

MATHEMATISCHES FORSCHUNGSINSTITUT OBERWOLFACH

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Coagulation and Fragmentation Models

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ABSTRACT. Analysis of coagulation and fragmentation is crucial to understanding many processes of scientific and industrial importance. In recent years this has led to intensified research activities in the areas of differential equations, probability theory, and combinatorics. The purpose of the workshop was to bring together people from these different areas working on various aspects of coagulation and fragmentation. We believe that the insights resulting from the interactions which have been stimulated that week should lead to further advances both in the development of mathematical techniques and in new applications.

Mathematics Subject Classification (2000):

Primary: 60 Probability theory and stochastic processes.

Secondary: 35 Partial differential equations scheme of the International Mathematical Union,
10 Probability and Statistics,

11 Partial Differential Equations.

Introduction by the Organisers

Historically deterministic equations were used for modelling the dynamics of the density of clusters of different sizes in a medium that evolves by coagulation and/or fragmentation. An alternative stochastic approach uses the distribution of a typical particle in systems undergoing a random evolution. This approach provides tools for deriving limit equations, it easily extends to more general interactions and, finally, it shares the familiar advantages of particle-based methods for computing distributions in high dimensions. The stochastic theory is undergoing intense development, both at a theoretical level, in the construction of models and analysis

of their properties, and at a computational level. Major mathematical challenges in the field of coagulation and fragmentation models are related to phase transitions due to fast coagulation (gelation) or fast fragmentation (formation of dust), and to explicit descriptions of the structure of partitions (e.g. allelic partitions induced by random mutations in models for the evolution of populations). A further direction of intensive study is the detailed analysis of particular coagulation and fragmentation processes, where special features (e.g., scaling properties) allow links to be made to Brownian motion and other Lévy processes, also to some interesting problems in random combinatorics.

Major topics that have been discussed during the workshop include :

1. Spatial models of coagulation and fragmentation
Models incorporating diffusion; scaling limits; derivation from particle dynamics; equilibrium measures for coagulation-fragmentation processes; formation of structured particles; diffusion limited aggregation
2. Phase transitions in coagulation and fragmentation models
Gelation effects; shattering transition (appearance of dust in fragmentation); explosion phenomena; computation of the gelation time; uniqueness issues; convergence of particle systems
3. Aspects of random combinatorics
Links to random graphs and trees; genealogy for certain large populations dynamics; mutation and allelic partitions; stochastic coalescents with multiple collisions (Λ -coalescents) and fragmentations
4. Computational issues
Approximation and numerics; analysis of algorithms; Monte Carlo issues around sensitivity in initial conditions and kernel parameters

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Abstracts

Exchangeable coalescents and flows of bridges

JEAN-FRANÇOIS LE GALL

(joint work with Jean Bertoin)

Exchangeable coalescents are Markov processes with values in the set of all partitions of \mathbf{N} , which describe the scaling limits of the ancestry process in populations with a large fixed size. They were introduced independently by Pitman and Sagitov, and were discussed later by Schweinsberg, Möhle and many others. An exchangeable coalescent is a coalescent process (meaning that the state of the process at time t is a random partition of \mathbf{N} whose blocks are merged together as time increases) which satisfies a natural exchangeability condition. An important subclass is the class of the Λ -coalescents, where at most one set of blocks can coalesce at any given time. Special cases of Λ -coalescents are the famous Kingman coalescent, the Bolthausen-Sznitman coalescent which arose in connection with certain models of spin glass theory, and more generally the so-called beta-coalescents. In this lecture, we first describe a remarkable connection between exchangeable coalescents and flows of bridges on the time interval $[0, 1]$. A bridge is a process with exchangeable increments and nondecreasing sample paths, which starts from 0 at time 0 and ends at 1 at time 1. A flow of bridges is then a collection $(B_{s,t})$ of bridges, indexed by pairs (s, t) of real numbers such that $s < t$, which satisfies the composition rule $B_{s,u} = B_{s,t} \circ B_{t,u}$ as well as the obvious stationarity and independence properties. The one-to-one correspondence between exchangeable coalescents and flows of bridges leads to certain generalized Fleming-Viot processes (already discussed by Donnelly and Kurtz), which are measure-valued duals to the Λ -coalescents. The duality relation makes it possible to derive properties of the coalescents using information from the Fleming-Viot processes. As a typical application, we investigate the small time behavior of the number of blocks in a Λ -coalescent under a regular tail assumption on the measure Λ . Sharper results have been obtained recently by Berestycki, Berestycki and Schweinsberg, but only in the special case of beta-coalescents.

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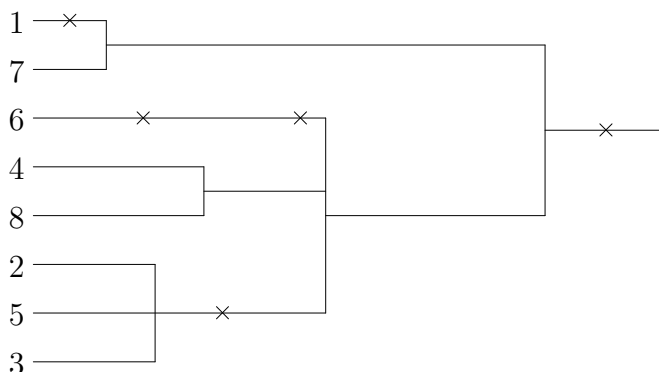
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**Asymptotics of the allele frequency spectrum associated with the
Bolthausen-Sznitman coalescent**

CHRISTINA GOLDSCHMIDT

(joint work with Anne-Laure Basdevant)

We imagine a coalescent process as modelling the genealogy of a sample from a population which is subject to neutral mutation. We work under the assumptions of the infinitely many alleles model so that, in particular, every mutation gives rise to a completely new type in the population. Mutations occur as a Poisson process of rate ρ along the branches of the coalescent tree. The *allelic partition* groups together individuals of the same allelic type, and is obtained by tracing each individual's lineage back in time to the most recent mutation. An example of this construction is given below.



The allelic partition here is $\{1\}, \{2, 3, 5\}, \{4, 7, 8\}, \{6\}$. Let $N_k(n)$ be the number of blocks of size k in the allelic partition, when we start with a sample of n individuals and let $N(n) = \sum_{k=1}^n N_k(n)$. The *allele frequency spectrum* is the vector $(N_1(n), N_2(n), \dots)$ of block counts.

We are interested in the distribution of the allele frequency spectrum associated with the Λ -coalescents, a class of exchangeable coalescent processes introduced by Pitman [10] and Sagitov [11]. Each such process corresponds to a finite measure Λ on $[0, 1]$. Since the state of a Λ -coalescent is an exchangeable random partition of \mathbb{N} for all times and the mutation occurs in a symmetric manner, the allelic partition is, itself, exchangeable. This entails that there exists a sequence of underlying random block frequencies $F_1 \geq F_2 \geq \dots \geq 0$ such that $\sum_{i=1}^{\infty} F_i \leq 1$. The allelic partition could then be viewed as the partition created by sampling from these (unknown) frequencies in an i.i.d. manner, according to Kingman's paintbox process. For a general exchangeable random partition, the quantities $N_k(n)$, $k \geq 1$, and $N(n)$ (thought of the numbers of boxes discovered by the first n samples) have recently been of particular interest; see Gnedin, Hansen and Pitman [8] and the references therein.

