# MULTIPLICATIVE COALESCENCE

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Abstract. We examine models of coalescence, where particles in a medium join together at rates dependent on their masses. In particular, for the multiplicative coalescent, where this rate is proportional to the product of the masses, we have several methods by which to find solutions of the governing ODEs, as introduced by Smoluchowski. A principal concern is to demonstrate existence and uniqueness of solutions to these equations for as general a class of initial conditions as possible. The dynamics are equally applicable to a finite-volume stochastic model, and we examine how much of the theory carries over the limit as the number of particles tends to $\infty$.

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## 1. Introduction

1.1. **Motivation.** It is natural to seek a mathematical model for the class of particle models in which, over time, smaller particles join to form larger ones. Scale makes no difference: polymers are built up dynamically from simple molecular units, as are galaxies and other large cosmic objects. Models of *coalescence*[1] were introduced to provide a mathematical description of all these systems.

In the situations above, it is important to consider which properties of the particles are relevant to the coalescent process, and which can be ignored, under suitable mean-field assumptions. For example, consider two clumps of foam on the surface of a cup of coffee. These will coalesce when they meet. But a complete mathematical description would require knowledge of the position and time-dependent velocities of the foam clusters, as well as their precise shape, boundary conditions, and the rule describing how they join if they collide. This is likely to be too complicated for study.

Instead, attention is most usefully restricted to situations where these properties are not relevant. Often this is achieved by considering a continuum of particles, or assuming that their speeds are very large relative to the rate of coalescence, hence absorbing local properties into a global average. Then the coalescent process is determined entirely by the masses of the particles.

[1] or *coagulation* or *aggregation*, and others depending on the physical context.

It is not hard to see why this carries applications in more theoretical mathematics. A model in which objects merge at rates related to their sizes (which is equivalent to mass in many contexts) is similar in flavour to existing processes in probabilistic combinatorics. Kingman's process for partitions of the unit interval, and the process recording how descendents are shared in population evolution both have the features of coalescence. In particular, the case of coalescence with a multiplicative kernel has a direct correspondence with component sizes in a random graph process.

1.2. **Models.** Assume that the rate of coalescence of two particles is given by a 'nice' function of their masses only. In particular, we examine the multiplicative kernel, where the rate of coalescence is proportional to the product of the masses. Then there are essentially two ways to proceed. In this essay, we mainly consider a continuum of particles, and thus a *deterministic* process. The evolution of the system can be described through a system of ODEs, as studied first by Smoluchowski.

The solutions for some of the most important kernels turn out to be phrased best in terms of the component sizes of classical Galton-Watson branching processes. This is a reminder of the underlying stochastic formulation of the coalescent process. And so, alternatively, we can consider *stochastic models* for the coalescent process. Here the dynamics are similar to the continuum described by Smoluchowski. But by treating only finitely many particles, the process is open to the theory of Markov processes. It is important for the credibility of the models that these finite stochastic systems converge in some suitable sense to the solutions to the deterministic equations.

The theory of these coagulation processes emerged at a similar time to the development of random graph processes. It turns out that the stochastic coalescent with multiplicative kernel and a standard graph process on finitely many vertices are essentially the same random object. The formation of the giant component in such a graph process has been much analysed in the literature. This turns out to be the natural analogue of gelation, and so existing results about graphs can be used in the context of coalescence.

1.3. **Outline.** The main goal of this essay is to introduce the models that describe coalescent processes, and discuss three essentially different ways to solve Smoluchowski's coagulation equations when the kernel is multiplicative. Different methods will allow us to consider initial conditions and the nature of the masses with different levels of generality.

Because of the explicit way in which the system has been defined, we would expect to be certain of the existence and uniqueness of solutions. In fact, a result of Norris in [21] shows that under a suitably perverse choice of kernel and initial conditions, Smoluchowski's equations have multiple solutions. It is therefore important to show that for models where the parameters have a more obvious physical interpretation, solutions are as we would expect.

When all particles initially have unit mass, we can control the distributions using the machinery of complex analysis. We exploit the fact that the densities $n(x,t)$ have similar forms for each mass $x$. As McLeod showed in the first 'pure mathematical' paper on the topic [19], induction will guarantee existence for $t \in [0,1]$. On examining the solutions, it is apparent that a phase transition occurs at $t = 1$, after which, counter-intuitively, mass is no longer preserved. We discuss how to interpret this physically as the formation of particles with infinite mass which are not accounted for in the governing equations, an effect referred to as *gelation*. We then consider some of the progress of Kokholm in [14], which shows that these methods can be adapted to prove uniqueness after gelation as well.

A more modern approach, first seen in [15], considers the generating function of the distributions $n(x,t)$, and a PDE which it satisfies. Questions of existence and uniqueness are then essentially governed by characteristics and the existence of an inverse function which specifies probability distributions. These can be examined entirely separately from the model. We consider a remark in [8] which exploits an equivalence with the generating functions of branching processes to move from uniqueness to existence in the monodisperse case. As part of this, we discuss some of the theory of branching processes, and provide an unusual proof about the distribution of the total population size in a Galton-Watson process, using a combinatorial approach.

To demonstrate the power of PDE applications, we consider instead a more complicated model of Bertoin introduced in [5], where particles are assigned *arms* which perform the coagulations but are then exhausted. This has similarities to the multiplicative version of Smoluchowski's model. Here, the generating functions need to track two parameters, arms and mass, but much of the theory carries through. We supply a full proof of existence and uniqueness using PDEs for this model, addressing some of the technical points omitted in the previous section. We discuss how these *limited aggregation* models also share properties with generalised branching processes, and some of the consequences of this equivalence.

Finally we will review the most general result to date about existence and uniqueness of solutions to Smoluchowski's equations, due to Norris [22]. Here we will be able to treat both pre- and post-gelation behaviour for a very general class of initial conditions, and for the continuous mass case as well. In fact, we will even be able to relax the dependence on the additive structure of the masses. A key feature of this proof is that we will assume that infinite particles continue to interact with finite particles in the natural physical extension of the original dynamics. We will work in slightly less abstraction than Norris, considering only the multiplicative kernel, rather than the relevant generalisations he examines. We give a full proof of existence and uniqueness for this case, and show that we can use this to describe the gelation time very precisely.

*A word on notation.* There are about as many choices for denoting the densities in the literature as there are papers. Here we will stick to the convention $n(x,t)$ for the density of mass $x$ particles at time $t$ wherever it is reasonable. However, as is often the case, notation suggests the approach. McLeod and Kokholm treat the densities as a process for

each $x$ evolving in time, as indicated by the choice $n_x(t)$. In the PDE analysis, $x$ appears in the generating function, and so for clarity ought to be an argument of the density. On the other hand, in Norris's approach, it makes sense to view Smoluchowski's dynamics as a statement about time evolution of measures, so for this environment we shall use $\mu_t(\cdot)$ instead, to indicate implicitly this greater generality.

1.4. **Notes and Acknowledgements.** The author's intention for this essay was to present the three main approaches to Smoluchowski's equations, in particular for the multiplicative kernel, in a single integrated narrative. As such, many of the results are reproduced almost directly from the original papers. The aim was to provide the motivation and intermediate steps that the author felt would have aided his own understanding on first reading the material. He has tried to indicate clearly when such passages arise, but apologises in anticipation of the inevitable omissions.

Many thanks to Prof. Norris for his comments on a draft of this essay, and for suggesting such an interesting set of papers to read. Thanks also to Chris Williams for his diligent proof-reading. The author enjoyed his reciprocal role in this arrangement, though still feels that he knows very little about elliptic curves.

## 2. Introduction to the Models for Coalescence

2.1. **A general description.** We draw heavily on the review paper by Aldous [3] for the notation and motivation of this introduction.

Consider the evolution of concentrations of particles[2] in some medium, defined by their masses only. At any time, there is a chance that two particles with masses $x$ and $y$ will coalesce to form a single particle with mass $x + y$. The masses may be *discrete*, taking positive integer values, or *continuous*, taking any positive real value. In particular, though it may help at times to think of a particle achieving 'infinite' mass, this is not permitted, at least initially.

A typical coalescence may be described as

$$\{x, y\} \to \{x + y\}.$$

The assumption is that different coalescences (that is, the above for different values of $x$ and $y$) occur at different rates or with different probabilities. Given a specified particle with mass $x$, we assume that the instantaneous rate at which it is involved in a coalescence with a particle with mass $y$ is proportional to the number (or density) of mass $y$ particles. Define the *coalescent kernel*, $K(x, y)$, to be the constant of proportionality in this relation. Informally, $K(x, y)$ specifies the relative likelihood of the given coalescence when there are equal numbers of each mass.

[2]Often *clusters*, and even *monomers* or *galaxies* in the literature, depending on context.

At this point there are two separate ways to establish a model. We can take $K(x, y)$ to be a pure rate if the number of particles is sufficiently large that the model is deterministic. Then by considering which coalescences form and remove particles with mass $x$, we can describe the densities of different masses through a system of differential equations. Alternatively, we can take the number of particles to be 'small' (that is, finite, or a natural extension of finite), and consider $K(x, y)$ as a rate in the sense of a continuous-time Markov process. This can be formulated on a finite state-space, but it is also advantageous to consider a more technical coupling.

2.1.1. *The multiplicative kernel.* We generally demand symmetry: $K(x, y) = K(y, x)$. Note that scaling $K(x, y)$ by a constant $c$ is equivalent to rescaling time by $c^{-1}$. A typical kernel considered in the applied science literature is:

$$K(x, y) = (x^{1/3} + y^{1/3})(x^{-1/3} + y^{-1/3})$$

which describes coalescence in a Brownian motion continuum [3].

The three kernels which have proved most tractable to theoretical analysis are:

- $K(x, y) = 1$.
- $K(x, y) = x + y$, the *additive kernel*.
- $K(x, y) = xy$, the *multiplicative kernel*, which is the focus of this essay.

## 2.2. **Deterministic model.**

2.2.1. *Discrete masses.* We now formalise the model introduced by Smoluchowski [24]. We assume a continuum of particles, and for now discrete masses, so introduce the notation:

$$n(x, t) := \text{density of mass } x \text{ particles at time } t.$$

Then the number of coalescences $\{x, y\} \to \{x + y\}$ in time interval $[t, t + dt]$ is assumed to be

$$\frac{1}{2} n(x, t) n(y, t) K(x, y) dt. \tag{2.1}$$

Note that the factor of $\frac{1}{2}$ arises because of the symmetry between

$$\{x, y\} \to \{x + y\} \quad \text{and} \quad \{y, x\} \to \{x + y\}.$$

Consider the rates of coalescences which form a particle of mass $x$, and the rates of coalescences in which a particle of mass $x$ merges with some other. Using (2.1), these can be equated with the derivative of $n(x, t)$. The result is a set of equations often referred to as *Smoluchowski's coagulation equations*:

$$\frac{d}{dt} n(x, t) = \frac{1}{2} \sum_{y=1}^{x-1} K(y, x - y) n(y, t) n(x - y, t) - n(x, t) \sum_{y=1}^{\infty} K(x, y) n(y, t). \tag{2.2}$$

In the case of multiplicative coalescence, $K(x,y) = xy$, this final term is

$$-xn(x,t)\sum_{y=1}^{\infty} yn(y,t).$$

The expression $\sum yn(y,t)$ represents the total mass in some suitable sense. The verbal description of the dynamics suggests that this should be constant in time.

2.2.2. *Continuous masses.* The case where particle masses are continuous is similar. Here, define:

$$n(x,t)dx := \text{density of mass } [x, x+dx] \text{ particles at time } t$$

and assume that the number of coalescences of particles with masses in $[x, x+dx]$ and $[y, y+dy]$ in time $[t, t+dt]$ is

$$\frac{1}{2}n(x,t)n(y,t)K(x,y)dxdy. \tag{2.3}$$

Now Smoluchowski's equations have the form:

$$\frac{d}{dt}n(x,t) = \frac{1}{2}\int_0^x K(y,x-y)n(y,t)n(x-y,t)dy - n(x,t)\int_0^{\infty} K(x,y)n(y,t)dy. \tag{2.4}$$

In this essay, at least initially we shall focus on the discrete case, but much of the theory carries over to the continuous setting.

2.2.3. *Initial conditions for the multiplicative coalescent.* When $K(x,y) = xy$, the discrete version of Smoluchowski gives:

$$\frac{d}{dt}n(x,t) = \frac{1}{2}\sum_{y=1}^{x-1} y(x-y)n(y,t)n(x-y,t) - n(x,t)x\sum_{y=1}^{\infty} yn(y,t). \tag{2.5}$$

We have previously discussed how the case $K(x,y) = cxy$ is the same as $K(x,y) = xy$ up to a constant factor rescaling of time. Suppose reasonably that the initial conditions give all particles the same mass $y$. Call the resultant process $n_y(x,t)$, so

$$n(x,0) = \delta_y(x).$$

Because $K(x,y)$ is homogeneous in $x$ and $y$, we have that:

$$n_y(x,t) = n_1\left(\frac{x}{y}, y^2 t\right).$$

Thus in the discrete case, we will generally consider *monodisperse* initial conditions $n(x,0) = \delta_1(x)$.

This would suffice as an initial condition in the continuous case as well. However, here we normally define the process over $t \in (-\infty, \infty)$. So it is more natural to demand the *standard* multiplicative coalescent be invariant under a class of time-mass rescalings[3]. A

[3]In the same fashion as a *standard* Brownian motion.

consequence of this is that the process forms from infinitissimely small particles at $t = -\infty$. The existence of such a process is non-obvious, and is demonstrated for example in [2] by a suitable rescaling of random graph processes around the critical point.

2.3. **Stochastic models for coalescence.** By using a continuum of particles, the previous model as defined by Smoluchowski's equations was deterministic. Now we consider coalescence in a finite-volume setting.

2.3.1. *Marcus-Lushnikov processes.* The model analogous to Smoluchowski's, proposed by Marcus [18] and developed by Lushnikov in [16] and [17], retains the mean-field assumption that the process is controlled only by particle masses. However, here we consider a finite collection of particles with masses $x_1, \ldots, x_k \in \mathbb{N}$. Define the total mass $N := \sum x_i$. Then we specify the dynamics by:

$$\text{Given particles with masses } x_i \text{ and } x_j \text{ coalesce at rate } \frac{K(x_i, x_j)}{N}.$$

The term $\frac{1}{N}$ specifies the density of a given particle, as in (2.1).

Normally we arrange the particle masses in non-increasing order, with

$$ML_i^{(N)}(t) := \text{ mass of the } i\text{th largest particle at time } t.$$

Then $(ML_i^{(N)}(t) : i \geq 1)$ is a continuous-time Markov chain on (finite) state-space $\Pi_N^{\downarrow}$, the set of non-increasing partitions of $[N]$.

