (2011).