For Kingman’s coalescent, the distribution of the allele frequency spectrum is known completely and is given by the celebrated *Ewens sampling formula* [7]:

$$q(m_1, m_2, \dots) := \mathbb{P}(N_1(n) = m_1, N_2(n) = m_2, \dots) = \frac{n! \theta^{\sum_{i \geq 1} m_i}}{(\theta)_n \prod_{j \geq 1} j^{m_j} m_j!},$$

where $\theta = 2\rho$ and $(\theta)_n = \theta(\theta + 1) \dots (\theta + n - 1)$. For no other Λ -coalescent (apart from the degenerate star-shaped coalescent with $\Lambda = \delta_1$) is $q(m_1, m_2, \dots)$ known explicitly, although Möhle [9] has proved a recursion that it must satisfy. However, Berestycki, Berestycki and Schweinsberg [2, 3] have recently proved asymptotic results for the Beta coalescents with $\alpha \in (1, 2)$; that is, the coalescents corresponding to

$$\Lambda(dx) = \frac{1}{\Gamma(\alpha)\Gamma(2 - \alpha)} x^{1-\alpha}(1 - x)^{\alpha-1} dx.$$

In this case $n^{\alpha-2}N(n) \xrightarrow{p} \frac{\rho\alpha(\alpha - 1)\Gamma(\alpha)}{2 - \alpha}$

and, for $k \geq 1$, $n^{\alpha-2}N_k(n) \xrightarrow{p} \frac{\rho\alpha(\alpha - 1)^2\Gamma(k + \alpha - 2)}{k!}$ as $n \rightarrow \infty$.

The Bolthausen-Sznitman coalescent [4] is the $\alpha = 1$ Beta coalescent i.e. $\Lambda(dx) = dx$. It has several nice properties and seems to be more tractable than most other Λ -coalescents. A significant difference between it and the Beta coalescents with $\alpha \in (1, 2)$ is that the Bolthausen-Sznitman coalescent does not come down from infinity; that is, it has infinitely many blocks for all time. The main result of [1] gives the corresponding (and rather different) asymptotics for the allele frequency spectrum of the Bolthausen-Sznitman coalescent:

Theorem. As $n \rightarrow \infty$,

$$\frac{\log n}{n} N_1(n) \xrightarrow{p} \rho$$

and, for $k \geq 2$,

$$\frac{(\log n)^2}{n} N_k(n) \xrightarrow{p} \frac{\rho}{k(k - 1)}.$$

As a corollary, we obtain that $\frac{\log n}{n} N(n) \xrightarrow{p} \rho$.

The proof of this theorem involves proving a fluid limit result for the path of the coalescent with mutations, using the method described in Darling and Norris [5]. We need to add some structure in order to follow the mutations and so (following Dong, Gnedin and Pitman [6]) we allow individuals to be in two possible states: *active* (unmutated) or *frozen* (mutated). Blocks may contain both active and frozen individuals, and the status of an individual is ignored by the operation of coalescence. At rate ρ , any block containing active individuals receives a mutation. A block can contain individuals which were frozen at different times, but all those frozen at the same time form a block in the final allelic partition. The process continues until all individuals are frozen. Now suppose that we start with n active individuals in singleton blocks. For $k \geq 1$, let $X_k^n(t)$ be the number of blocks containing k active individuals at time t . Let $Z_k^n(t)$ be the number of blocks of

size k in the final allelic partition which have already been formed by time t . Let $T_n = \inf\{t \geq 0 : \sum_{k=1}^n X_k^n(t) = 0\}$. Then

$$(X_1^n(t), X_2^n(t), \dots, Z_1^n(t), Z_2^n(t), \dots)_{0 \leq t \leq T_n}$$

is a Markov jump process whose terminal value is of interest to us. We show that

$$\left(\frac{1}{n} X_1^n \left(\frac{t}{\log n} \right), \frac{\log n}{n} X_2^n \left(\frac{t}{\log n} \right), \frac{\log n}{n} X_3^n \left(\frac{t}{\log n} \right), \dots, \right. \\ \left. \frac{\log n}{n} Z_1^n \left(\frac{t}{\log n} \right), \frac{(\log n)^2}{n} Z_2^n \left(\frac{t}{\log n} \right), \frac{(\log n)^2}{n} Z_3^n \left(\frac{t}{\log n} \right), \dots \right)_{0 \leq t \leq (\log n) T_n}$$

behaves asymptotically like the deterministic function

$$(x_1(t), x_2(t), x_3(t), \dots, z_1(t), z_2(t), z_3(t), \dots)_{t \geq 0},$$

$$\text{where } \quad x_1(t) = e^{-t}, \quad x_k(t) = \frac{te^{-t}}{k(k-1)}, \quad k \geq 2, \\ z_1(t) = \rho(1 - e^{-t}), \quad z_k(t) = \frac{\rho}{k(k-1)}(1 - e^{-t} - te^{-t}), \quad k \geq 2.$$

Heuristically, then, $(\log n)T_n$ should not be too far from $\inf\{t \geq 0 : \sum_{k=1}^{\infty} x_k(t) = 0\} = \infty$. It is possible to show rigorously that we do, indeed, have

$$\frac{\log n}{n} Z_1^n(T_n) \sim z_1(\infty) = \rho \quad \text{and} \quad \frac{(\log n)^2}{n} Z_k^n(T_n) \sim z_k(\infty) = \frac{\rho}{k(k-1)}, \quad k \geq 2,$$

as stated in the Theorem. See [1] for a full proof.

We remark that this fluid limit is unusual in two respects. Firstly, we scale time *down* rather than up and, secondly, different co-ordinates of the process have different scalings.

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On the number of cuts needed to isolate the root of a random recursive tree

MARTIN MÖHLE

(joint work with Michael Drmota, Alex Iksanov and Uwe Rösler)

Let T be a rooted deterministic tree. Meir and Moon [7] introduced the following procedure to isolate the root of T by successive deletions of edges. Delete one edge chosen at random. Now consider only the subtree containing the root and delete in it one edge at random. Repeat the last step until the root is isolated. With $X(T)$ we denote the (random) number of cuts needed to isolate the root of T .

A *recursive tree* is a rooted tree with $n \in \mathbb{N} := \{1, 2, \dots\}$ vertices $1, \dots, n$ such that the root has label 1 and the labels of the vertices on the unique path from the root to any other vertex form an increasing sequence. A tree T_n is called a *random recursive tree* with n vertices if T_n is uniformly distributed on the set of all $(n-1)!$ recursive trees with n vertices.

We are interested in the number $X_n = X(T_n)$ of cuts needed to isolate the root of a random recursive tree with n vertices. Note that both the tree and the cuts are random. It is well known that $(X_n)_{n \in \mathbb{N}}$ satisfies the recursion

$$(1) \quad X_1 = 0 \quad \text{and} \quad X_n = 1 + X_{n-D_n}, \quad n \in \{2, 3, \dots\},$$

where D_n is a random variable independent of X_2, \dots, X_{n-1} with distribution $P(D_n = k) = n/((n-1)k(k+1))$, $k \in \{1, \dots, n-1\}$. The random variable X_n can be interpreted as the absorption time $\inf\{k \geq 0 : J_k = 1, J_0 = n\}$ of a strictly decreasing Markov chain $(J_k)_{k \geq 0}$ with state space \mathbb{N} and transition probabilities $P(J_{k+1} = j | J_k = i) = i/((i-1)(i-j)(i-j+1))$, $j \in \{1, \dots, i-1\}$. Note that X_n coincides with the number of collision events that take place in the Bolthausen-Sznitman coalescent, restricted to the set $\{1, \dots, n\}$, until there is just a single block (Goldschmidt and Martin [3]).