Alternatively, can take the state-space to be:

$$\{(n_1, \ldots, n_N) \in \mathbb{N}^N : \sum x n_x = N\}.$$

Here, for each $x$ we are tracking the number of particles with mass $x$ at time $t$, say $ML^{(N)}(x, t)$. It is easy to show that this is equivalent to the original setup under the natural transformation. These are both called *Marcus-Lushnikov processes*. The context will determine whether $i$th component size or number of mass $x$ components is more useful.

2.3.2. *The stochastic coalescent.* Note that under either interpretation $(ML^{(N)}(t))$ requires a different state space for each integer $N$. When the coalescent kernel is homogeneous, we can couple this set of processes by rescaling to consider partitions of the unit interval $[0, 1]$. This will be useful when we consider $N \to \infty$ limits.

We take as state-space the set of (not necessarily finite) non-increasing partitions of 1:

$$\mathcal{P} := \{\mathbf{x} = (x_1, x_2, \ldots) : x_1 \geq x_2 \geq \ldots > 0, \sum x_i = 1\}.$$

We now declare that given particles with masses $x_i$ and $x_j$ coalesce at rate $K(x_i, x_j)$. This defines a Markov process $(X_i(t), i \geq 1)$ on $\mathcal{P}$, called the *stochastic coalescent*.

*Notes.* (1) For the multiplicative kernel $K(x,y) = xy$, we can couple $X_i(t)$ and $ML_i^{(N)}(t)$ by:

$$X_i(t) = N^{-1} ML_i^{(N)}(N^{-1}t)$$

for any initial conditions suitable for $ML^{(N)}$, as

$$N^{-1}\Pi_N^{\downarrow} \subset \mathcal{P}.$$

(2) This generality comes at a price. Each $ML^{(N)}$ is a finite state-space Markov chain, but $\mathcal{P}$ is not countable. So we want to show some regularity condition for $(X(t))$. In [2], it is demonstrated that the multiplicative stochastic coalescent is a Feller process, which implies the Strong Markov property amongst others.

2.4. **Random graphs.** The additive and multiplicative coalescent processes have much in common with graph processes. I will give the briefest of summaries, borrowing from the introduction of [7], of the most important random graph models, as introduced by Erdős and Rényi [11]. Then we will prove a very easy result showing equivalence between a simple random graph process and the Marcus-Lushnikov process for a multiplicative kernel.

2.4.1. *Basic Models.* We consider probability spaces with elements drawn from $\mathcal{G}_n$, the set of graphs on $n$ labelled vertices.

- For each integer $0 \le m \le n$ define:

  $$\mathcal{G}(n,m) := \{G \in \mathcal{G}_n : e(G) = m\}.$$

  Then define $G_{n,m}$ to be the random variable uniformly distributed on $\mathcal{G}(n,m)$. So

  $$\mathbb{P}(G_{n,m} = H) = 1(e(H) = m)\binom{N}{m}^{-1}.$$

- *Binomial model*: Here, take $\mathcal{G}_n$ to be the probability space, and some $0 < p < 1$. Then define a random variable $G_{n,p}$ on $\mathcal{G}_n$ by including each of the $\binom{n}{2}$ edges independently with probability $p$. Then

  $$\mathbb{P}(G_{n,p} = H) = p^{e(H)}(1-p)^{n-e(H)}.$$

  Notice that the model is 'binomial' in the sense that

  $$e(G_{n,p}) \sim \mathrm{Bi}(n,p).$$

  Also note that sometimes we write $G(n,p)$ instead of $G_{n,p}$.
- *Graph processes*: Set $N := \binom{n}{2}$ for ease of notation. Now we take as probability space the set of nested graph sequences:

  $$\{E_n{}^4 = G_{n,0} \subset G_{n,1} \subset \ldots \subset G_{n,N} = K_n : e(G_{n,t}) = t \quad \forall t\}.$$

[4] $E_n :=$ the empty graph on $n$ vertices.

We then define $(G_{n,t})_{t=0}^N$ to be the random variable uniformly distributed on this set. Notice that the process describing which edge is added at time $t$:

$$(E(G_{n,t})\backslash E(G_{n,t-1}), 1 \leq t \leq N)$$

is uniformly chosen from the set of permutations on $[N]$.

- *Coupling*: Note that the random graph process is a coupling of the random variables[5] $(G_{n,m}, 1 \leq m \leq N)$. We have a similar construction for $(G_{n,p}, 0 \leq p \leq 1)$. Supply to each edge $e$ independent $U[0,1]$ random variables, say $(X_e, e \in E(K_n))$. Then construct $G_{n,p}$ by the rule:

$$e \in E(G_{n,p}) \iff X_e \leq p.$$

2.4.2. *Random graphs and the multiplicative Marcus-Lushnikov process.* At a very informal level, the link between the multiplicative coalescent and random graph processes is the following. In a standard Erdős-Rényi graph process $\mathcal{G}(n,t)$, at a given time $t$, the probability that the next edge added will join given components of sizes $x$ and $y$ is proportional to the number of edges joining these components. As they are disjoint, this is equal to $xy$.

Now we consider an equivalence more concretely. The proof is a more detailed version of that given in [23].

**Proposition 2.1.** The process $ML^{(N)}(t)$ with monodisperse initial conditions is equal in distribution to the process of component sizes in $G(n, 1-e^{-t})$.

*Note.* The latter is defined as a process by coupling in the natural way. With $X_e \sim U[0,1]$ as before, edge $e$ appears at time $t$ iff $X_e \leq 1-e^{-t}$. In particular, note that

$$\mathbb{P}(X_e = X_f : \text{some } e \neq f) = 0,$$

and $1-e^{-t}$ is strictly increasing and continuous from 0 to 1 as a function of $t \in [0,\infty)$. So this process is equal in distribution to the ordinary random graph process $(G_{n,t})_{t=0}^N$ up to deterministic time change.

*Proof.* With this notation, the appearances of distinct edges are independent and

$$\mathbb{P}(\text{edge } e \text{ appears after time } t) = e^{-t/N}.$$

Therefore, the appearance times of edges are independent $\text{Exp}(\frac{1}{N})$ random variables. In particular, the edge process is memoryless, and so the component size process is Markov. It is also now clear that the rate of appearance of an edge to join given components with sizes $x$ and $y$ is $\frac{xy}{N}$. Hence we have two Markov chains with identical transition rates and the same initial conditions. □

[5]Or, more precisely, of the probability spaces on which they are defined.

## 3. Smoluchowski's Equations: Solutions and Probabilistic Interpretations

The first topic which we address is the deterministic model for coalescence with a multiplicative kernel. We recall the statement of Smoluchowski's equations (2.5) for discrete masses in this case:

$$\frac{d}{dt}n(x,t) = \frac{1}{2}\sum_{y=1}^{x-1} y(x-y)n(y,t)n(x-y,t) - n(x,t)x\sum_{y=1}^{\infty} yn(y,t).$$

3.1. **Uniqueness of solution with monodisperse initial conditions.** We consider solutions to (2.5) with monodisperse initial conditions: $n(x,0) = \delta_1(0)$. For such a solution, we define the moments

$$m_1(t) = \sum_{x=1}^{\infty} xn(x,t) \quad \text{and} \quad m_2(t) = \sum_{x=1}^{\infty} x^2 n(x,t).$$

Note that by considering what happens before and after a typical coalescence $\{x,y\} \to \{x+y\}$, it is natural to suppose that $m_1(t)$ and $m_2(t)$ will be constant and increasing respectively.

**THEOREM 3.1.** Suppose we are given a solution $n(x,t)$ to (2.5) with $n(x,0) = \delta_1(x)$ for $t \in [0,T]$ for some $T < 1$ and for which $m_2(t)$ is absolutely and uniformly convergent on this same interval. Then $n(x,t)$ is the only such solution.

*Proof from* [19]. We have $n(x,t)$ differentiable (in $t$) for each $x$, so certainly these are also continuous. Continuity of $\frac{dn(x,t)}{dt}$ then follows for each $x$ because it is expressed as a uniformly convergent sum of uniformly continuous functions. The convergence assumption on $m_2(t)$ is a strong one. It implies that $m_1(t)$ is also absolutely and uniformly convergent on $[0,T]$. This allows us to define and rearrange the following infinite sums:

$$\sum_{x=1}^{\infty} x^2 n(x,t)\sum_{y=1}^{\infty} yn(y,t) = \frac{1}{2}\sum_{x=1}^{\infty} x\sum_{y=1}^{x-1} y(x-y)n(y,t)n(x-y,t). \tag{3.1}$$

Thus it is possible to multiply each equation in (2.5) by $x$ and sum to obtain

$$\sum_{x=1}^{\infty} x\frac{dn(x,t)}{dt} = \frac{1}{2}\sum_{x=1}^{\infty} x\sum_{y=1}^{x-1} y(x-y)n(y,t)n(x-y,t) - \sum_{x=1}^{\infty} x^2 n(x,t)\sum_{y=1}^{\infty} yn(y,t) = 0. \tag{3.2}$$

Now, by the uniform continuity discussed above, we can integrate and apply the monodisperse initial conditions to obtain

$$m_1(t) = \sum_{x=1}^{\infty} xn(x,t) = 1, \tag{3.3}$$

the statement about conservation of mass which we had expected. Now we make the obvious substitution in (2.5), giving:

$$\frac{d}{dt}n(x,t) = \frac{1}{2}\sum_{y=1}^{x-1} y(x-y)n(y,t)n(x-y,t) - n(x,t)x. \tag{3.4}$$

Uniqueness of $n(x,t)$ can now be verified[6] one at a time (in $x$), as each is defined by $n(0,t),\ldots,n(x-1,t)$. □

It is straightforward to show by induction on $x$ that if there is a solution, it has the form:

$$n(x,t) = c(x)t^{x-1}\frac{e^{-xt}}{x},$$

where $c(x)$ is a constant defined inductively by:

$$c(1) = 1, \quad \text{and} \quad c(x+1) = \frac{x+1}{2x}\sum_{y=1}^{x} c(y)c(n+1-y).$$

This can be expressed explicitly as:

$$n(x,t) = \frac{x^{x-2}}{x!}t^{x-1}e^{-xt}.$$

In [19], McLeod goes on to show that this solution does indeed have the crucial property that $m_2(t) < \infty$ on any $[0,T] \subset [0,1)$.

We can describe these distributions in terms of a probabilistic model. We have the relation:

$$n(x,t) = \frac{1}{x}B(t,x), \tag{3.5}$$

where $B(t,x)$ is the *Borel distribution*. This can be defined as the distribution of total population sizes in a Galton-Watson branching process, with a single time 0 ancestor and generation law $\sim \mathrm{Po}(t)$. See [25] for a calculation of the distribution. Note that this also motivates why the solution cannot be extended beyond $t = 1$. Also note that the structure defining the distribution is different for each $t$, and there isn't a particularly obvious coupling. Aldous shows in [3], using details from [1], the existence of a single stochastic object, related to the *Yule process*, which encodes the solution to Smoluchowski's equations for all times $t$.

3.2. **Existence and uniqueness up to $t = \infty$.** Let us summarise what we know so far. We can exploit uniqueness to nest the solutions found by McLeod to cover the interval $[0,1)$. This solution is unique and has second moment bounded on any interval $[0,T] \subset [0,1)$. Moreover, the solution found has the form given above, which can clearly be extended to the whole time interval $[0,\infty)$. However, it can easily be checked that these fail to solve

[6]Because the general equation $f' + \lambda f = g$ has unique solution: $f = e^{-\lambda t}(c + \int_0^t e^{\lambda u}g(u)du)$.

(2.5) for $t > 1$. In fact it is clear why the proof cannot be extended into this region. It can be calculated that the second moment $m_2(t)$ diverges to $\infty$ at $t = 1$.

With this motivation, it makes sense to see how much progress can be made if we relax the restriction on the second moment. While it is tempting to insist on uniform convergence or continuity of the total mass (ie. the first moment $m_1(t)$), in fact all that is required for what follows is that $m_1(t) < \infty$ at all times $t$.

We now paraphrase [14], showing global existence and uniqueness of solutions to (2.5) with monodisperse initial conditions. A discussion of the phase transition at $t = 1$ will follow in the next section, as things will be more clear once we have seen a concrete example.

We consider solutions to a version of Smoluchowski's equations where the original particles are retained during a coalescence. So a typical coalescence is

$$\{x, y\} \to \{x, y, x + y\}.$$

Then the equations governing the dynamics are:

$$c(x,t) = \frac{1}{2}\sum_{y=1}^{x-1} y(x-y)c(y,t)c(x-y,t), \tag{3.6}$$

with initial conditions $c(x, 0) = \delta_1(x)$. Note, obviously, there is no expectation that mass will be conserved here. However, as in Theorem 3.1, we can solve these uniquely, globally in time, by induction:

$$c(x,t) = x^{x-2}\frac{t^{x-1}}{x!}.$$

The following theorem relates this solution of the modified equations (3.6) to a global solution of (2.5). Essentially, the distributions are the same, but a time-dependent rescaling, with a phase transition at $T = 1$, is required to move to the coalescent case. First, define:

$$\phi(t) = \begin{cases} t & \text{for } 0 \le t \le 1 \\ 1 + \log t & \text{for } 1 < t < \infty \end{cases}.$$

(This will turn out to be the integral over time of the total mass, or first moment.)

The proof is essentially copied from [14], but in a slightly different order, and with fleshed out explanation in places, in particular the evaluation of the important contour integral in the lemma.

**THEOREM 3.2.** (1) If we set

$$n(x,t) = c(x,t)e^{-x\phi(t)} \quad x = 1, 2, \ldots, t \in [0, \infty), \tag{3.7}$$

then for each $x$, $n(x,t) \in C^1[0,\infty)$ and has a convergent first moment:

$$m_1(t) = \sum_{x=1}^{\infty} xn(x,t) = \begin{cases} 1 & t \in [0,1] \\ 1/t & t \in (1,\infty) \end{cases}.$$

Furthermore, $n(x,t)$ satisfies (2.5) for all $t$.

(2) In addition, if for some $T > 0$ and for each $x \in \mathbb{N}$ suppose we are given $n(x,t) \in C^1[0,T)$ such that $\sum_{x=1}^{\infty} xn(x,t)$ converges for $t \in [0,T)$ and which satisfies (2.5). Then $n(x,t)$ is defined by (3.7) for $t \in [0,T)$.

*Proof.* We consider uniqueness. Assume that $T$ and $n(x,t)$ are given as in (2). We want to consider a time interval $[0,T_1)$ on which $m_1(t)$ is continuous. The existence of such an interval is clear from (2.5). $n(1,t)$ is positive on some interval $[0,T_1')$ and so continuity of $m_1(t) = \sum xn(x,t)$ follows from

$$\frac{dn(1,t)}{dt} = -n(1,t)\sum_{x=1}^{\infty} xn(x,t).$$

Take $T_1$ to be the supremum of all such $T_1'$ which are less than $T$. We hope to show that $T_1$ is in fact equal to $T$. Now we consider an inverse of (3.7) to lift uniqueness of (3.6) to uniqueness of (2.5). So define analogues to $\phi$ and $c$:

$$\psi(t) = \int_0^t \sum_{x=1}^{\infty} xn(x,u)du, \quad \text{and} \quad b(x,t) = n(x,t)e^{x\psi(t)}, \quad t \in [0,T_1).$$

The initial condition $b(x,0) = \delta_1(x)$ is now clear, and as $\psi \in C^1[0,T_1)$,

$$\frac{db(x,t)}{dt} = \left(\frac{dn(x,t)}{dt} + xn(x,t)\sum yn(x,t)\right)e^{x\psi(t)} = \frac{1}{2}\sum_{y=1}^{x-1} y(x-y)b(y,t)b(x-y,t).$$

So $b(x,t)$ satisfies the same system (3.6) as $c(x,t)$ and so these are in fact equal. We want to perform a similar argument for $\psi$ and $\phi$. Observe that

$$t\frac{d\psi(t)}{dt} = \sum_{x=1}^{\infty} xn(x,t) = t\sum_{x=1}^{\infty} xc(x,t)e^{-x\psi(t)} = \sum_{x=1}^{\infty} x^{x-1}\frac{(te^{-\psi(t)})^x}{x!}. \tag{3.8}$$

We now need a technical result about complex functions to proceed rigorously.

**Lemma 3.3.** The power series

$$f(z) = \sum_{k=1}^{\infty} k^{k-1}\frac{z^k}{k!}$$

has radius of convergence $e^{-1}$. It is uniformly convergent and therefore continuous on this disc, and is $C^\infty$ in the interior. Furthermore, $f$ satisfies the relations:

$$f(z) = ze^{f(z)} \text{ and } |f(z)| \leq 1, \quad |z| \leq e^{-1}$$

$$f(we^{-w}) = w, \quad |w| \leq 1.$$

In addition, $f$ is increasing on the real interval $[0,e^{-1}]$, with $f(0) = 0$ and $f(e^{-1}) = 1$.

*Proof.* Convergence and the other regularity properties follow from the Stirling approximation $\frac{k^{k-1}z^k}{k!} \sim k^{-3/2}(ze)^k$. We now consider the domain $|w| < 1$ and fixed $|z| < e^{-1}$. Then $|ze^w| < 1$ holds, and so by Rouché's theorem, the equation $w - ze^w = 0$ has the same number of solutions for $|w| < 1$ as the equation $w = 0$, that is, a single solution. Now we can apply the residue theorem to see that the solution is

$$\frac{1}{2\pi i}\oint_{|w|=1} w\frac{\frac{d}{dw}(w-ze^w)}{w-ze^w}dw = \frac{1}{2\pi i}\oint_{|w|=1}(1-ze^w)\frac{dw}{1-\frac{ze^w}{w}}$$
$$= \sum_{k=0}^{\infty}\frac{1}{2\pi i}\oint_{|w|=1}\frac{(1-ze^w)(ze^w)^k}{w^k}dw,$$

where this last equality follows from uniform convergence. Now proceed using Cauchy's differentiation formula, taking the $(k-1)$th derivative of $g(w) = (1-ze^w)(ze^w)^k$.

$$\frac{1}{2\pi i}\oint_{|w|=1}\frac{g(w)dw}{w^k} = \frac{g^{(k-1)}(0)}{(k-1)!} = \frac{1}{(k-1)!}\left[k^{k-1}z^k - (k+1)^{k-1}z^{k+1}\right].$$

We now rearrange to express the solution (to $w - ze^w$, recall) as a series in $z$:

$$\sum_{k=0}^{\infty}\frac{1}{2\pi i}\oint_{|w|=1}\frac{(1-ze^w)(ze^w)^k}{w^k}dw = \sum_{k=0}^{\infty}z^k\left[\frac{k^{k-1}}{(k-1)!} - \frac{k^{k-2}}{(k-2)!}\right] = \sum_{k=0}^{\infty}\frac{k^{k-1}}{k!}z^k = f(z).$$

This proves that $f(z) = ze^{f(z)}$, and $|f(z)| \le 1$ for $|z| < e^{-1}$, a result which can be extended by continuity to the closed disc as necessary. When $|w| < 1$, we have $|we^{-w}| < e^{-1}$ and so

$$f(we^{-e}) = we^{-w}e^{f(we^{-w})} \quad \Rightarrow \quad f(we^{-w}) = w,$$

by uniqueness of $f$. Again, this can be extended by continuity to the closed disc $|w| \le 1$. This last result shows that the inverse of $f$ is increasing on $[0,1]$ which proves the final assertion, that $f$ is increasing on $[0, e^{-1}]$. □

Immediately, we consider the RHS of (3.8), which converges, so by the lemma, must have $0 \le te^{-\psi(t)} \le e^{-1}$. We can also rewrite (3.8) as:

$$t\frac{d\psi(t)}{dt} = f(te^{-\psi(t)}), \quad t \in [0, T_1). \tag{3.9}$$

We now restrict attention to the largest time interval $[0, T_2) \subset [0, T_1)$ for which we have the strict relation $te^{-\psi(t)} < e^{-1}$. We can now use the smoothness of $f$ shown in the lemma to show that $\psi \in C^\infty[0, T_2)$, with $t\frac{d\psi(t)}{dt} < 1$ in this region also. Then for $0 < t < T_2$:

$$\frac{d\psi(t)}{dt} = \frac{1}{t}f(te^{-\psi(t)}) = e^{-\psi(t)}e^{f(te^{-\psi(t)})} = e^{-\psi(t)+t\frac{d\phi(t)}{dt}}.$$

Differentiating and cancelling gives $\frac{d^2\psi(t)}{dt^2} = 0$ in this range, and so $\psi(t) = t$ on $[0, T_2)$. By the definition of $T_2$, and the fact that $te^{-t} < e^{-1}$ for $t < 1$, we conclude that $T_2 = \min\{1, T_1\}$.

If $T_1 \leq 1$, then we have verified $\psi(t) = \phi(t)$ and $b(x,t) = c(x,t)$ for $t \in [0, T_1)$, hence in this interval, $n(x,t)$ must be the solution described in the statement of the theorem. Then by definition of $T_1$, we must have $T_1 = T$. Otherwise, when $T_1 > 1$, we find a bounding argument to demonstrate the equality $\psi(t) = \phi(t)$ on $[0, T_1)$. Precisely,

$$te^{-\psi(t)} \leq e^{-1} \quad \Rightarrow \quad \psi(t) \geq 1 + \log t, \quad t \in [0, T_1)$$

and by the lemma,

$$\frac{d\psi(t)}{dt} = \frac{1}{t} f(te^{-\psi(t)}) \leq \frac{1}{t}, \quad t \in (0, T_1).$$

So we have an integral sandwich for $t \in [1, T_1)$:

$$1 + \log t \leq \psi(t) \leq \psi(1) + \int_1^t \frac{du}{u} \leq 1 + \log t.$$

Again, therefore, we have $\psi(t) = \phi(t)$ for $t \in [0, T_1)$ and as before can conclude that $T_1 = T$. So $n(x,t)$ has the form specified in the statement of the theorem.

We can now easily verify the outstanding claims in the first part of the theorem:

$$\sum_{x=1}^{\infty} xn(x,t) \overset{(3.8)}{=} \frac{1}{t} f(te^{-\phi(t)}) = \frac{d\phi(t)}{dt} \overset{\text{lemma}}{=} \begin{cases} 1 & t \in [0,1] \\ 1/t & t \in (1, \infty) \end{cases}.$$

Thus, from the definition of $n(x,t)$:

$$\frac{dn(x,t)}{dt} = \left( \frac{dc(x,t)}{dt} - x \frac{d\phi(t)}{dt} \right) e^{-x\phi(t)}$$

$$\overset{(3.6)}{=} \left( \frac{1}{2} \sum_{y=1}^{x-1} y(x-y)c(y,t)c(x-y,t) - x \sum_{y=1}^{\infty} yn(y,t) \right) e^{-x\phi(t)}$$

$$= \frac{1}{2} \sum_{y=1}^{x-1} y(x-y)n(x,t)n(x-y,t) - x \sum_{y=1}^{\infty} yn(y,t).$$

This shows that the expression for $n(x,t)$ given does indeed have all the required properties. □

*Remarks.*

- As we would expect, this solution agrees with that of McLeod in the pre-gelation region $[0, 1)$.
- The fact that the distributions given as the solutions have nice complex analytic properties is crucial to this proof. In particular, we know that the phase transition happens at $t = 1$. In general, this gelation time and the distributions will depend strongly on the initial conditions, and so in this author's opinion it seems unlikely that this argument could be adapted for a substantially more general setting.

3.3. **Gelation: Interpretations of the phase transition.** As has been mentioned in passing, there is a phase transition at $t = 1$. We call this the *gelation time*, $T_{gel}$. We consider some properties in this specific case:

- $m_2(t) < \infty$ for all $t < 1$, but $m_2(T_{gel}) = \infty$.
- The key step in McLeod's solution was the deduction that mass is conserved: $m_1(t) \equiv 1$ on $[0, T_{gel}]$. We have seen in the statement of Theorem 3.2 that mass is not conserved for $t > T_{gel}$.
- To define the gelation time formally in a more general context, we have two options. One is to define $T_{gel}$ as the divergence time of the second moment. The alternative is to set it as the supremum of times up to which Smoluchowski's equations (2.2) have a solution for which mass is constant.
- Apart from a few recent results, for example [13] and [21], the majority of interest in coalescence has been restricted to the pre-gelation phase. While some work in more applied directions assume implicitly that the two definitions are equivalent, this author has been unable to find any reference either to the existence or non-existence of a proof or counterexample of this under general conditions. For the time being, we will make it clear which definition we are using, when necessary.
- It is reasonable to view this physically as the loss of mass because of the formation of particles with infinite mass. Such particles are not accounted for in Smoluchowski's equations. However, for the multiplicative kernel, the rate of loss of mass $x$ particles is dependent only on the density of such particles and the total mass, so (2.5) remains a valid description of the densities of finite mass particles beyond $T = 1$, provided the infinite components do not further coalesce with finite ones. These are sometimes referred to as *gel* and *sol* respectively.
- Note that it is not the case that there is a single infinite particle. Infinite mass particles are formed at times 1 and $1 + t'$ for all $t' > 0$. Since these do not interact further once they have been formed, infinite particles formed at different times cannot be the same!
- So-called Flory models, where coalescences between gel and sol particles are permitted have been discussed in chemistry literature, eg. [27]. A discussion of this will be unavoidable when we address the model of cluster coagulation introduced in [22], and it will be seen that such an extension is entirely possible.

## 4. Generating Functions and Branching Processes

We now examine a method for demonstrating existence and uniqueness of solutions up to gelation for the multiplicative kernel in a wider range of settings. With discrete masses, we consider the generating function of the distributions and the evolution of these in time. In this context, (2.5) transforms into a quasi-linear PDE which can be solved explicitly for monodisperse initial conditions. However, now we can also appeal to general PDE theory to guarantee the existence of solutions to Smoluchowski's equations.

Such methods are generally described as standard, but this author has been unable to find any source with a definitive claim to be the first application of this method. We follow the notation and direction of Deaconu and Tanré in [8], but will explicitly find the characteristics and the solution in the monodisperse case (of their Proposition 2.2). We then discuss a remark of the same authors, which shows a link between the multiplicative solution and branching processes that had been generally known, but not previously considered in this way. The majority of this study of PDE methods concerns a recent *limited aggregation* model of Bertoin from [5] which demonstrates that this approach works equally well in a more general setting with two-dimensional parameters.

## 4.1. **PDE methods for the multiplicative coalescent.**

4.1.1. *A generating function.* Recall Smoluchowski's equations (2.5) for the multiplicative kernel:

$$\frac{d}{dt}n(x,t) = \frac{1}{2}\sum_{y=1}^{x-1} y(x-y)n(y,t)n(x-y,t) - n(x,t)x\sum_{y=1}^{\infty} yn(y,t).$$

We are now going to assume $T_{gel}$ is defined as the supremum of the set of times $T$ for which a solution to (2.5) preserves mass, that is:

$$\text{for } t < T_{gel}: \quad \frac{d}{dt}\sum_{x=1}^{\infty} xn(x,t) = 0.$$

From now on, we restrict attention to solutions for $t \in [0, T_{gel})$, and assume that $\sum xn(x,t) = 1$ for all such times, since we can renormalise time and mass appropriately. For the monodisperse case then, from the previous section, we know $T_{gel} = 1$.

We observe that $(xn(x,t))_x$ is now a probability distribution on $\mathbb{N}$ at each time $t < T_{gel}$, which motivates considering the generating function:

$$G(s,t) = \sum_{x=1}^{\infty} xn(x,t)s^x.$$

We restrict attention to the domain $t \leq 1$ and $|s| \leq 1$, where we know the series converges. We now assume (2.5) holds, and observe that in the time region we are considering, the first sum on the RHS looks like a discrete convolution, and in the second term $\sum yn(y,t)$ vanishes. Following this thought through, we see that $G$ satisfies the following quasi-linear PDE:

$$\begin{cases} \partial_t G(s,t) = \frac{s}{2}\partial_s(G^2)(s,t) - s\partial_s G(s,t) \\ G(s,0) = s \\ G(1,t) = 1, \quad t \leq 1, |s| \leq 1 \end{cases} \tag{4.1}$$

Conversely, given a solution $G$ of (4.1), the assertion $G(1,t) = 1$ means that, if $G$ is a suitable power series at all, we can write:

$$G(s,t) = \sum_{x=1}^{\infty} p(x,t)s^x,$$

where $p(x,t)$ is a probability distribution on $\mathbb{N}$ for each $t$. If we now set

$$n(x,t) := \frac{1}{x}p(x,t) \text{ for each } x \in \mathbb{N}, t \leq 1,$$

then by reversing the previous argument it is clear that $n(x,t)$ satisfies the Smoluchowski equations.