Panholzer [9] derived the asymptotics of the j th moment of X_n , $j \in \mathbb{N}$. In particular, $\mu_n := E(X_n) \sim n/\log n$, $E(X_n^2) \sim n^2/\log^2 n$ and $\sigma_n^2 := \text{Var}(X_n) \sim n^2/(2 \log^3 n)$, from which the weak law of large numbers follows immediately, i.e. $X_n/\mu_n \rightarrow 1$ in probability as $n \rightarrow \infty$. A natural and for many years open problem was to find the following weak limiting behaviour of X_n . As $n \rightarrow \infty$,

$$(2) \quad \frac{\log^2 n}{n} X_n - \log n - \log \log n \xrightarrow{d} X,$$

where X is a 1-stable random variable with characteristic function $E(e^{itX}) = e^{it \log |t| - \frac{\pi}{2}|t|}$, $t \in \mathbb{R}$. Panholzer [9] already mentioned that it is impossible to verify (2) via an approach based on the method of moments. Contraction methods (see, for example, Neininger and Rüschenendorf [8]) seem to be not or at least not directly applicable. An analytic proof of (2), based on a singularity analysis of the

generating function $f(s, t) := \sum_{n \in \mathbb{N}} \mathbb{E}(s^{X_n})t^{n-1}$, was given in [1]. Applications to the number of collisions, the total branch length, and the number of segregating sites of the Bolthausen-Sznitman coalescent appeared in [2].

Shortly later, a completely different, purely probabilistic proof of (2) was provided in [4]. This probabilistic proof is based on a coupling related to the random walk $(S_n)_{n \geq 0}$, $S_0 := 0$, $S_n := \xi_1 + \dots + \xi_n$, where ξ_1, ξ_2, \dots are independent copies of a random variable ξ with distribution $P(\xi = k) = 1/(k(k+1))$, $k \in \mathbb{N}$.

It turns out that this coupling method can be extended to any recursion of the form (1) as long as the random variable D_n is independent of X_2, \dots, X_{n-1} and has a distribution of the form

$$(3) \quad P(D_n = k) = \frac{p_k}{p_1 + \dots + p_{n-1}}, \quad k, n \in \mathbb{N}, k < n,$$

for some proper probability distribution $p_k = P(\xi = k)$, $k \in \mathbb{N}$. Asymptotic results for absorption times of Markov chains under the assumption (3) are studied in [5]. These results are in particular applied to the number X_n of collisions in beta($a, 1$)-coalescents with parameter $0 < a < 2$. The results indicate that the two parameter values $a = 1$ and $a = 2$ play a kind of threshold-role when studying the limiting behaviour of X_n . The coupling method is not applicable for $a \geq 2$. However, the boundary case $a = 2$ can be treated separately via asymptotics of moments and contraction methods [6].

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Collisions and freezing events in coalescents with multiple mergers

ALEXANDER GNEDIN

(joint work with Yuri Yakubovich)

The Pitman–Sagitov Λ -coalescent is a continuous-time Markov process describing the random coagulation of an infinite system of particles that collide in bulks and merge by collisions to form new particles [8, 9]. Restricting the process to n particles, each j -tuple of them is merging into a single particle at some rate $\lambda_{n,j}$ (for $j = 2, \dots, n$), so that the total rate of collision among n particles is

$$\lambda_n = \sum_{j=2}^n \binom{n}{j} \lambda_{n,j}.$$

Pitman [8] showed that the consistency of restricted coalescent processes for various values of n amounts to an integral representation of the rates

$$\lambda_{n,j} = \int_0^1 x^{j-2} (1-x)^{n-j} \Lambda(dx).$$

with some finite measure Λ on $[0, 1]$, which by the virtue of a time-change can be reduced to a normalised measure, so we assume $\Lambda[0, 1] = 1$.

Letting the time ticking at the collision events, we can represent the decaying number of particles by means of a decreasing Markov chain, which we denote \mathcal{M}_n for the coalescent starting with n particles. Dong, Gnedin and Pitman [5] characterised all Markov chains on \mathbb{N} that appear in this way, and demonstrated that the *decrement matrix* q of such a chain (which is a lower-triangular transition matrix whose entries satisfy a nonlinear recursion) uniquely determines Λ and the collision rates through the relation $q(n, n-j+1) = \lambda_{n,j}/\lambda_n$, hence determines fully the law of the coalescent process. For instance, Kingman's coalescent with only binary collisions ($\Lambda = \delta_0$) corresponds to \mathcal{M}_n with the deterministic path $n, n-1, \dots, 1$. Note that \mathcal{M}_n decrements from n to $n-j+1$ if the first collision among n particles takes j of them. The number of collisions C_n is thus the number of jumps the chain \mathcal{M}_n needs to move from n to the terminal state 1.

The large- n asymptotics of many interesting functionals like C_n are to a great extent determined by the behaviour of the underlying measure Λ near zero. Here we discuss a family of measures with the power-like behaviour

$$(1) \quad \Lambda[0, x] = Ax^\alpha + O(x^{\alpha+\varsigma}) \text{ as } x \downarrow 0, \text{ with } 0 < \alpha < 1 \text{ and } \varsigma > 0.$$

This covers some beta-coalescents [1, 2], with $\Lambda = \text{Beta}(\alpha, 2-\alpha)$ (we mean $\varsigma = 1$ and $0 < \alpha < 1$ as in (1)), but excludes the Bolthausen–Sznitman coalescent for which Λ is the uniform distribution [4].

Let J_n denote the random multiplicity of the first collision, so

$$\mathbb{P}(J_n = j) = q(n, n-j+1) \quad j = 2, \dots, n,$$

and the size of the first jump of \mathcal{M}_n is $J_n - 1$. It turns out that under assumption (1) J_n converges in distribution:

$$\lim_{n \rightarrow \infty} \mathbb{P}(J_n = j) = (2 - \alpha) \frac{(\alpha)_{j-2}}{j!} \quad j = 2, 3, \dots,$$

where $(\alpha)_j$ stays for the rising factorial. This quasi-stationarity of decrements allows us to construct stochastic bounds J_n^+ and J_n^- to satisfy

$$J_n^+ \leq_d J_b \leq_d J_n^-$$

for sufficiently large n and for all b in the range $n \geq b \geq n^\nu$ for some constant $\nu < 1$. The distributions of J_n^+ and J_n^- depend on ν and three further parameters, which can be chosen to guarantee that the mean values both converge to $1/(1 - \alpha)$. Comparing the Markov chain \mathcal{M}_n with two random walks, whose negative jumps are $J_n^+ - 1$ and $J_n^- - 1$, correspondingly, we are lead to the following law of large numbers for the number of collisions.

Theorem. *If the measure Λ satisfies assumption (1) then $n^{-1}C_n$ converges to $1 - \alpha$ in probability.*

Coupling arguments also allow us to derive a limit theorem for C_n from Feller's renewal theorem for random walks [6]. However, it is by far not enough that J_n^+ and J_n^- have asymptotically the same means, since we also need that the limit laws for the approximating random walks hold with the same scaling. This objective can be achieved by a still finer tuning of the parameters of distributions for $J_n^+ - 1$ and $J_n^- - 1$, but the tuning requires explicit control of the error term in (1), which restricts the range of ς .

Theorem. *Let the measure Λ satisfy (1) with $\varsigma > \max\left\{\frac{(2-\alpha)^2}{5-5\alpha+\alpha^2}, 1-\alpha\right\}$. Then, as $n \rightarrow \infty$, we have the convergence in distribution*

$$\frac{C_n - (1 - \alpha)n}{(1 - \alpha)n^{1/(2-\alpha)}} \rightarrow_d \mathcal{S}_{2-\alpha}$$

to a stable random variable $\mathcal{S}_{2-\alpha}$ with the characteristic function

$$(2) \quad \mathbb{E} [e^{iu\mathcal{S}_{2-\alpha}}] = \exp\left(-e^{-i\pi\alpha \operatorname{sign}(u)/2}|u|^{2-\alpha}\right).$$

Note that the most important case $\varsigma = 1$ is always covered.

A variation of the Λ -coalescent is the (Λ, ρ) -coalescent with freeze [5], in which every particle can be withdrawn from the collision process (frozen) at certain rate $\rho > 0$. In a biological context, which motivated this kind of model [7], a freeze event corresponds to a mutation in the population which leads to formation of a new allele and, consequently, of a new block in the partition of the population by alleles. Let F_n be the number of frozen particles ever generated by the (Λ, ρ) -coalescent starting with n particles.

A Markov chain \mathcal{L}_n which captures all relevant information has now the state-space $\mathbb{N} \times \mathbb{Z}_+$, and the initial state $(n, 0)$. The first component counts the number of remaining active particles, while the second component counts the number of

frozen particles. The state (b, m) changes by a j -fold collision to $(b - j + 1, m)$, and in the event of freeze to $(b - 1, m + 1)$. The number of mutations F_n is the final value of the second component as \mathcal{L}_n enters a state $(1, \bullet)$.

Like for \mathcal{M}_n , the decrements of \mathcal{L}_n in the first component can be satisfactorily approximated by J_n^+ and J_n^- on the major part of the path. However, the probability of freeze varies substantially along the path, since the probability is asymptotic to $\text{const } b^{\alpha-1}$ at state (b, m) . A natural way to circumvent the difficulty is to further subdivide the trajectory of \mathcal{L}_n into smaller pieces on which the probability of freeze can be approximated by a constant.

Theorem. *Suppose that the measure Λ satisfies assumption (1) with $\varsigma = 1$. Then for $n \rightarrow \infty$ the number of frozen particles F_n satisfies:*

$$\text{for } 0 < \alpha < 2 - \sqrt{2}, \quad \frac{F_n - \rho(1-\alpha)(2-\alpha)n^\alpha}{\sqrt{\rho(1-\alpha)(2-\alpha)n^{\alpha/2}}} \rightarrow_d \mathcal{N},$$

$$\text{while for } 2 - \sqrt{2} < \alpha < 1, \quad \frac{F_n - \rho(1-\alpha)(2-\alpha)n^\alpha}{\beta n^{(3\alpha-1-\alpha^2)/(2-\alpha)}} \rightarrow_d \mathcal{S}_{2-\alpha},$$

where \mathcal{N} is the standard Normal distribution, $\mathcal{S}_{2-\alpha}$ is determined by (2) and $\beta = \left(\frac{\rho(1-\alpha)(2-\alpha)}{A(3\alpha-1-\alpha^2)}\right)^{1/(2-\alpha)}$.

Closely related results with the same kind of phase transition have been obtained in [3] for the total length of branches of the coalescent tree at a fixed time.

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Beta coalescents and populations with large family sizes

JASON SCHWEINSBERG

(joint work with Julien Berestycki, Nathanaël Berestycki)

Coalescents with multiple collisions, also known as Λ -coalescents, are coalescent processes in which many clusters can merge at once into a single cluster. These processes were introduced by Pitman [10] and Sagitov [11]. In recent years, there has been a surge of interest in these processes, motivated in part by potential biological applications.

Before defining these processes precisely, we recall the definition of Kingman's coalescent, which was introduced in [8]. Kingman's coalescent has the property that only two clusters merge at a time, and each pair of clusters merges at rate one. More precisely, the n -coalescent is a Markov process, taking its values in the set of partitions of $\{1, \dots, n\}$ and starting from the partition of $\{1, \dots, n\}$ into singletons, such that each transition that involves merging two blocks of the partition occurs at rate 1, and no other transitions are possible. Kingman's coalescent is a Markov process taking its values in the set of partitions of the positive integers whose restriction to $\{1, \dots, n\}$ is the n -coalescent.

Coalescents with multiple collisions are also Markov processes taking their values in the set of partitions of the positive integers that are defined by their restrictions to $\{1, \dots, n\}$. The restriction of a coalescent with multiple collisions to $\{1, \dots, n\}$ has the property that whenever there are b blocks, each transition in which k blocks merge into one occurs at some rate $\lambda_{b,k}$, which does not depend on n or on the sizes of the blocks. Pitman [10] showed that for some finite measure Λ on $[0, 1]$, the merger rates must satisfy

$$(1) \quad \lambda_{b,k} = \int_0^1 x^{k-2} (1-x)^{b-k} \Lambda(dx).$$

The coalescent process whose transition rates satisfy (1) is called the Λ -coalescent. To understand the meaning of the measure Λ , note that any finite measure Λ on $[0, 1]$ can be written as $\Lambda = a\delta_0 + \Lambda_0$, where δ_0 is the unit mass at zero and $\Lambda_0(\{0\}) = 0$. We can think of the Λ -coalescent as having the following two types of transitions:

- 1) Each transition that involves two blocks merging into one happens at rate a .
- 2) Consider a Poisson process on $[0, \infty) \times (0, 1]$ with intensity $dt \times p^{-2}\Lambda_0(dp)$. If (t, p) is a point of this Poisson process, then at time t , we flip an independent coin for each block which comes up heads with probability p , and merge the blocks whose coins come up heads.

Thus, the measure Λ determines the rates at which different multiple mergers occur. Kingman's coalescent is the case in which Λ is a unit mass at zero, so $a = 1$ and Λ_0 is the zero measure. The Λ -coalescent in which Λ is the uniform distribution on $[0, 1]$ is called the Bolthausen-Sznitman coalescent and was introduced in [6].