4.1.2. *Solutions of the PDE.* So now we have a direct equivalence between solutions to (2.5) and solutions to the system (4.1). We immediately exploit this by reposing Theorem 3.1 in this setting.

**Proposition 4.1.** The PDE (4.1) has a unique solution.

*Proof.* Rather than appealing to general results, for this case we work in detail, using the method of characteristics. First, we write the dynamic equation in (4.1) as

$$-\partial_t G + s(G-1)\partial_s G = 0.$$

Then solve for the characteristics:

$$\frac{ds}{dt} = s(1-G) \quad \Rightarrow s(t) = s_0 e^{(1-G)t}.$$

Now applying the initial condition $G(s,1) = s$, we must have

$$G(s,t) = z, \quad \text{where } s = ze^{(1-z)t}$$

$$\iff ste^{-t} = zte^{-zt} \iff G(s,t) = \frac{1}{t}f(ste^{-t}),$$

where $f$ is the inverse of the function $g : w \mapsto we^{-w}$. This exists on $[0, e^{-1}]$, as $g$ is strictly increasing on $[0,1]$, or by reference to Lemma 3.3. The result $G(1,t) = 1$ follows from the second point of the same lemma. □

We check that this gives the same solution as McLeod's argument:

$$G(s,t) \overset{\text{lemma}}{=} \frac{1}{t}\sum_{x=1}^{\infty} \frac{x^{x-1}}{x!}(ste^{-t})^k = \sum_{x=1}^{\infty} xn(x,t)s^k$$

$$\Rightarrow n(x,t) = \frac{k^{k-2}}{k!}t^{k-1}e^{-kt}.$$

*Remarks.*

- The requirement to use the lemma from the previous proof is obviously not ideal. However, demonstrating the existence of $f$ was not necessary for the proof of existence of a solution. Furthermore, while checking $G(1,t) = 1$ through the lemma was very straightforward, we could also apply the equivalence discussed previously. A solution to the first two equations in (4.1) corresponds to a solution of Smoluchowski's equations for some pre-gelation interval, for which we know mass is conserved, which then, again by the equivalence, shows that $G(1,t) = 1$ for the range of $t$ under discussion.
- The proof makes it clear that this result can be extended to more general initial conditions. Indeed, provided the initial distribution $n(x,0)$ gives a total mass of 1, we can replace (4.1) by:

$$\begin{cases} \partial_t G(s,t) = \frac{s}{2}\partial_s(G^2)(s,t) - s\partial_s G(s,t) \\ G(s,0) = \sum xn(x,t)s^x \\ G(1,t) = 1, \quad t \leq T \leq T_{gel}, |s| \leq 1 \end{cases}, \tag{4.2}$$

  and the same proof will suffice, but it will not in general be possible to solve for $G(s,t)$ explicitly.
- We are deliberately ignoring the question of whether any solution $G(s,t)$ has a suitable expression as a generating function. Such considerations are of course important, and will be treated with full rigour in the second model which we examine using PDE methods.

## 4.2. **A first discussion of branching processes.**

4.2.1. *Background and definitions.* A *Galton-Watson branching process* is a stochastic process, describing a simple model for evolution of a population. At each stage of the evolution, a new generation is induced by every member of the current generation producing some number of 'offspring' with identical and independent (both across all generations and within generations) distributions. Such processes were introduced by Galton and Watson [12] to examine the evolution of surnames through history.

More precisely, we specify an *offspring distribution*, a probability distribution supported on $\mathbb{N}_0$. Then define a sequence of random variables $(Z_n, n \in \mathbb{N})$ by:

$$Z_{n+1} = Y_1^n + \ldots + Y_{Z_n}^n,$$

where $(Y_k^n, k \geq 1, n \geq 0)$ is a family of i.i.d. random variables with the offspring distribution $Y$. We say $Z_n$ is the size of the $n$-th generation. From now on, assume $Z_0 = 1$ and then we call $(Z_n, n \geq 0)$ a Galton-Watson process. We also define the *total population size* to be

$$X := Z_0 + Z_1 + Z_2 + \ldots,$$

noting that this might be infinite. For our purposes, $Y$ will generally be distributed according to a Poisson distribution, with parameter $t$, for which we denote the total population

size[7] as $X_t$. We refer to the case $X$ finite as *extinction*, and can easily check[8] by Markov's inequality or martingale arguments that extinction occurs almost surely when $\mathbb{E}Y \leq 1$, excepting the trivial case $Y = \delta_1$.

Branching processes have proved particularly amenable to treatment using generating functions. In particular, conditional on the event $Z_1 = k$, we have:

$$X|Z_1 = k \quad \stackrel{d}{=} \quad 1 + X^1 + \ldots + X^k,$$

where $X^1, \ldots, X^k$ are independent copies of $X$. If $f$ is taken to be the generating function of $\xi$ and $G$ the generating function of $X$, then as a result we have the relation

$$G(s) = sf(G(s)).$$

4.2.2. *Total population size generating function.* We take $f(s,t)$ to be the generating function of a Poisson random variable with parameter $t$, and $G(s,t)$ the generating function of the corresponding total population size. We will show that $G(s,t)$ satisfies (4.1). This has the following consequences:

- We know by uniqueness of solution with characteristics that (4.1) has at most one solution. This therefore confirms that a solution exists, and has the form of the generating function, which is necessary if it is to apply to the coalescent structure.
- We will be able to calculate $n(x,t)$ directly, without making reference to complex analytic properties of function, just by using the combinatorial structure of branching processes. In particular, we have two ways of describing the distribution of the total population size. The generating function identity given above will be used to prove that $G(s,t)$ satisfies (4.1), while Dwass's Theorem, a result with purely probabilistic statement, can be used to calculate the distribution explicitly.

To show that $G(s,t)$ satisfies (4.1), we exploit two results. Firstly, as before:

$$G(s,t) = sf(G(s,t),t) \quad s,t \in [0,1]. \tag{4.3}$$

Note that $t \leq 1$ guarantees that it is a probability distribution on $\mathbb{N}_0$ rather than $\mathbb{N}_0 \cup \{\infty\}$, and so the radius of convergence is at least 1, with equality for $t = 1$. See Durrett [9] for a proof in the case $t = 1$. In particular, this gives $G(t,1) = 1$. $G(0,s) = 0$ is clear from definitions. Secondly, we can calculate the probability generating function and corresponding derivatives of a $\mathrm{Po}(t)$ random variable explicitly:

$$\left\{ \begin{array}{c} f(s,t) = \sum_{k=0}^{\infty} e^{-t} \frac{t^k}{k!} s^k = e^{-t(1-s)}, \\ \Rightarrow \quad \partial_s f(s,t) = tf(s,t), \quad \partial_t f(s,t) = (s-1)f(s,t). \end{array} \right. \tag{4.4}$$

[7] Confusingly, in some sources, the total population size is $Z$, with corresponding Poisson population size $Z_t$.

[8] See for example [9] for an fuller exposition.

We can now solve:

$$\partial_s G = f(G,t) + stf(G,t)\partial_s G \quad \Rightarrow \quad \partial_s G = \frac{f(G,t)}{1-stf(G,t)},$$

$$\partial_t G = s(G-1)f(G,t) + stf(G,t)\partial_t G \quad \Rightarrow \quad \partial_t G = \frac{s(G-1)f(G,t)}{1-stf(G,t)},$$

$$\Rightarrow \quad \partial_t G = s(G-1)\partial_s G,$$

which is precisely the statement of (4.1).

4.2.3. *A result of Dwass and derivation of the Borel distributions.* To calculate the coefficients of $G(s,t)$, that is $\mathbb{P}(X_t = k)$, we use a general result about branching processes.

**Proposition 4.2** (Dwass [10])**.** For a general branching process with a single time-0 ancestor and offspring distribution $Y$ and total population size $X$:

$$\mathbb{P}(X=k) = \frac{1}{k}\mathbb{P}(Y^1 + \ldots + Y^k = k-1), \quad k \geq 1 \tag{4.5}$$

where $Y^1, \ldots, Y^k$ are independent copies of $Y$.

It is now clear how to proceed in the case $Y = Y_t \sim \text{Po}(t)$. We know that Poisson distributions satisfy

$$Y^1 + \ldots + Y^k \sim \text{Po}(kt)$$

$$\Rightarrow \quad kn(k,t) = \mathbb{P}(X=k) = \frac{1}{k}\left[e^{-kt}\frac{(kt)^{k-1}}{(k-1)!}\right],$$

and this agrees with the solution given previously. We now give a proof of Dwass's result via a combinatorial argument. The author is unsure whether or not this approach is original. Much of the literature gives a proof using generating functions.

*Proof (of Proposition).* For motivation, consider the following. It is natural to consider a branching process as a tree, with the time-0 ancestor as the root. Suppose the event $\{X = k\}$ in (4.5) holds, which means that the tree has $k$ vertices. Now consider the numbers of offspring of each vertex in the tree. Since every vertex except the root has exactly one parent, and there are no vertices outside the tree, we must have $Y^1 + \ldots + Y^k = k-1$ where $Y^1, \ldots, Y^k$ are the offspring numbers in some order. However, observe that this is not sufficient. For example, if $Y^1$ is the number of offspring of the root, and $k \geq 2$, then we must have $Y^1 \geq 1$.

We can define the branching process in a more subtle way via a coupling that allows us to exploit this more carefully. Formally, take $(Y^1, Y^2, \ldots)$ a set of i.i.d. random variables with the same distribution as $Y$. Now construct the branching process as follows. Using graph theoretic notation, define a root $v_1$. Then demand that $v_1$ has $Y^1$ children, and so if $Y^1 > 0$, define $v_2, \ldots, v_{1+Y^1}$ to be $v_1$'s children. Then take the smallest $v_n$ (ordered by index) which hasn't been treated yet, and demand that it has $Y^n$ children, labelled with the smallest available indices. Continue. It is clear that this is equivalent to the definition

previously given. And when $\mathbb{E}Y \leq 1$, this process terminates after some almost surely finite number of iterations, giving a tree which has a breadth-first labelling[9].

The key observation is that the following are equal:

$$X = \inf\{k \geq 1 : Y^1 + \ldots + Y^k = k - 1\}.$$

Or in other words, as events

$$\{X = k\} = \{Y^1 + \ldots + Y^k = k - 1\} \cap \{Y^1 + \ldots + Y^j \geq j,\ \forall 1 \leq j \leq k - 1\}.$$

So it will suffice to prove:

$$\mathbb{P}\left[Y^1 + \ldots + Y^j \geq j,\ \forall 1 \leq j \leq k-1 \middle| Y^1 + \ldots + Y^k = k - 1\right] = \frac{1}{k}. \tag{4.6}$$

We observe that the joint distribution of $(Y^1, \ldots, Y^k)$ is unchanged under cyclic permutations of the indices. We will show that given $Y^1 + \ldots + Y^k = k - 1$, there is precisely one cyclic permutation of the indices for which initial segments of the sum are bounded suitably. For ease of notation, we define $z_i = Y^i - 1$, hence $z_i \in \{-1, 0, 1, 2, \ldots\}$ for each $i$. The following lemma will therefore provide precisely what is required.

**Lemma 4.3.** With $z_i$ as above, if $z_1 + \ldots + z_n = -1$, then there is precisely one $\sigma \in C_n$, the cyclic group acting on $[n]$, such that, defining $w_i = z_{\sigma(i)} \quad \forall i \in [1, n]$, we have:

$$w_1 \geq 0, \quad w_1 + w_2 \geq 0, \quad \ldots, \quad w_1 + \ldots + w_{n-1} \geq 0.$$

*Proof.* We first check uniqueness. Let $\tau := (12 \ldots n) \in C_n$. It suffices to check that the result cannot hold simultaneously for $\sigma = \mathrm{id}$ and for $\sigma = \tau^k$ where $1 \leq k \leq n - 1$. This is simple. If this holds for such a $\sigma$, then

$$\begin{aligned} w_{\sigma(1)} + \ldots + w_{\sigma(n-k)} = z_{k+1} + \ldots + z_n \geq 0, \quad \text{and} \quad z_1 + \ldots + z_k \geq 0, \\ \Rightarrow \quad -1 = z_1 + \ldots + z_n \geq 0. \end{aligned}$$

For existence, define

$$k := \arg\min_{j \in [1,n]} (z_1 + \ldots + z_j).$$

If there are multiple $j$ at which the function is minimised, then take $k$ to be the least such $j$. Then claim that $\sigma := \tau^k$ satisfies the statement of the lemma. For, taking $w_i = z_{\sigma(i)}$,

$$w_1 + \ldots + w_j = \begin{cases} (z_1 + \ldots + z_{k+j}) - (z_1 + \ldots + z_k) \geq 0 & k + j \leq n \\ (-1 + z_1 + \ldots + z_{j+1-n}) - (z_1 + \ldots + z_k) > -1 & k + j > n \end{cases},$$

by definition of $k$. In particular, notice that by assumption all $z_i \in \mathbb{Z}$, and so the second case also gives $w_1 + \ldots + w_j \geq 0$. □

This completes the proof of the proposition. □

[9]For what follows, a depth-first labelling would be satisfactory also. Or indeed any labelling such that whenever the resultant tree has $k$ vertices, the offspring distributions of these vertices were given in the construction by $Y^1, \ldots, Y^k$. The breadth-first labelling is described because it is simplest, and most similar to the generational ordering given in the original construction.

4.3. **PDEs applied to other models.** Deaconu and Tanré continue in [8] to specify similar PDE descriptions of Smoluchowski's equations in the discrete setting with constant and additive kernels, as well as for continuous mass distributions, here considering Laplace transforms as the natural continuous analogue of generating functions. Time and space constraints prevent a fuller discussion here.

Instead we consider a more complicated system, the *symmetric model* introduced by Bertoin in [5]. In Smoluchowski's equations coagulation rates are governed entirely by the additive quantity of particle mass. In a chemical model, the covalent bonds can form between molecules only when they have suitable numbers of lone pairs of electrons. In particular, molecules can be formed which are no longer available for further bonding. Motivated by this system, we consider now that the particles have some finite number of *arms* with which they perform the coagulations. That is, an arm grabs an arm on a different particle, then the particles are joined, but the arms used for the coagulation are now exhausted. A generating function will now require two arguments, but a PDE approach is still profitable.