Coalescent processes are of interest in biology because they can be used to describe the genealogy of a population. If one samples n individuals from a population and follows their ancestral lines backwards in time, the ancestral lines will coalesce. Consider a population with infinitely many generations and N individuals in each generation. Assume the distribution of the N family sizes ν_1, \dots, ν_N is exchangeable, and is the same in each generation. To describe the genealogy of the population, sample n individuals at random from the population in generation zero and define a discrete-time Markov chain $(\Psi_{n,N}(m))_{m=0}^{\infty}$, where $\Psi_{n,N}$ is the partition of $\{1, \dots, n\}$ such that i and j are in the same block if and only if the i th and j th individuals in the sample have the same ancestor in generation $-m$. Let c_N be the probability that two individuals chosen at random from one generation have the same ancestor in the previous generation. Möhle and Sagitov [9] have shown that under suitable regularity conditions, the continuous-time processes $(\Psi_{n,N}(\lfloor t/c_N \rfloor), t \geq 0)$ converge as $N \rightarrow \infty$ to a limiting coalescent process. When family sizes are small enough that it is unlikely that three or more of the sampled ancestral lines will merge simultaneously, the processes $(\Psi_{n,N}(\lfloor t/c_N \rfloor), t \geq 0)$ converge to Kingman's n -coalescent. However, Sagitov [11] showed that if very large family sizes are possible, then Λ -coalescents can arise in the limit because multiple ancestral lines coming from a large family will coalesce at the same time.

To focus on what seems to be a natural special case, consider a model in which the numbers of offspring of the N individuals are independent, and N of these offspring are chosen at random to form the next generation. Suppose the probability of having k or more offspring is $Ck^{-\alpha}$ for some constant C . It was shown in [13] that if $\alpha \geq 2$, the genealogy is described by Kingman's coalescent because large families are rare. However, when $1 \leq \alpha < 2$, the genealogy is described by a Λ -coalescent in which Λ is the Beta($2 - \alpha, \alpha$) distribution. A continuous version of this result appears in [5]. Bertoin and Le Gall [4] had previously shown that the Bolthausen-Sznitman coalescent (which is the beta coalescent when $\alpha = 1$) gives the genealogy of a continuous-state branching process introduced by Neveu. These results indicate that the beta coalescents are natural models of the genealogy of populations with large family sizes and provide motivation for further study of beta coalescents.

We focus here on properties of beta coalescents that are of potential interest in genetics. Consider a beta coalescent restricted to $\{1, \dots, n\}$, which represents the genealogy of a sample of size n from a population. Suppose mutations occur at times of a Poisson process of rate θ along each lineage. When we examine the DNA of the n sampled individuals, we can observe which mutations each individual acquired. Let S_n be the total number of mutations in the tree. This is called the number of segregating sites because as long as each mutation takes place at a different site on the DNA, the number of sites on the DNA at which not all n segments agree will be the number of mutations. Define the allelic partition to be the partition of $\{1, \dots, n\}$ such that i and j are in the same block if and only if the i th and j th individuals in the sample got exactly the same set of mutations. Let $M_{k,n}$ be the number of mutations that are acquired by k of the n sampled

individuals, and let $N_{k,n}$ be the number of blocks of size k in the allelic partition. The sequence $(M_{1,n}, \dots, M_{n-1,n})$ is called the site frequency spectrum, and the sequence $(N_{1,n}, \dots, N_{n,n})$ is called the allele frequency spectrum.

Considerable progress has been made in recent years towards understanding the behavior of these quantities. It is well-known that for Kingman's coalescent, $S_n/\log n \rightarrow_p \theta$, and the distribution of S_n is asymptotically normal. It was shown in [2] that for the beta coalescent with $1 < \alpha < 2$, we have

$$\frac{S_n}{n^{2-\alpha}} \rightarrow_p \frac{\theta\alpha(\alpha-1)\Gamma(\alpha)}{2-\alpha}.$$

For the Bolthausen-Sznitman coalescent, it was shown in [7] that $(\log n)S_n/n \rightarrow_p \theta$, and the asymptotic distribution of S_n is a stable law of index one.

For Kingman's coalescent, the distribution of the allelic partition is given by the famous Ewens sampling formula. In this case, $E[M_{k,n}] = \theta/k$ for $k = 1, 2, \dots, n-1$, and for fixed k , we have $E[N_{k,n}] \rightarrow \theta/k$ as $n \rightarrow \infty$. Asymptotics for the site and allele frequency spectra for the beta coalescents were worked out in [3], where it was shown that

$$\frac{M_{k,n}}{S_n} \rightarrow_p \frac{(2-\alpha)\Gamma(k+\alpha-2)}{\Gamma(\alpha-1)k!}$$

for all k and that the same result holds when $M_{k,n}$ is replaced on the left-hand side by $N_{k,n}$. Recently, detailed asymptotics for the allele frequency spectrum for the Bolthausen-Sznitman coalescent were obtained in [1].

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Coalescent with rebirth

VLADA LIMIC

(joint work with A. Greven, A. Winter)

The goal of the talk was to motivate the construction of the process called the *coalescent with rebirth* from [6] that arises naturally in the asymptotic study of spatial Moran models and similar particle systems evolving on two-dimensional lattice. Neither the talk, nor this extended abstract, attempt to show the full strength of the results and techniques in [6]. Rather, a certain asymptotic phenomenon is described in a simpler and already potentially interesting setting.

It is well known, see for example [2], that coalescing random walks are dual to the voter model. In an analogous way, the spatial coalescent (with delay), see [5], is dual to the spatial Moran models. This duality turns out to be a very powerful tool for studying asymptotic behavior of the voter (and alike) models, due to the fact that the partitions formed from coalescing random walks started at “sparse” configurations, when viewed on appropriate scale, converge to the Kingman coalescent [7]. The original result verifying the above fact was proved by Cox [2] in the case of coalescing simple symmetric random walks on d -dimensional tori. In [5], we extend his analysis to the case of delayed spatial coalescent, and this enables us to characterise the asymptotic behavior of voter-like models in transient ($d \geq 3$) dimensions. The one-dimensional setting was understood some time ago due to the work of Arratia [1]. However, the critical recurrent dimension $d = 2$, which is also interesting from the perspective of applications in biology, seems to be more difficult to handle. In [6] we focus on the analysis of coalescent processes, and we postpone the analysis of the particle systems until future work.

A predecessor of the coalescent with rebirth is the “frozen coalescent” of Cox and Griffeath [3], and indeed, we build on their analysis. One advantage of our approach are the weak limits in the sense of Skorokhod topology, and not solely in the sense of finite-dimensional distributions.

The coalescent with rebirth evolves formally (see [6] for a rigorous construction) according to the following dynamics: starting with infinitely many particles/blocks, each pair of blocks coalesces at rate 1, and immediately upon each coalescing event (in which two blocks merge to one) a new particle is reborn/created.

The following figure represents a simpler process, where the “rebirth” is performed at times I_2 , and I_3 . Denote by

$$(1) \quad (K_{I_*}^{b;I_1,I_2,I_3}, K_{I_*}^{g;I_1,I_2,I_3}, K_{I_*}^{w;I_1,I_2,I_3})$$

the triple consisting of the numbers of black, grey and white blocks, respectively, in the configuration at time I_* .

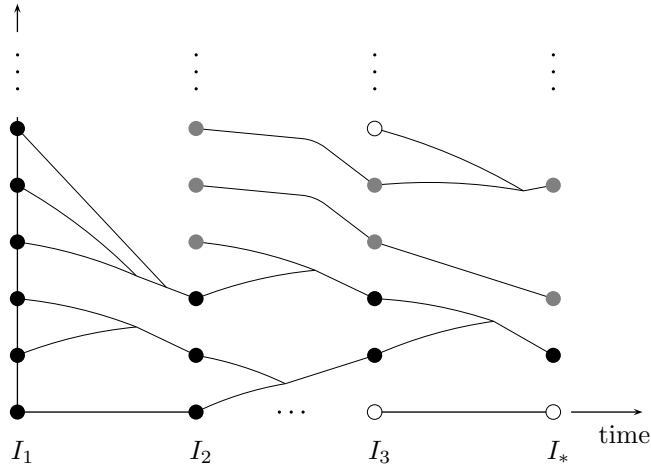


Figure 1

Next fix a large parameter t , and three boxes $[-\sqrt{t^{\alpha_i}}, \sqrt{t^{\alpha_i}}]^2 \cap \mathbb{Z}^2$, $i = 1, 2, 3$,

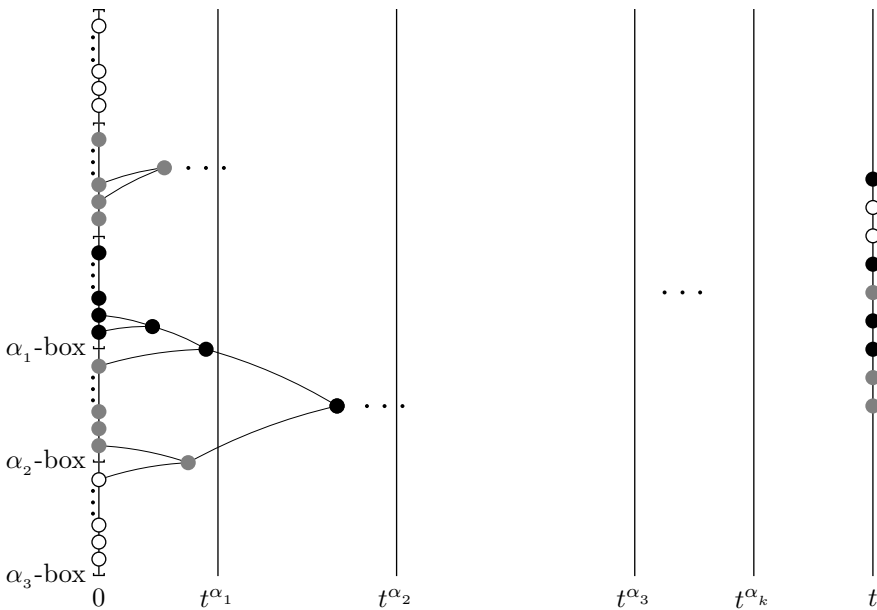


Figure 2

where $0 < \alpha_1 < \alpha_2 < \alpha_3$. We refer to $[-\sqrt{t^{\alpha_i}}, \sqrt{t^{\alpha_i}}]^2 \cap \mathbb{Z}^2$ as the α_i -box. Consider configurations of up to several (stochastically bounded, say) particles situated at each site of $[-\sqrt{t}, \sqrt{t}] \cap \mathbb{Z}^2$. We are interested in the state of the spatial coalescent started from the above configuration at time 0 and observed at time t .

It turns out (as we prove in [6]) that, for t large, after initial short period of coalescence, the remaining blocks in the α_i -box do not interact until the time t^{α_i} , and after this time they evolve approximately as the (non-spatial) Kingman coalescent, however with the logarithmic time change. An essential indication of this behavior is the Erdős-Taylor [4] formula for regular two-dimensional walks saying that, for $z \in \mathbb{R} \setminus \{(0, 0)\}$, and $0 < \gamma < \beta$

$$\lim_{t \rightarrow \infty} P^{zt^{\gamma/2}}(\text{the walk does not visit origin before time } t^\beta) = \frac{\gamma}{\beta} = e^{-\log(\beta/\gamma)}.$$

In Figure 2, the colors (shades) of the particles match on purpose those in Figure 1 to illustrate the correspondence between the **space** for the spatial coalescent (with no rebirth) and the **time** for the coalescent with rebirth.

A consequence of a general theorem from [6] is that, asymptotically as $t \rightarrow \infty$,

- 1) there is a diverging number of black blocks present in the system at time t^{α_1} ,
- 2) the black blocks interact among themselves according to a time-changed Kingman coalescent during the time interval $[t^{\alpha_1}, t^{\alpha_2}]$,
- 3) there is a diverging number of grey blocks present in the system at time t^{α_2} ,
- 4) the black and grey blocks interact jointly according to a time-changed Kingman coalescent during the time interval $[t^{\alpha_2}, t^{\alpha_3}]$,
- 5) there is a diverging number of white blocks present in the system at time t^{α_3} ,
- 6) all the blocks (black, grey and white) interact according to a time-changed Kingman coalescent during the time interval $[t^{\alpha_3}, t]$.

In conclusion, if one denotes by (N_t^b, N_t^g, N_t^w) the triple consisting of the numbers of black, grey and white blocks in the spatial coalescent system at time t , then

$$(N_t^b, N_t^g, N_t^w) \xrightarrow{t \rightarrow \infty} (K_0^{b;\log \alpha_1, \log \alpha_2, \log \alpha_3}, K_0^{g;\log \alpha_1, \log \alpha_2, \log \alpha_3}, K_0^{w;\log \alpha_1, \log \alpha_2, \log \alpha_3}),$$

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Spatially Structured Coalescents

NATHANAËL BERESTYCKI

(joint work with O. Angel, A. Hammond, V. Limic)

Many models from the field of mathematical population genetics lead to a description of the genealogical tree of a population by a coalescent process first introduced by Kingman in 1982 [3, 4], now known as Kingman's coalescent. A fascinating mathematical object, Kingman's coalescent has also permitted much important theoretical progress in population genetics. From a quantitative point of view, it serves as the basic model to evaluate genetic diversity in a well-mixed population at a neutral locus, and when an individual doesn't typically have a large number of offsprings. While this situation is now well-understood, there has been a lot of interest recently in trying to analyze more sophisticated models which depart from these oversimplifying hypotheses.

For instance, in the case where natural selection cannot be ignored (e.g., viral populations), or when there is large variation in the offspring distribution of a typical individual (e.g., marine species), there is convincing evidence that the use of coalescents which allow for *multiple collisions* is more appropriate than Kingman's coalescent. These processes, called Λ -coalescents, have been introduced and studied by Pitman [6] and Sagitov [7]. We defer to the next section for precise definitions and some background on these processes.

In this paper, we study spatially structured coalescent processes which describe the genealogy of a population when we also try to take into account geographic factors such as migration, isolation, etc. These processes, introduced by Limic and Sturm [5], bear the name of *spatial coalescents*. They can be informally described as follows. We are given a locally finite graph $G = (V, E)$, and we view each vertex $v \in V$ as the site of a colony. Each edge represents potential migratory routes between two adjacent colonies. Initially, we are given n particles on the graph, which represents in biological terms a sample of the population at the present time. When we follow the ancestral lineages of these individuals backward in time, two things can happen. Particles which are on the same site, coalesce according to some mechanism, be it Kingman's coalescent or, more generally, a Λ -coalescent. Simultaneously, every particle performs simple random walk in continuous time, with some given rate $\theta > 0$. These two rules reflect the idea that individuals typically reproduce within their own colony (so that only particles on the same site may coalesce), and occasionally there is a rare migration event, which corresponds to the random walk motion of particles. In the case where the coalescence mechanism is simply Kingman's coalescent, we note that this model bears close connections with Kimura's *stepping-stone model*.