4.3.1. *Statement of the symmetric model.* We consider again a collection of particles under a mean-field assumption. This time, a particle is described by its mass, and by some non-negative number of available arms. We define:

$$n_t(a,m) = \text{ density of particles with mass } m, \text{ } a \text{ arms at time } t, \quad a \in \mathbb{N}_0, m \in \mathbb{N}.$$

In a typical coalescence, distinct particles are joined using an arm from each, which is no longer available in the new particle. The typical transition is then

$$\{(a,m),(a',m')\} \to (a+a'-2, m+m').$$

Rather than consider a general kernel $K(a,a',m,m')$, instead we assume that pairs of arms (from different particles naturally) grab each other at the same unit rate. So the above coalescence happens at rate

$$aa' n_t(a,m) n_t(a',m').$$

Note that this is in appearance similar to the rate for the multiplicative kernel in Smoluchowski's model. As in that case, we can describe the evolution of densities by a system of ODEs:

$$\frac{d}{dt} n_t(a,m) = \frac{1}{2} \sum_{a'=1}^{a+1} \sum_{m'=1}^{m-1} a'(a-a'+2) n_t(a',m') n_t(a-a'+2, m-m') - a n_t(a,m) \sum_{a'=1}^{\infty} \sum_{m'=1}^{\infty} a' n_t(a',m'). \tag{4.7}$$

To avoid the requirement to write lots of double sums everywhere, we introduce the measures

$$\langle f, n_t \rangle = \sum_{a=0}^{\infty} \sum_{m=1}^{\infty} f(a,m) n_t(a,m)$$

$$\text{and } \langle\langle g, n_t\rangle\rangle = \sum_{a,a'=0}^{\infty} \sum_{m,m'=1}^{\infty} g(a, a', m, m') n_t(a, m) n_t(a', m').$$

for general functions $f : \mathbb{N}_0 \times \mathbb{N} \to \mathbb{R}_{\geq 0}$ and $g : \mathbb{N}_0^2 \times \mathbb{N}^2 \to \mathbb{R}_{\geq 0}$. We can now express (4.7) more succintly as the single equation:

$$\frac{d}{dt}\langle f, n_t\rangle = \frac{1}{2}\langle\langle [f(a + a' - 2, m + m') - f(a, m) - f(a'm')]aa', n_t\rangle\rangle \tag{4.8}$$

for $f$ bounded[10]. We assume that the initial conditions specify monodisperse mass, that is

$$n_0(a, m) = \mu(a)\delta_1(m),$$

where $\mu$ is a measure on $\mathbb{N}_0$. In particular, we do not require $\mu$ to be a probability distribution. By the statement of the model, the total number of arms will decrease in time. However, we generally assume that $\mu(a)$ has mean 1. From now on, call these mass 1 particles *monomers*.

Observing the similarity to the multiplicative coalescent process, we need to consider what gelation means in this symmetric limited aggregation model. We would like it to be the case that any infinite mass particle formed in finite time also has an infinite number of arms. Then we will be able to characterise gelation by divergence of a second moment of distribution of arms, rather than of mass. This is more useful as the transition rate is specified in terms of arms. We observe that sequences of coalescences of the form

$$\{(1, n), (2, 1)\} \to (1, n + 1)$$

will generate infinite particles with a single arm. However, the rate of all such transitions is the constant 2, and so the infinite particles do not form in finite time. Very informally, the formation of infinite mass particles in finite time requires transition rates to be unbounded for the finite size particles which end up forming the infinite mass. But transition rates are proportional to the number of arms, which means that the number of arms of particles which make up the infinite mass is unbounded as we approach the gelation time. We can now define the *gelation time* in terms of the second moment of the distribution of arms:

$$\Gamma_\infty := \sup\{t \geq 0 : \langle a^2, n_t\rangle < \infty\}.$$

4.3.2. *A suitable PDE.* We follow the direction of Bertoin in Section 3 of [5], giving full details wherever the original author directs the reader to adapt the methods of his Section 2. First we define $A_t := \langle a, n_t\rangle$, the mean number of arms.

[10](4.7) gives this result for $f = \delta(a, m)$, but we extend to linear combinations and eventually bounded $f$ in the usual way

**Proposition 4.4.** For all $t < \Gamma_\infty$, $A_t$ satisfies the equation $\frac{d}{dt}A_t = -A_t^2$.

*Proof.* This appears to be true by taking $f(a,m) = a$ in (4.8). But there, $f$ must be bounded, so instead we appeal to convergence results. Because $t < \Gamma_\infty$, we have:

$$\langle a, n_t\rangle = \sum_{a=0}^{\infty}\sum_{m=1}^{\infty} a n_t(a,m) < \infty$$

$$\Rightarrow A_t^2 = \sum_{a,a'=0}^{\infty}\sum_{m,m'=1}^{\infty} a^2 a'^2 n_t(a,m) n_t(a',m') < \infty.$$

In other words, the function $a^2a'^2$ is integrable with respect to the measure $\langle\langle\cdot, n_t\rangle\rangle$. Because $a, a' \in \mathbb{N}_0$, we have $aa' \le a^2a'^2$ and so by Dominated Convergence, $aa'$ is also integrable. Now we observe that

$$A_t = \lim_{k\to\infty} \uparrow \langle a \wedge k, n_t\rangle. \tag{4.9}$$

This is helpful because (4.8) holds for $f(a,m) = a \wedge k$. This convergence is uniform on compact intervals, because of the bounded second moment. We observe the very crude bound

$$aa'|(a + a' - 2) \wedge k - (a \wedge k) - (a' \wedge k)| \le aa'(2k + a + a') \le aa'(2k + 2aa').$$

The function on the right hand side of (4.9) is integrable, and so by Dominated Convergence, so is the function inside the modulus on the left hand side. Observe the pointwise limit

$$\lim_{k\to\infty} (a + a' - 2) \wedge k - (a \wedge k) - (a' \wedge k) = -2.$$

Now apply the full form of Dominated Convergence:

$$\frac{d}{dt}A_t = \lim_{k\to\infty}\frac{d}{dt}\langle a \wedge k, n_t\rangle \overset{(4.8)}{=} \lim_{k\to\infty}\frac{1}{2}\langle\langle[(a + a' - 2) \wedge k - (a \wedge k) - (a' \wedge k)]aa', n_t\rangle\rangle$$

$$\overset{\text{DC}}{=} -\langle\langle a^2a'^2, n_t\rangle\rangle = -A_t^2.$$

□

We immediately solve this to obtain

$$A_t = \frac{A_0}{1 + tA_0}. \tag{4.10}$$

From now on, assume $A_0 = 1$, by rescaling time and arms if necessary. Now we define the generating function

$$g_t(x,y) := \langle x^a y^m, n_t\rangle, \quad x, y \in [0,1].$$

Then substituting $x^a y^m$ into (4.7) gives

$$\frac{d}{dt}g_t(x,y) = \frac{d}{dt}\langle x^a y^m, n_t\rangle$$

$$= \frac{1}{2}\sum_{a,a'\geq 1}\sum_{m,m'\geq 1}\left[x^{a+a'-2}y^{m+m'} - x^a y^m - x^{a'}y^{m'}\right] aa' n_t(a,m)n_t(a',m')$$

$$= \frac{1}{2}\left(\sum_{a\geq 1}\sum_{m\geq 1} a x^{a-1}y^m n_t(a,m)\right)^2 + \sum_{a,a'\geq 1}\sum_{m,m'\geq 1} x^a y^m a n_t(a,m) a' n_t(a',m')$$

$$= \frac{1}{2}\left(\sum_{a\geq 1}\sum_{m\geq 1} a x^{a-1}y^m n_t(a,m)\right)^2 + A_t\sum_{a\geq 1}\sum_{m\geq 1} a x^a y^m n_t(a,m)$$

$$\frac{d}{dt}g_t(x,y) = \frac{1}{2}\left(\partial_x g_t\right)^2 - xA_t\partial_x g_t(x,y). \tag{4.11}$$

We want to get rid of squares of derivatives, so it turns out to be more convenient to consider instead

$$k_t(x,y) := \partial_x g_t(x,y) = \sum_{a=1}^{\infty}\sum_{m=1}^{\infty} a x^{a-1}y^m n_t(a,m).$$

Unsurprisingly, we also have: $\frac{d}{dt}k_t(x,y) = \partial_x \frac{d}{dt}g_t(x,y)$. Now differentiate with respect to $x$ in (4.11):

$$\frac{d}{dt}k_t(x,y) = k_t(x,y)\partial_x k_t(x,y) - A_t k_t(x,y) - xA_t\partial_x k_t(x,y)$$

$$\frac{d}{dt}k_t(x,y) = \left(k_t(x,y) - \frac{x}{1+t}\right)\partial_x k_t(x,y) - \frac{1}{1+t}k_t(x,y), \quad x,y\in[0,1] \tag{4.12}$$

The boundary condition is $n_0(a,m) = \mu(a)\delta_1(m)$, where $\mu(a)$ is assumed to have mean 1. So the following is a probability measure:

$$\nu(a) := (a+1)\mu(a+1), \quad a\in\mathbb{N}_0.$$

We can then obtain initial conditions for $k_t(x,y)$:

$$k_0(x,y) := \partial_x g_0(x,y) = \partial_x\left[\sum_{a=0}^{\infty} x^a y\mu(a)\right] = \sum_{a=0}^{\infty} x^a y\nu(a).$$

From now on, these are assumed to be the boundary conditions for the PDE (4.12).

4.4. **Analysis of Bertoin's PDE.** We will show first that this PDE has a solution for $t <$ some $T$. Then, we prove that if this solution is a generating function satisfying the necessary boundary conditions it is the only such solution. And finally that the solution found *is* a suitable generating function.

4.4.1. *Finding solutions.* We proceed with a method of characteristics. We consider characteristics for $0 \le s \le 1$ satisfying initial conditions $x(0,0) = r$, $u(s,0) = k_0(s,y)$ and

$$\frac{dx}{dt} = \frac{x}{1+t} - u, \quad \frac{du}{dt} = -\frac{u}{1+t}.$$

The solution is then

$$u(s,t) = \frac{k_0(s,y)}{1+t}, \quad x(s,t) = s(1+t) - tk_0(s,y).$$

We conclude that $k_t(x,y) = u(s(x,y),t)$, where $s(\cdot,y)$ is the inverse of the map $s \mapsto s(1+t) - tk_0(s,y)$. The derivative of this map is

$$1 + t - t\partial_x k_0(s,y) \ge 1 + t - t\partial_x k_0(1,1) = 1 + t - t\sum_{a=0}^{\infty} a\nu(a),$$

and this final quantity is positive for $t < T$ where

$$\text{for } M := \sum_{a=0}^{\infty} a\nu(a), \quad T = \begin{cases} \infty & M \le 1 \\ (M-1)^{-1} & M > 1 \end{cases}. \tag{4.13}$$

Thus we have an inverse map, say $h_t(x,y)$. We clarify that this satisfies

$$x = h_t(x,y)(1+t) - tk_0(h_t(x,y),y). \tag{4.14}$$

We therefore have a solution to (4.12):

$$k_t(x,y) = \frac{1}{1+t} k_0(h_t(x,y),y)).$$

Since we defined $h_t$ as an inverse, this can be expressed as

$$k_t(x,y) = \frac{h_t(x,y)}{t} - \frac{x}{t+t^2}, \quad t < T, x, y \in [0,1]. \tag{4.15}$$

4.4.2. *From PDE solutions to the original model.* Now we assume that we have a solution of (4.12) such that $k_t$ is a generating function for each $t \in [0,t)$. We need to check that inverting $k_t(x,y)$ gives a solution to (4.7). If $k_t$ solves (4.12), then because of the previous solution method, (4.15) holds. $k_0(1,1) = 1$ by assumption, so it is easy to check by (4.14) and uniqueness that $h_t(1,1) = 1$ for all $t$, and so from (4.15):

$$k_t(1,1) = \frac{1}{1+t},$$

which is precisely what remained to be shown to establish the correspondence between generating function solutions of (4.12) and solutions to (4.7).

The final assertion to be shown is that the solution to (4.12) is a generating function in a suitable sense to be inverted to give a solution to the original problem (4.8). We have the initial condition

$$k_0(x,y) = \sum_{a=0}^{\infty} x^a y\nu(a) = yk(x), \text{ say.}$$

Now define:

$$h(x,y) := \frac{1}{t}[(1+t)h_t(x,y) - x]$$

$$\text{And so from (4.14): } h(x,y) = yk\left(\frac{x}{1+t} + \frac{t}{1+t}h(x,y)\right).$$

We now require a technical step (stated more generally as Lemma 3 in [5]) to show that this identity, and the fact that $k(x)$ has a power series expansion, is sufficient to ensure that $h(x,y)$ also has a power series expansion. This essentially allows us to adjust the Lagrange inversion theorem, which is posed for single-variable functions, for this case where $h$ is dependent on $x$ and $y$, but $k$ is a function of $x$ only.

Define $l(y) := k(\frac{x+ty}{1+t})$. Note that the argument is $\leq 1$. This is a generating function (with respect to $y$) of a measure, which can be checked to be:

$$\lambda(a) = \sum_{n=a}^{\infty} \binom{n}{a}(1+t)^{-n}x^{n-a}\nu(n).$$

We now have the central equation: $h(x,y) = yl(h(x,y))$. Since $l(0) > 0$, we can appeal to the Lagrange inversion theorem[11] and obtain

$$h(x,y) = \sum_{n=1}^{\infty} \frac{y^n}{n}\lambda^{*n}(n-1).$$

We can now translate this back to an expression in $x$ and $\nu$. The final result is

$$h(x,y) = \sum_{a=0}^{\infty}\sum_{m=1}^{\infty} x^a y^m \frac{1}{m}\binom{a+m-1}{a}\frac{t^{m-1}}{(1+t)^{a+m-1}}\nu^{*m}(a+m-1),$$

$$\Rightarrow k_t(x,y) = \sum_{a=0}^{\infty}\sum_{m=1}^{\infty} x^a y^m \frac{t^{m-1}}{m(1+t)^{a+m}}\binom{a+m-1}{a}\nu^{*m}(a+m-1). \tag{4.16}$$

It only remains to check that $T$ as defined by the existence of a suitable inverse map in (5.13) agrees with the critical time $\Gamma_\infty$ defined as the divergence time of the second moment of arms. Observe that

$$\langle a^2, n_t\rangle = A_t + \partial_x k_t(1,1),$$

and $A_t$ is bounded (as it is decreasing), and so it suffices to find the divergence time of $\partial_x k_t(1,1)$.

$$\partial_x k_t(1,1) \overset{(4.15)}{=} \frac{1}{t}\partial_x h_t(1,1) - \frac{1}{t+t^2}. \tag{4.17}$$

$$\text{But by (4.14):} \quad x = h_t(x,1)(1+t) - tk_0(h_t(x,1),1),$$

$$\Rightarrow 1 = \partial_x h_t(1,1)(1+t) - t\partial_x h_t(1,1)\partial_x k_0(h_t(x,1),1)$$

$$= \partial_x h_t(1,1)(1+t) - t\partial_x h_t(1,1)\partial_x k_0(1,1) \overset{(5.13)}{=} \partial_x h_t(1,1)(1+t) - Mt\partial_x h_t(1,1)$$

[11] See, for example, Theorem 5.1.1 in [26].

$$\Rightarrow \quad \partial_x h_t(1,1) = [1+(1-M)t]^{-1},$$
$$\Rightarrow \quad \partial_x k_t(1,1) \overset{(4.17)}{=} \frac{M}{(1+t)(1+(1-M)t)}.$$

This is bounded for $t \in [0,T'] \subset [0,T)$, and diverges to $\infty$ as $t \uparrow T$, so we can conclude that $T = \Gamma_\infty$.