Our main results give some information about the limiting behavior of this process as the size of the sample n tends to infinity, at both small and large time-scales. Our main results are in the case where at time $t = 0$ all particles are located at the origin o of G . The only general assumptions we make on G are that

it is connected and has bounded degrees, though some of our results give more detailed descriptions of the behaviour when G is the d -dimensional lattice.

Theorem. *Suppose the local coalescence is Kingman’s coalescent, and fix G and $t > 0$. Then there are constants $c, C > 0$ such that*

$$P \left(c \leq \frac{N^n(t)}{\text{Vol } B(o, \log^* n)} \leq C \right) \xrightarrow{n \rightarrow \infty} 1,$$

where $\text{Vol } B(o, r)$ is the volume of the ball of radius r around o .

Remark. *The function $\log^*(n)$ is the inverse of the tower function:*

$$(1) \quad \text{Tow}(n) = e^{\text{Tow}(n-1)} := \underbrace{e^{e^{\dots^e}}}_{n \text{ times}}.$$

Thus, $\log^*(n) = \inf\{m \geq 1 : \text{Tow}(m) \geq n\}$. The function $\log^*(n)$ tends to infinity with n , but at a very slow rate. For instance, when $n = 10^{78}$ (the total number of atoms in the universe), $\log^*(n) = 4$. For all practical purposes, $\log^*(n)$ is a constant equal to 3.

The behaviour in Theorem contrasts with the non-spatial case, where $N^n(t)$ is known to converge (without renormalization) to a finite random variable N_t . In the lattice case $G = \mathbb{Z}^d$, we see that $N^n(t)$ diverges as $\log^*(n)^d$, i.e. extremely slowly. Even on a regular tree, where the balls have maximal volume given the degrees, the volume is only $e^{c \log^*(n)}$.

Our next result deals with the biologically relevant case where the coalescence mechanism is not Kingman’s, but one known as the Beta-coalescent, with parameter $1 < \alpha < 2$. (See, e.g., [1, 2]). Our result is easier to state when the graph G is simply \mathbf{Z}^d . It states that for this process, the number of particles that survive up to a fixed constant time is of order $(\log \log n)^d$, rather than $(\log^* n)^d$ in the case of Kingman’s coalescent.

Theorem. *Let $1 < \alpha < 2$, and suppose the local coalescence is a Beta($2 - \alpha, \alpha$)-coalescent, and fix G and $t > 0$. Then there are constants $c, C > 0$ such that*

$$P \left(c \leq \frac{N^n(t)}{(\log \log n)^d} \leq C \right) \xrightarrow{n \rightarrow \infty} 1.$$

The next result concerns the case of more general Λ -coalescents. Our result states that no matter what the geometry graph G looks like, spatial coalescents are always globally divergent. Let $N^n(t)$ be the number of particles at time $t > 0$ when initially there was n particles at some given vertex o of G .

Theorem. *For any measure Λ and any infinite G and $t > 0$, we have $N^n(t) \rightarrow \infty$ almost surely as $n \rightarrow \infty$.*

This should be compared with the behaviour in the non-spatial case. There, $N^n(t)$ is either tight or diverges, depending on Λ . In the spatial case divergence is universal.

While the above theorems consider the state of the system at a fixed time t , we also give relatively precise estimates for the number of particles who survive for a long time. Here the diffusion of particles plays a more important role, and the results depend in a fundamental way on the underlying graph. We focus on the case $G = \mathbb{Z}^d$. When $d = 1, 2$ or 3 , this case bears special biological relevance. For instance, when $d = 1$, one should think of coastal marine species, since the coast is essentially a one-dimensional object. When the coalescence mechanism is Kingman's, our results take the following form.

Theorem. *Let $G = \mathbb{Z}^d$, let $m = \log^*(n)$, and fix $\delta > 0$. Then there exists some constants $c > 0$ and $C > 0$ (depending only on the d, δ) such that if $d > 2$*

$$\mathbb{P}\left(cm^{d-2} < N^n(\delta m^2) < Cm^{d-2}\right) \xrightarrow[n \rightarrow \infty]{} 1,$$

while if $d = 2$ then

$$\mathbb{P}\left(c \ln m < N^n(\delta m^2) < C \ln m\right) \xrightarrow[n \rightarrow \infty]{} 1.$$

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Structured population dynamics : the method of generalized entropy

BENOIT PERTHAME

The notion of Relative Entropy Inequality is standard for Markov processes and several linear Partial Differential Equations that are conservation laws written as parabolic, hyperbolic or integral equations.

Biological applications lead naturally to birth and death processes that can be described by zeroth order terms. They also lead to models where several structuring variables enter (age, size of individuals, physiological character or level of some proteins for cells) and several balance laws combine together (number of individuals, total biomass, total protein content) but no significant conservation law follows. Then the dynamics is strongly driven by these birth and death processes, more than by flux exchanges.

In this talk, we introduce the notion of General Relative Entropy Inequality that applies to PDEs that are not in conservation form. We show how the eigenelements come in the definition of the entropy and we give several types of applications of the General Relative Entropy Inequality: a priori estimates and existence of solution, long time asymptotic to a steady state or attraction to periodic solutions. This last point is motivated by the question: can tumor growth be seen as a lost of circadian control?

This talk is taken from papers with P. Michel, S. Mischler and L. Ryzhik; J. Clairambault and F. Bekkal-Brikci; J. Carrillo and S. Cuadrado.

Coagulation models with nonlocal drift

BARBARA NIETHAMMER

(joint work with M. Herrmann, P. Laurençot, J. Velázquez)

In this talk we consider models of the form

$$(1) \quad \partial_t f + \partial_x \left((x^\alpha u(t) - 1) f \right) = J(f, f)$$

where $f = f(x, t)$ is a number density of e.g. particles of size $x \in [0, \infty)$, $\alpha \in (0, 1]$ and $J(f, f)$ is a typical coagulation term of the form

$$(2) \quad J(f, f) = \frac{1}{2} \int_0^x K(x-y, y) f(x-y) f(y) dy - f(x) \int_0^\infty K(x, y) f(y) dy$$

with a symmetric coagulation kernel $K(x, y)$. The so-called mean-field $u(t)$ is a nonlocal term and determined by the constraint that the first moment of f is conserved, that is

$$(3) \quad \int_0^\infty x f(t, x) dx = \rho.$$

In particular we are interested in the two cases that

$$(1) \quad \alpha = 1/3 \quad \text{and} \quad K(x, y) = (x + y)/t$$

$$(2) \quad \alpha = 1 \quad \text{and} \quad K(x, y) = 2$$

Our motivation to investigate the first case is that the model has been suggested as a possible regularization of the classical LSW mean-field model [3, 7] for Ostwald Ripening; the second case we study as a simpler toy model.