4.5. **Remarks on the symmetric model.**

- Of course, it is worth mentioning explicitly that $k_t(x,y)$ in (4.16) can be inverted to obtain the solution for $n_t(a,m)$:
$$n_t(a,m) = \frac{(a+m-2)!}{a!m!} t^{m-1}(1+t)^{-(a+m-1)} \nu^{*m}(a+m-2).$$
- This argument has demonstrated the power of PDE methods. Uniqueness remains similarly straightforward: recall that in McLeod's proof this followed from uniqueness of solutions to a first-order ODE, while here it follows from the PDE's characteristics covering the whole space. Existence on the other hand now follows much more simply: solving a quasi-linear PDE and applying the Lagrange inversion theorem to verify that the solution is a generating function may require lots of notation, but is less mathematically involved than the complex analysis in Kokholm's method.
- Note that this is the first model where we are able to specify the critical gelation time explicitly in terms of the initial distribution. Observe that it is determined, roughly speaking, by the second moment (of arms) in the initial distribution. This is perhaps unsurprising, given that the transition rates are quadratic functions of the number of arms present. It shall be seen in the next study that this carries over to the multiplicative kernel for standard coalescence.
- Indeed this symmetric model has other similarities to our main object of study. We have previously commented on the similarities of the sets of equations (2.5) and (4.7) governing the dynamics. But we also have similarities in solutions. Bertoin remarks that taking $\mu \sim \mathrm{Po}(1)$ gives a model where the infinite time distribution[12] is the same as the distribution at the gelation time $T = 1$ in our previous model of a standard multiplicative coalescent with monodisperse initial conditions. It would be interesting if there were a 'nice' reason for this equivalence, but this author cannot find one, nor any reference to the existence of such an argument.

4.6. **The emergence of the giant component in a random graph process.** In the study of random graph processes, a great deal of attention was given to the emergence of the so-called *giant component*. Precisely, $G(n,p)$ exhibits a phase transition at $p = \frac{1}{n}$. For $p > \frac{1}{n}$, the random graph will almost surely (in a suitable $n \to \infty$ limit sense) have a component with $O(n)$ vertices, while for $p < \frac{1}{n}$ almost surely all components will be small,

[12] Of mass - all arms have been exhausted by $t = \infty$.

that is, $O(\log n)$. We suspect there may be a similar phase transition for other random graph models.

As an application of the previous section, we now consider the giant component in two models connected to the coalescent processes discussed, and show (non-rigorously) that the criterion for this emergence is the same as the condition for gelation in the continuum model.

4.6.1. *Sparse uniform random graphs.* Consider graphs on $N$ vertices with degree sequence $d_1, \dots, d_N$ which sum to $2M$ say. We consider a graph chosen uniformly from this set. Let $\mu_N = \frac{1}{N}\sum_{i=1}^{N} \delta_{d_i}$, the corresponding probability measure. Suppose we now let $N \to \infty$ and $\mu_N \to \mu$, some probability measure. We will not concern ourselves with the precise statement of this limit now. We consider the probability that in the limit, this graph has an infinite component.

We can relate the component sizes to branching processes as follows. Fix an edge $e$, and consider the size of the component containing that edge, conditional on $e$ being present. The measure of the degree of one of the incident vertices is size-biased, that is, $d\mu(d)$. We will be interested in the number of edges out of this vertex other than $e$, so we consider instead the measure of the *outer degree* $\nu(d) = (d+1)\nu(d+1)$. The crucial assumption is that the number of vertices is sufficiently large that we may assume that the degrees of all vertices we consider are independent, and that any finite component almost surely contains no cycles. Now we may treat the component of $e$ as a Galton-Watson branching process with two progenitors.

The offspring distribution is $\nu$ as defined before. We normalise by assuming $\nu$ is a probability distribution $\sum_d \nu(d) = 1$, and so we can calculate the criterion for extinction, which corresponds to finiteness of the component.

$$\text{Extinction} \quad \iff \quad \mathbb{E}\nu > 1 \quad \iff \sum_{d \geq 1} d\nu(d) > 1.$$

Observe that this is precisely the condition given by (5.13) for gelation in Bertoin's symmetric model. This observation is unsurprising. After all, a finite-volume version of Bertoin's dynamics produces precisely such a random graph once all the arms have been exhausted. We observed much earlier that the Marcus-Lushnikov process for the multiplicative kernel was in some sense exactly the same as the standard Erdős-Rényi graph process. This is not the case here: the finite-volume stochastic model for these dynamics is not exactly the same as the uniform degree-specified graph. Apart from anything else, the symmetric model does not allow cycles, and it is certainly not obvious that the final graph left has the uniform distribution on the set of possible graphs.

However, we would not be surprised if even this crude analogy respected the phase transition. Informally, the differences between the finite-volume symmetric model[13], and the

[13] which is shown in [6] to converge to the continuum process.

*uniform sparse random graph*, as described previously, derive from local properties. In the $N \to \infty$ limit, the dependence on local structure is much weaker, and assumptions that everything is independent are more reasonable.

We can in fact see a stronger relation between the continuum symmetric model, and the branching process discussed. When $T = \infty$, that is, gelation does not occur, the solution (4.16) induces a limit concentration

$$n_\infty(a, m) = 1_{a=0} \frac{1}{m(m-1)} \nu^{*m}(m-2), \quad a \in \mathbb{N}, m \geq 2. \tag{4.18}$$

Remember that we discounted the possibility that a monomer initially has 0 arms, hence there are no mass 1 particles left at $t = \infty$. It can further be checked that when $T = \infty$, provided $\nu \neq \delta_1$ (that is $\mu \neq c\delta_2$):

$$\sum_{m=2}^{\infty} n_\infty(a, m) = \mu(\mathbb{N}),$$

from which we conclude that infinite size particles are not produced as time tends to $\infty$. Proving this identity requires an application of the Lagrange inversion formula. The reason it fails to hold analytically in the case $\nu = \delta_1$ is that LIF requires $\nu(0) \neq 0$.

The proposition of Dwass that we proved in an earlier section can easily be extended to describe a branching process which has two time 0 progenitors. Denoting by $X_2$ the total population size of such a process, we have:

$$\mathbb{P}(X_2 = k) = \frac{2}{k} \nu^{*k}(k-2), \quad k \geq 2. \tag{4.19}$$

A proof is given in the original paper [10], but we can also adapt the method of proof from the previous section. This time, we use a depth-first labelling, so the constructions of the two trees are disjoint. Thus since it does not matter which order we construct the trees, we get a factor of $\frac{2}{k}$, rather than $\frac{1}{k}$. We note the similarity to (4.18).

By the branching process equivalence, under these independence assumptions, the size of the component containing an edge is given by (4.19). But when a component has $k$ vertices, there are $(k-1)$ choices for the initial edge, and 2 orderings of the arms making up that edge. So we conclude that:

$$n_\infty(a, k) = 1_{a=0} \frac{1}{2(k-1)} \cdot \frac{2}{k} \nu^{*k}(k-2),$$

as previously deduced.

4.6.2. *Coagulation with mating and oriented, sparse graphs.* We now examine in passing Normand's model for limited aggregation [20]. This is essentially the same as Bertoin's symmetric model as previously discussed, only now we assume that arms are either male or female, and coagulations occur only between a male and a female arm. The motivation

for this is partly chemical. If all the arms of a particle have the same gender, then this provides a toy model for ionic bonding, where anions and cations bond over time.

Now, particles are characterised by $(a, b, m)$ where $a, b \in \mathbb{N}_0$ are the number of male and female arms respectively, and $m \in \mathbb{N}$ is the mass as before. Then a typical coalescence is

$$\{(a, b, m), (a', b', m')\} \to (a + a' - 1, b + b' - 1, m + m').$$

Furthermore, we assume that all male/female pairs are activated independently at unit rate, and so the above coalescence happens at rate $ab' + a'b$.

As in the case of the symmetric model, Normand demonstrates existence and uniqueness of solutions to the continuum equations. He assumes all particles at time 0 are monomers, then uses generating functions, here with three arguments, and PDEs. Checking the technical details about inversions of power series is more challenging in this situation because of the extra parameter. We remark, in particular, on the case where the total number of arms is specified, and then genders are chosen uniformly at random, independently. This is the same as the symmetric model, up to trivial changes of normalisation.

We assume that the mean number of male and female arms is initially equal, and so, by reference to the underlying dynamics, should always be equal. Then it is reasonable to assume that there is a well-defined limit distribution, corresponding to the state of the system once there are no longer any arms left to coagulate. As for the symmetric model, [20] provides a precise condition for gelation, the appearance of particles with infinitely many arms (of either gender), to occur:

$$\text{Gelation occurs at finite time } T \quad \iff \langle ab, n_0\rangle + \sqrt{\langle a^2 - a, n_0\rangle\langle b^2 - b, n_0\rangle} > 1.$$

As before, we assume that at time 0 all particles are monomers, so $n_0 = \mu$, a measure on $\mathbb{N} \times \mathbb{N}$, specifiying the numbers of arms of each gender.

We now consider an oriented sparse random graph. That is, a uniformly chosen graph with given degree sequence as before, for which each edge is given a direction. For this, we have to specify the sequence of pairs of in-degrees and out-degrees. We assume, naturally, that the sum of the in-degrees is equal to the sum of the out-degrees. We are interested in the existence of a giant component as before. In particular, we wonder whether the criterion for emergence of a giant component will depend on the oriented pairs of degree sequence, or merely on the unoriented degree sequence.

As before, we assume we have a measure on the pairs of oriented degrees $\mu_N(a, b) \to \mu(a, b)$ as $N \to \infty$. Again, take the number of vertices to be sufficiently large that we can assume independence and ignore cycles. Now, we consider the component size of a given oriented edge, assuming it exists. We shall use a branching process calculation as before. We call the vertices at either end of the edge the *head* and *tail* with obvious ordering. Then the

(outer[14]-)degree distribution for the vertex at the head is size-biased and shifted by 1 with respect to in-degree, and the distribution for the tail is size-biased and shifted by 1 with respect to out-degree. With suggestive notation, call these distributions:

$$\nu_m(a,b) = (a+1)\mu(a+1,b) \quad \text{and similarly} \quad \nu_f(a,b) = (b+1)\mu(a,b+1).$$

Here, we call a vertex in the branching process *male* if it lies at the head of the edge joining it to its ancestor, and *female* if it lies at the tail. Thus the component may be described as a *two-type Galton-Watson branching process*. In such a system, male and female ancestors give birth (individually rather than in pairs, or suchlike) to male and female offspring, but according to different distributions, $\nu_m$ and $\nu_f$. In this particular case, we begin with one male and one female progenitor. It is clear for the same reasons as in the symmetric model that such a process with these offspring distributions gives a good approximation to Normand's continuum model. We would therefore hope that the condition for a giant component in the oriented sparse graph model is the same as the condition for gelation in the continuum mating setting.

The properties of such a branching process can still be described using generating functions. Take $G_m, G_f$ to be the generating functions of the total population sizes started from male and female ancestors respectively, and $f_m(x,y), f_f(x,y)$ the generating functions of $\mu_m, \mu_f$. Then these must satisfy:

$$\begin{cases} G_m(z) &= z f_m(G_m(z), G_f(z)) \\ G_f(z) &= z f_f(G_m(z), G_f(z)) \end{cases}$$

The extinction probability is a function of both offspring distributions. We have to consider the expected number of male and female children of male and female parents. Define:

$$\mathbb{E}_m a = \sum_{a,b} a\nu_m(a,b), \quad \mathbb{E}_m b = \sum_{a,b} b\nu_m(a,b),$$

and similarly for $\mathbb{E}_f$. Note that because the out-edges of a vertex give rise to male children, we have that $\mathbb{E}_m b$ is the expected number of male offspring of a male parent, and so forth. Then it is relatively straightforward to show (see [4] for a full explanation) that if we take $\rho$ the largest eigenvalue of the matrix

$$M := \begin{pmatrix} \mathbb{E}_m b & \mathbb{E}_m a \\ \mathbb{E}_f b & \mathbb{E}_f a \end{pmatrix},$$

the branching process becomes extinct almost surely iff $\rho \leq 1$. Observing that

$$\sum_{a,b} a(b+1)\mu(a,b+1) = \langle ab, \mu \rangle,$$

and similarly for the other three case, we deduce that $\rho$ satisfies the quadratic equation:

$$0 = \rho^2 - 2\langle ab, \mu\rangle \rho + \left[ \langle ab, \mu \rangle^2 - \langle a(a-1), \mu \rangle \langle b(b-1), \mu \rangle \right].$$

[14] That is, *outer* in the sense of a branching process - counting only edges which haven't already been considered. We count both arriving and departing edges in the oriented model.

So we have a giant component iff

$$\rho = \langle ab, \mu\rangle + \sqrt{\langle a^2 - a, \mu\rangle\langle b^2 - b, \mu\rangle} > 1.$$

Thus we obtain a precise condition for the emergence of the giant component in the oriented sparse graph model. We observe that it is dependent on the distributions of both in- and out-degrees, and so is different to the unoriented case. In addition, we observe that the condition for the giant component here is the same as the condition required for gelation with monomer initial distributions in Normand's model.

## 5. Cluster Coagulation

One of the principle motivations for a treatment of coalescence as described by Smoluchowski was to describe the formation of polymers. In this setting, we observe that there are multiple possibilities for the outcome of a coalescence of two polymers, $A$ and $B$ say, depending on which atoms are bonded in the transition. For example, whether butane or its isomer methylpropane is formed as a result of a reaction is dependent (locally) on the geometry of the collision, at least in this toy model. As explained in the introduction, tracking all of the physical properties necessary to describe this explicitly is totally impractical, but we want to find a way to develop the idea of coalescence that is not entirely controlled by the additive quantity of mass. The following model introduced by Norris [22] allows us to work in this higher generality.

5.1. **Mathematical description of cluster model.** We now assume that the coalescing elements, which in this context we call *clusters*, are drawn from some set $E$ equipped with a $\sigma$-algebra $\mathcal{E}$ which turns it into a measure space. In particular, note that for the original model discussed, $E = \mathbb{N}$ with Dirac measure. Of course, this measure-theoretic approach draws no distinction between a discrete and a continuous setting. The clusters have mass described by a measurable function $m : E \to \mathbb{R}_+$.

When two clusters $x$ and $y$ coagulate, the cluster formed can theoretically be any element of $E$. So now a typical coalescence is

$$\{x, y\} \to A, \text{ understood to mean: } \{x, y\} \to z, \quad z \in A,$$

where $A \in \mathcal{E}$ is a measurable set of clusters. We say the rate of such coagulations is $K(x, y, A) \in [0, \infty)$. For well-definedness, we need $K(x, y, \cdot)$ to be a measure on $\mathcal{E}$, and in order to formulate meaningful equations about the rate of formation of clusters in $A$, we also require $K(x, y, A)$ to be measurable as a function of $(x, y)$ for fixed $A \in \mathcal{E}$. $K(x, y, \cdot)$ will be the *coagulation kernel*, provided it satisfies the natural requirements extending from the Smoluchowski model:

- Define the total rate of coagulation of clusters $x$ and $y$ as $\bar{K}(x, y) := K(x, y, E)$. We insist that this is finite for every pair $x, y$, so as not to break down the mean-field assumption.

- Symmetry: $K(x, y, A) = K(y, x, A)$ for all $x, y \in E$ and $A \in \mathcal{E}$.
- Mass preservation: we demand that almost all coagulations satisfy mass-preservation. This can be stated as:

$$m(z) = m(x) + m(y) \text{ for almost all } z \text{ w.r.t. measure } K(x, y, \cdot), \quad \forall x, y \in E.$$

We view a cluster coagulation process as an evolution of non-negative measures on the space $\mathcal{E}$. Call this space of measures $\mathcal{M}^+$. Here we describe evolution of measures through an integral form, as time-derivatives of measures are not very tractable in this generality. Instead we describe an operator $L$ on $\mathcal{M}^+$, corresponding roughly to rate of change of the measure, by its action on the measure of a function $f$, from a class of functions to be determined later.

$$\langle f, L(\mu)\rangle := \frac{1}{2}\int_{E\times E\times E} [f(z) - f(x) - f(y)]K(x, y, dz)\mu(dx)\mu(dy). \tag{5.1}$$

Observe as motivation the similarity to (4.8). Now, as for Smoluchowski's equations, we can define a *local solution* (or *K-coagulant*) as a measurable map[15] $t \mapsto m_t : [0, T) \to \mathcal{M}^+$ satisfying:

$$\langle f, \mu_t\rangle = \langle f, \mu_0\rangle + \int_0^t \langle f, L(\mu_s)\rangle ds, \quad t < T, \tag{5.2}$$

for $f$ in the class of functions $S$. It is natural to demand that $S$ contains all bounded, non-negative measurable functions supported on $m^{-1}(B)$ for $B$ a compact set of masses in $(0, \infty)$. To avoid allowing mass to enter at 0, we also include in $S$ the function $m(x)1_{m(x)\le 1}$. From now on, we assume $S$ to be the $\pi$-system generated by this class of functions.

We also demand that $\langle f, \mu_0\rangle < \infty$ for all $f \in S$. Note that this is not quite the same as demanding that initial mass is finite, as the function $m(x) \notin S$. Recalling the earlier requirement of the kernel and that $\bar{K}(x, y) < \infty$, we also insist on the finiteness of the following quantity. This essentially demands that an infinite number of coagulations cannot happen locally (in mass) before it happens globally (except near 0):

$$\int_0^t \int_{m^{-1}(B)\times E} \bar{K}(x, y)\mu_s(dx)\mu_s(dy)ds < \infty, \quad \text{compact } B \subset (0, \infty), t < T.$$

Now consider the action on the mass of this evolution. The presence of the term $[f(z) - f(x) - f(y)]$ in (5.1) shows that, if it is defined, $\langle \phi(m), \mu_t\rangle \le 0$ for all sublinear functions $\phi$. But it is easy to see that any non-negative sublinear function is a monotone limit of sublinear functions on bounded support which are genuinely linear near 0. And $\langle \cdot(m), \mu_t\rangle$ is certainly defined for these functions, and so by Fatou and monotone convergence, the result holds. In particular, taking $\phi = \mathrm{id}$ shows that the total mass density $\langle m, \mu_t\rangle$ is non-increasing in $t$. In particular, we seek *conservative* solutions for which this quantity is finite and constant in time. If this mass density is constant precisely until some finite time

[15] In the sense that $t \mapsto \mu_t(A)$ is measurable for each $A \in \mathcal{E}$.

$S$, then we say *gelation* happens at $S$. Note that at the moment we make no claim about a relation between $S$ and $T$, the time up to which the solution is defined.

While in [22], the assumption is the more general one that $\bar{K}(x,y) \leq \phi(m(x))\phi(m(y))$ for $\phi$ sublinear, in this treatment, we restrict attention to the multiplicative kernel:

$$\bar{K}(x,y) = m(x)m(y).$$

Norris demonstrates that in a real continuous setting $E = (0,\infty)$, for this multiplicative kernel, that solutions to (5.2) are unique when the second moment $\langle x^2, \mu_t\rangle < \infty$. And if this moment is bounded initially, then there exists a well-defined gelation time, a function of the initial distribution $\mu_0$, and in particular $\geq \langle x^2, \mu_0\rangle^{-1}$, up to which the solution is *strong*, that is,

$$\int_0^t \langle x^2, \mu_s\rangle ds < \infty.$$

We will present the third of the three main theorems in the first section of [22], which discusses a multiplicative kernel process which allows for interaction between the infinite mass clusters and the finite masses. Norris treats this situation for *eventually multiplicative kernels* where $\bar{K}$ is bounded for small masses, and multiplicative for large masses in a suitable sense, and this doesn't pose too many more difficulties than our work.

5.2. **Post-gelation cluster behaviour and the main result.** For Smoluchowski's model, we have a loss of mass starting at the gelation time $T_{gel}$. The most natural way to account for this in the language of the model is that at this time coalescences happen for particular chains of large masses sufficiently fast that 'infinite mass' particles are formed. These are not considered in the governing equations (2.2), and so they are effectively inert. They do not interact with each other or the finite particles after they are formed.

This might fit the model in some situations, say if the infinite particle's mass causes it to leave the medium or to perform a phase transition which means it is no longer reacting with other particles. But for the multiplicative kernel, it is natural to think of particles as collections of monomers. The coalescences occur because monomers are joining uniformly at random to other monomers, and, informally, taking the other monomers in the particle with them. This is certainly the case in a random graph process as described in the introduction. And with this framework, we would assume - unless there were specific reasons otherwise - that there would be no distinction in the dynamic treatment of monomers in finite particles, and in an infinite particle.

Tempting though it might be to consider a mass measure on $\mathbb{N}\cup\{\infty\}$, it is more convenient to record mass in infinite clusters by the difference between initial mass and current mass (of finite clusters). Concretely, we define $S$, an operator analogous to $L$, by:

$$\langle f, S(\mu)\rangle = \langle f, L(\mu)\rangle - \langle m, \mu_0 - \mu_t\rangle\langle mf, \mu_t\rangle. \tag{5.3}$$

We will then be searching for families of measures which satisfy:

$$\mu_t = \mu_0 + \int_0^t S(\mu_s)ds. \tag{5.4}$$

Note that $\langle m, \mu_0 - \mu_t\rangle$ is the mass in infinite clusters. $\langle mf, \mu_t\rangle$ gives the (rate) of loss of finite clusters through coagulation with infinite clusters, weighted by $f$. We now see that we can describe the solutions to this system.

**THEOREM 5.1.** Assume $\bar{K}(x,y) = m(x)m(y)$, that is $\bar{K}$ a multiplicative kernel. Suppose further that $\langle m+1, \mu_0\rangle < \infty$. Then there is a unique solution to (5.4) starting from $\mu_0$.

*Proof.* In the statement of the model, we consider measures supported on $\mathbb{R}$, where finite clusters are also affected by infinite clusters. But suppose that instead we make this threshold finite. That is, for some $R < \infty$, we consider the induced measure on clusters with mass $\leq R$. We would expect to be able to derive an equation similar to (5.4) which treats coagulations involving small mass clusters in a integral, with a corrective term for mass lost over the $> R$ threshold.

Concretely, suppose we have a solution $(\mu_t)_{t\geq 0}$. Set $\nu_t = 1_{m\leq R}\mu_t$, and for any $f \in S$, apply (5.4) to the function $1_{m\leq R}f$. Then[16]:

$$\frac{d}{dt}\langle f, \nu_t\rangle = \frac{d}{dt}\langle 1_{m\leq R}f, \mu_t\rangle = \frac{1}{2}\int_{E\times E\times E}\left[f(z)1_{m(z)\leq R} - f(x)1_{m(x)\leq R} - f(y)1_{m(y)\leq r}\right]$$
$$\times K(x,y,dz)\nu_t(dx)\nu_t(dy) - \langle m, \mu_0 - \mu_t\rangle\langle mf1_{m\leq R}, \mu_t\rangle.$$

The integral term above can be rewritten as follows. The factor of 2 arises from the obvious symmetry between $x$ and $y$:

$$= \frac{1}{2}\int_{E\times E\times E}\left[f(z)1_{m(z)\leq R} - f(x) - f(y)\right]K(x,y,dz)\nu_t(dx)\nu_t(dy)$$
$$-2\cdot\frac{1}{2}\int_{E\times E\times E} f(x)K(x,y,dz)\nu_t(dx)[\mu_t - \nu_t](dy).$$

Remembering that $\bar{K}(x,y) = m(x)m(y)$, this second integral can be separated as

$$\langle m(x)f, \nu_t\rangle\langle m(y), \mu_t - \nu_t\rangle,$$

where $m(x)$ and $m(y)$ are abuses of notation to indicate how each $m$ arises from the integral. Note also that $\langle mf1_{m\leq R}, \mu_t\rangle = \langle mf, \nu_t\rangle$, and so we can rearrange the original equation to obtain:

$$\frac{d}{dt}\langle f, \nu_t\rangle = \frac{1}{2}\int_{E\times E\times E}\left[f(z)1_{m(z)\leq R} - f(x) - f(y)\right]K(x,y,dz)\nu_t(dx)\nu_t(dy) - \lambda_t\langle mf, \nu_t\rangle, \tag{5.5}$$

[16] We treat time-derivatives in the *weak* sense. That is, the following is true after integration with respect to $t$.

where $\lambda_t := \langle m, \mu_0 \rangle - \langle m, \nu_t \rangle$ measures how much mass is contained in clusters with mass $> R$ at time $t$. We now substitute $m1_{m \leq R}$, which is certainly bounded, into the above, to obtain:

(5.6)
$$\frac{d}{dt}\lambda_t = -\frac{d}{dt}\langle m, \nu_t \rangle = \frac{1}{2}\int_{E\times E} [m(x) + m(y)] 1_{m(x)+m(y)>R} \bar{K}(x, y)\nu_t(dx)\nu_t(dy) + \lambda_t \langle m^2, \nu_t \rangle,$$

where we make use of the condition that $m(z) = m(x) + m(y)$ for $K(x, y, \cdot)$-almost all $z$.

Our aim is to solve this pair of equations (5.5) and (5.6) for given $R$, and show that the solutions are unique. This will make it possible to take a limit as $R \to \infty$ in a well-defined way. The proof of this lemma is therefore the key part of the result. The proof represents the third approach to demonstrating uniqueness and existence of Smoluchowski-type equations that we will see in this essay. Essentially, we approximate solutions in a similar way to Euler's method for ODEs, then use completeness of the space of functions under consideration to force uniqueness. We have completeness of the normed space because we are assuming the functions have compact support. This explains why the reduction we have just performed was important.

We first need to set up some notation. Here we are considering the coupled processes $(\nu_t, \lambda_t)_{t\geq 0}$, so we find a space for these to operate on. Define:

$$\langle (f, a), (\mu, \lambda) \rangle = \langle f, \mu \rangle + a\lambda,$$

in an obvious abuse of notation, where the $\langle \cdot, \cdot \rangle$ on the RHS refers to the operator previously discussed. This holds for bounded measurable $f$ and $a \in \mathbb{R}$. As before, we define an operator $S_R$ with which to describe the measure evolution. With reference to the equations we are looking to solve, define:

$$\begin{aligned}\langle (f, a), S_R(\mu, \lambda) \rangle = &\frac{1}{2}\int_{E\times E\times E} [f(z) - f(x) - f(y)]\, K(x, y, dz)\nu(dx)\nu(dy) \\ &+\frac{1}{2}\int_{E\times E} a\,[m(x) + m(y)]\, 1_{m(x)+m(y)>R} m(x)m(y)\nu(dx)\nu(dy) \\ &+\lambda \int_E [am(x) - f(x)]\, m(x)\nu(dx),\end{aligned} \tag{5.7}$$

for $a \in \mathbb{R}$ and $f$ bounded, measurable and supported on $E_R := \{x : m(x) \leq R\}$. We also demand that $\nu$ is supported on $E_R$. The equations under consideration can now be summarised as:

$$(\nu_t, \lambda_t) = (\nu_0, \lambda_0) + \int_0^t L(\nu_s, \lambda_s)ds. \tag{5.8}$$

**Lemma 5.2.** For every $\nu_0 \in \mathcal{M}$, that is with finite total variation, and also supported on $E_R$ and $\lambda_0 \in [0, \infty)$, (5.8) has a unique solution $(\nu_t, \lambda_t)_{t\geq 0}$ starting from $(\nu_0, \lambda_0)$. That is, for all non-negative, bounded, measurable functions $f$ supported on $E_R$, and $a \in \mathbb{R}$:

$$\langle (f, a), (\nu_t, \lambda_t) \rangle = \langle (f, a), (\nu_0, \lambda_0) \rangle + \int_0^t \langle (f, a), S_R(\nu_s, \lambda_s) \rangle ds. \tag{5.9}$$

*Proof.* We will show that for any initial conditions, we have a unique solutions $(\nu_t, \lambda_t)_{0\le t\le T}$ where $T$ is an absolute constant. By starting again at $(\nu_T, \lambda_T)$ and so forth, uniqueness and existence for $t \in [0, \infty)$ follows. At no point have we assumed that $\nu_t$ is anything other than a signed measure, so to finish we will need to demonstrate that it is in fact non-negative. The main motivation for considering just a multiplicative kernel, rather than Norris's *eventually multiplicative* kernel is that we can verify this fact more easily.

So we first assume WLOG, by rescaling $\nu_0$ and $\lambda_0$ if necessary that

$$\langle m(x), \nu_0\rangle + \lambda_0 \le 1.$$

We also define the norm on $\mathcal{M} \times \mathbb{R}$

$$||(\nu, \lambda)|| := ||m\nu|| + |\lambda|,$$

which is complete, as a product norm of complete norms. Notice now that in the statement of (5.7), everything on the RHS is at most a quadratic function of $m\nu$ and $\lambda$. So because we have restricted mass to compact support, we may assume there exists an absolute constant $C < \infty$ dependent only on $R$ such that, for all $\nu, \nu' \in \mathcal{M}$ and $\lambda, \lambda' \in \mathbb{R}$,

$$||S_R(\nu, \lambda)|| \le C(R)||(\mu, \lambda)||^2, \tag{5.10}$$

$$||S_R(\nu, \lambda) - S_R(\nu', \lambda')|| \le C(R)||(\nu, \lambda) - (\nu', \lambda')|| \left(||(\nu, \lambda)|| + ||(\nu', \lambda')||\right). \tag{5.11}$$

We will use these bounds, and completeness, to show that an Euler-type approximation converges. We take $(\nu_t^0, \lambda_t^0) := (\nu_0, \lambda_0)$ for all $t$ and define inductively $(\nu_t^n, \lambda_t^n)$, continuous (in time) by:

$$(\nu_t^{n+1}, \lambda_t^{n+1}) := (\nu_0, \lambda_0) + \int_0^t S_R(\nu_s^n, \lambda_s^n)ds. \tag{5.12}$$

To exploit our bounds on the norms, see that as by assumption $||(\nu_t^0, \lambda_t^0)|| = ||(\nu_0, \lambda_0)|| \le 1$,

$$||(\nu_t^{n+1}, \lambda_t^{n+1})|| \le 1 + C\int_0^t ||(\nu_s^n, \lambda_s^n)||ds.$$

It is now easy to check by induction on $n$ that this gives:

$$||(\nu_t^n, \lambda_t^n)|| \le \frac{1}{1 - Ct}, \quad t \le C^{-1}, \quad \forall n.$$

In particular, taking a closed subinterval of this time range gives a uniform bound, say

$$||(\nu_t^n, \lambda_t^n)|| \le 2, \quad 0 \le t \le T := \frac{1}{2C}, \quad \forall n.$$

To apply completeness, we also need to bound the differences between these. Set $g_0(t) = ||(\nu_0, \lambda_0)||$ for all $t$, and define $g_n(t) := ||(\nu_t^n, \lambda_t^n) - (\nu_t^{n-1}, \lambda_t^{n-1})||$. Now:

$$g_{n+1}(t) = ||\int_0^t S_R(\nu_s^{n+1}, \lambda_s^{n+1}) - S_R(\nu_s^n, \lambda_s^n)ds|| \le \int_0^t ||S_R(\nu_s^{n+1}, \lambda_s^{n+1}) - S_R(\nu_s^n, \lambda_s^n)||ds$$

$$\overset{(5.11)}{\le} 4C\int_0^t g_n(s)ds, \quad t \le T.$$

We can therefore bound:

$$g_1(t) \le (4C)t, \quad g_2(t) \le \frac{(4C)^2}{2!}t^2, \quad g_n(t) \le \frac{(4C)^n}{n!}t^n, \quad t \le T.$$

In particular,

$$|g_n(t) - g_m(t)| \to 0 \quad \text{uniformly in } t \in [0,T] \text{ as } m,n \to \infty.$$

So now by completeness, we know that a function $(\nu_t, \lambda_t)_{t\le T}$ exists, and that it must satisfy (5.9) by taking a $n \uparrow \infty$ limit in (5.12). And we also have the machinery to show that it is unique. For suppose $(\nu_t, \lambda_t)$ and $(\nu'_t, \lambda'_t)$ are both solutions. Then, by continuity, and that $t \in [0,T]$, we have

$$\sup_{t\le T}\left[||(\nu_t,\lambda_t)|| + ||(\nu'_t,\lambda'_t)||\right] = D \le \infty.$$

Then, as before:

$$||(\nu_t,\lambda_t) - (\nu'_t,\lambda'_t)|| = ||\int_0^t \left[S_R(\nu_s,\lambda_s) - S_R(\nu'_s,\lambda'_s)\right] ds|| \le \int_0^t ||S_R(\nu_s,\lambda_s) - S_R(\nu'_s,\lambda'_s)||ds$$
$$\overset{(5.11)}{\le} CD\int_0^t \left[||(\nu_s,\lambda_s) - (\nu'_s,\lambda'_s)||\right] ds.$$

Then by the argument given for $g_n(t)$, conclude that

$$||(\nu_t,\lambda_t) - (\nu'_t,\lambda'_t)|| \le \frac{(CD)^n}{n!}t^n, \quad t \le T \quad \Rightarrow (\nu_t,\lambda_t)_{t\le T} = (\nu'_t,\lambda'_t)_{t\le T}.$$

Finally, we have to check that $\nu_t \ge 0$. First observe that taking $f = m$ in (5.5), all the terms on the RHS are non-positive. Therefore $\langle m, \nu_t\rangle$ is decreasing in time. So $\lambda_t$ is increasing by definition. Now take $B \in \mathcal{E}_R$. Take $f = 1_B$ in (5.5) and ignore positive terms, while also getting a factor of 2 from $x, y$ symmetry:

$$\frac{d}{dt}\nu_t(B) \ge -\int_{E\times E} 1_B(x)\bar{K}(x,y)\nu_t(dx)\nu_t(dy) - \lambda_t\langle m1_B, \nu_t\rangle$$
$$= -\langle m,\nu_t\rangle\langle m1_B,\nu_t\rangle - \lambda_t\langle m1_B,\nu_t\rangle = -\langle m,\nu_0\rangle\langle m1_B,\nu_t\rangle$$
$$\ge -R\langle m,\nu_0\rangle\nu_t(B), \quad t \le T.$$

We conclude that

$$\nu_t(B) \ge \nu_0(B)e^{-R\langle m,\nu_0\rangle t} > 0, \quad t \le T.$$

This holds for all measurable $B \in \mathcal{E}_R$, and so we have that $\nu_t \ge 0$ for $t \le T$. $\lambda_t \ge 0$ follows as it is increasing. This concludes the proof of the lemma. □

Now, to finish the proof of the theorem. We call the solution which we have just found $\nu_t^R$. Given $R < S < \infty$, observe that taking $\nu = \nu^S$ and $f = 1_{m\le R}$ in (5.7) gives a solution for $\nu = \nu_R$. In other words, by uniqueness:

$$\nu^R = 1_{m\le R}\nu^S.$$

So the measures:

$$\mu_t := \lim_{R\to\infty} \nu_t^R, \quad \text{and } \lambda_t := \lim_{R\to\infty} \lambda_t^R,$$

are well-defined, with $\lambda_t + \langle m, \mu_t\rangle = \langle m, \mu_0\rangle$ by monotone convergence. Finally, recalling that a solution to (5.4) only demands the required evolution of measures of functions with compact (in mass) support, we conclude that $\mu_t$ satisfies (5.4). □

5.2.1. *Notes on main result, and further implications.*

- In contrast to the previous methods, this proof of existence genuinely provides no suggestion as to what form the solution might take. In a way, this is not surprising. After all, this was achieved without describing the form taken by the clusters in $E$, and with essentially no restriction apart from finiteness in a suitable sense on the initial measure. We shall presently show that when $E = (0, \infty)$, that is the multiplicative coalescent, we can be more precise. In particular, we will be able to specify the gelation time as a function of the initial measure.
- The theorem also demonstrates existence and uniqueness of maximal (in time) conservative solutions with Smoluchowski's dynamics. Observe from the definition of $S$ (5.3) that when $\langle m, \mu_0\rangle = \langle m, \mu_t\rangle$, we have $S(\mu) = L(\mu)$. So any conservative solution on $t < T$ of (5.2) also satisfies (5.4) on that interval. And we have just shown uniqueness of solutions to (5.4) so we certainly have uniqueness for $t \le T$. Conversely, taking

$$T := \inf\{t : \langle m, \mu_t\rangle < \langle m, \mu_0\rangle\} \tag{5.13}$$

gives the gelation time and thus specifies the maximal conservative solution.

5.3. **Multiplicative coalescence on** $(0, \infty)$**.** We will now consider $E = (0, \infty)$, $m(x) = x$, and $K(x, y, dz) = xy\delta_{x+y}(dz)$. We assume $\langle m + 1, \mu_0\rangle < \infty$ and so by the theorem just proved, have $(\mu_t)_{t\ge 0}$ the unique solution to (5.4) for the multiplicative coalescent.

We first make a remark in the direction of showing that the two definitions of gelation time concur. Returning to the more general notation, for $t < T$, defined as in (5.13), we show that the dynamics of $m^2$ are also governed by the functional form of Smoluchowski's equation. Note that we cannot substitute $f = m^2$ in (5.1) as it is unbounded. However, we may take $f = m1_{m\le k}$, then subtract from the equation of mass conservation to obtain:

$$\langle m1_{m>k}, \mu_t\rangle = \langle m1_{m>k}, \mu_0\rangle$$
$$+\frac{1}{2}\int_0^t \int_{E^3} \left[m(z)1_{m(z)>k} - m(x)1_{m(x)>k} - m(y)1_{m(y)\ge k}\right] K(x, y, dz)\mu_s(dx)\mu_s(dy).$$

By almost sure mass conservation (in a coalescence), the integrand is non-negative, so by Dominated Convergence we can integrate w.r.t. $k$ inside the integral, obtaining:

$$\langle m^2, \mu_t\rangle = \int_0^\infty \langle m1_{m>k}, \mu_t\rangle dk$$
$$= \langle m^2, \mu_0\rangle + \frac{1}{2}\int_0^t \int_{E^3} \left[m(z)^2 - m(x)^2 - m(y)^2\right] K(x, y, dz)\mu_s(dx)\mu_(dy).$$

$$= \langle m^2, \mu_0 \rangle + \int_0^t \int_{E^3} m(x)^2 m(y)^2 \mu_s(dx)\mu_s(dx),$$

where the final equality follows from $\bar{K}(x,y) = m(x)m(y)$ and $m(z) = m(x) + m(y)$, $K(x,y,dz)$-almost everywhere.

We conclude with a theorem confirming that the gelation time of the multiplicative coalescent is related to the second moment of the initial mass measure, and that the two definitions are consistent. Recall we are in the continuous setting here, but the result applies equally well to the discrete case by considering discrete measures.

**THEOREM 5.3.** For the multiplicative coalescent described above, there is a unique time $T_{gel} < \infty$ such that:

$$\langle m, \mu_t \rangle = \langle m, \mu_0 \rangle, \quad \langle m^2, \mu_t \rangle < \infty, \quad 0 \le t < T_{gel},$$
$$\langle m, \mu_t \rangle < \langle m, \mu_0 \rangle, \quad t > T_{gel}, \quad \text{and} \quad \langle m^2, \mu_t \rangle \uparrow \infty \quad \text{as } t \to T_{gel}.$$

Furthermore, we have $T_{gel} = (\langle m^2, \mu_0 \rangle)^{-1}$.

*Proof.* Assume WLOG that $\langle m, \mu_0 \rangle = 1$. We consider the exponential moments:

$$m_t(p) := \langle m e^{-pm}, \mu_0 \rangle, \quad p \ge 0, t \ge 0.$$

By regularisation and (5.4), both partial derivatives exist:

$$\partial_p m_t(p) = -\langle m^2 e^{-pm}, \mu_t \rangle < 0, \quad p \in (0, \infty),$$
$$\partial_t m_t(p) = \langle m^2 e^{-pm}, \mu_t \rangle (m_t(p) - 1) < 0, \quad p > 0.$$

Thus by monotonicity and continuity, there is a unique function $t \mapsto p_t$ such that

$$m_t(p_t) = m_0(p_0), \quad t \le \tau(p_0), \quad \text{for some } \tau(p_0) < \infty.$$

Furthermore, this is continuous and differentiable, and satisfies $p_t \downarrow 0$ as $t \to \tau(p_0)$, when this is finite. We therefore have

$$0 = \frac{d}{dt} m_t(p_t) \langle m^s e^{-p_t m}, \mu_t \rangle \left[ m_t(p_t) - 1 - \frac{dp}{dt} \right].$$

Since $\langle m^2 e^{-p_t m}, \mu_t \rangle$ is positive, we can solve to obtain

$$p_t = p_0 - [1 - m_0 p(0)]\, t, \quad t < \tau(p_0).$$

Because we demanded $p_t \ge 0$, we may conclude that $\tau(p_0) = \frac{p_0}{1 - m_0(p_0)}$. Using that $\langle 1 - m, \mu_0 \rangle = 0$, we rearrange:

$$1 - m_0(p) = \langle 1 - m e^{-pm}, \mu_0 \rangle = \langle 1 - m + m^2 p - m^3 \frac{p^2}{2!} + \ldots, \mu_0 \rangle$$
$$= mp \int_0^m \left[ 1 - px + \frac{(px)^2}{2!} - \ldots \right] dx.$$

So,

$$\tau(p) = \left[ \langle m \int_0^m e^{-px} dx, \mu_0 \rangle \right]^{-1}, \quad p > 0.$$

In addition, by continuity, we have $\tau(0) = (\langle m^2, \mu_0\rangle)^{-1}$, so $\tau : [0,\infty) \to [\tau_0, \infty)$ is a continuous increasing bijection. Now for $p > 0$, we have

$$\langle m, \mu_{\tau(p)}\rangle = m_{\tau(p)}(0) = m_0(p) < m_0(0) = \langle m, \mu_0\rangle.$$

Thus:

$$\langle m, \mu_t\rangle \quad \begin{cases} = \langle m, \mu_0\rangle & t \le \tau(0) \\ < \langle m, \mu_0\rangle & t > \tau(0) \end{cases}.$$

So for $t < \tau(0)$, using the result shown before the theorem:

$$\frac{d}{dt}\langle m^2, \mu_t\rangle = \langle m^2, \mu_t\rangle^2,$$

$$\Rightarrow \quad \langle m^2, \mu_t\rangle = \frac{1}{\tau(0) - t}, \quad t < \tau(0).$$

Taking $T_{gel} := \tau(0)$ gives precisely the statement of the theorem. □

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