The classical LSW model is a mean-field model to describe coarsening of particles interacting by diffusional mass exchange. Under the assumption that the volume fraction of particles is small and that then particles interact effectively only via a common mean-field, denoted by $u = u(t)$, the model is given by

$$(4) \quad \partial_t f + \partial_x \left((x^{1/3} u(t) - 1) f \right) = 0$$

$$(5) \quad \int_0^\infty x f dx = \rho \quad \text{that is} \quad u(t) = \frac{\int_0^\infty f dx}{\int_0^\infty x^{1/3} f dx}$$

One particular interest in the LSW-theory is the study of convergence of f to self-similar form. It can be easily calculated that (4)-(5) has a one parameter family of self-similar solutions, all with compact support. The largest support has that member of the family which is exponentially smooth, the others behave like a power law at the end of the support. It has been established in [4] that the long-time behavior of solutions to (4)-(5) depends very sensitively on the behavior of the data at the end of their support. For convergence to any of the self-similar solutions behaving like a power law it is necessary for the data to be regularly varying at the end of their support with the same power. Sufficiency of this condition could also be established under some restrictions (see [4, 5, 6]).

In order to overcome this so-called weak selection of self-similar asymptotic states it has been suggested in [3] to take the occasional merging of particles into account which has been neglected in the mean-field ansatz. This amounts to adding a coagulation term with a kernel which is additive in self-similar variables such that we obtain equation (1) with $\alpha = 1/3$, $K(x, y) = \frac{x+y}{t}$. To emphasize that the volume fraction of particles is small, we replace ρ by $\varepsilon \ll 1$ in (3).

Going over to self-similar variables, that is $f(x, t) = \varepsilon t^{-2} F(z)$, $z = x/t$ and $u = \lambda t^{-1/3}$ we find the following equation for self-similar solutions:

$$(6) \quad -(1 + z - \lambda z^{1/3})F' = (2 - \frac{\lambda}{3}z^{-2/3})F + \varepsilon \left(\frac{1}{2}F \star F - F - zFm_0(F) \right)$$

with $F \star F(x) = \int_0^x F(x-y)F(y) dy$ and $m_0(F) = \int_0^\infty F(y) dy$.

As described before, for $\varepsilon = 0$ there exists one self-similar solution that is exponentially smooth. We call it F_{LSW} , it has support in $[0, 1/2]$ and a corresponding value of λ which is $\lambda_{LSW} = 3 \cdot 2^{2/3}$.

Lifshitz and Slyozov treat the coagulation term in (6) as a perturbation and construct an approximation of a solution by plugging F_{LSW} into and solve the resulting inhomogeneous linear ODE. Via asymptotic analysis they also found that the corresponding λ satisfies $\lambda_{LSW} - \lambda = O(1/\ln|\varepsilon|^2)$, that is the deviation of the mean-field is quite large. However, this construction leads only to an approximation of a solution, if indeed a fast decaying solution exists at all. Since this is not clear a-priori, a rigorous proof of the existence – and possibly uniqueness – of such a solution seems desirable. By setting up an appropriate fixed-point problem, we are able to show the following

Theorem [2] For any sufficiently small $\varepsilon > 0$ there exists a unique self-similar solution F_λ to (6) with $\lambda_0 - \lambda \sim \frac{1}{|\ln \varepsilon|^2}$ and which decays exponentially.

We should emphasize that uniqueness is only claimed within the class of fast decaying solutions, strictly speaking, the decay is of the order $\frac{1}{z^\gamma} e^{-Lz}$ where $\gamma > 1$ and L is sufficiently large.

Furthermore, we conjecture, that also solutions with algebraic decay exist. However, at this stage, our methods are not yet sufficient to prove this statement.

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Scaling dynamics in solvable models of coagulation

ROBERT PEGO

(joint work with Govind Menon)

We discuss the dynamical behavior of several mean-field models of coagulation that are ‘solvable’ in the sense that the Laplace transform converts the evolution equation for size distribution into a first-order PDE that can be studied by the method of characteristics. These models include Smoluchowski’s coagulation equations with rate kernels $K(x, y) = 2$, $x + y$ and xy , and models of ‘min-driven’ coagulation in which the smallest cluster combines with k others at random with probability p_k . The latter class of models was recently shown to be solvable by Gallay and Mielke [2] using a remarkable linearizing transformation.

In these models of coagulation, typical cluster size grows without bound as time progresses, and we must rescale to study nontrivial long-time dynamics. We aim to address the following issues:

- What scaling solutions exist? Here we seek *self-similar solutions*, or fixed points of the dynamics modulo scaling.
- What are the domains of attraction of these scaling solutions? These comprise the *universality classes* for dynamic scaling.
- What limit points are possible under scaling dynamics in general? We call the set of such points the *scaling attractor* of the system.
- How can we describe the dynamics on the scaling attractor? We call this the *ultimate dynamics* of the system.
- How complicated can the ultimate dynamics be?

While this is evidently stated in dynamical terms, there is a deep analogy with classical limit theorems of probability theory, related to the central limit theorem, stable laws, and infinite divisibility.

Our results for Smoluchowski’s equations appear in [3], [4] and [6]. Due to work of Carrasco & Duchon and Bertoin that established a rigorous connection between the kernel $K = x + y$ and Burgers turbulence model, in [5] we were able to classify domains of attraction for solutions of $u_t + uu_x = 0$ whose increments form a one-sided Lévy process with no positive jumps.

Associated with a size distribution measure solution ν_t of Smoluchowski's equation is a probability measure with distribution function

$$F_t(x) = \int_{(0,x]} y^\gamma \nu_t(dy) / \int_{(0,\infty)} y^\gamma \nu_t(dy)$$

($\gamma = 0, 1$, or 2 for $K = 2$, $x + y$ and xy resp.), and the dynamics defines an evolution on the space \mathcal{P} of probability measures on $(0, \infty)$ (prior to the gelation time for the xy kernel). Addressing the questions above we have the following results.

- *Scaling solutions.* Up to normalization, there is a one-parameter family of self-similar solutions, corresponding to distribution functions written $F_{\rho,\gamma}$ for $0 < \rho \leq 1$, $\gamma \in \{0, 1, 2\}$. The endpoint $\rho = 1$ delivers the unique (and classically-known) self-similar solution with finite $\gamma + 1$ st moment, and this solution has exponential decay as $x \rightarrow \infty$. For $0 < \rho < 1$, the solutions have infinite $\gamma + 1$ st moment and are directly related to important heavy-tailed distributions of probability theory — Mittag-Leffler distributions for $K = 2$, and Lévy stable laws of maximum skewness for $K = x + y$ and xy . For $K = x + y$ these solutions were first discovered by Bertoin by a different argument [1].
- *Domains of attraction.* The classical self-similar solution with $\rho = 1$ attracts all solutions with finite $\gamma + 1$ st moment in the weak topology. In general, the domains of attraction of self-similar solutions are characterized by the power-law behavior (more precisely, regular variation) of the $\gamma + 1$ st moment distribution: An initial size distribution measure ν_0 lies in the domain of attraction of the self-similar solution $F_{\rho,\gamma}$ if and only if

$$\int_0^x y^{\gamma+1} \nu_0(dy) \sim x^{1-\rho} L(x), \quad x \rightarrow \infty,$$

for some function L slowly varying at ∞ . There are no other self-similar solutions or domains of attraction.

- *Scaling attractor.* The (proper) scaling attractor corresponds in one-to-one fashion with eternal solutions of Smoluchowski's equation, and these have a Lévy-Khintchine representation for each solvable kernel, as established first for $K = x + y$ by Bertoin [1]. This parametrizes the set of scaling limit points in terms of measures satisfying certain finiteness conditions. The measures can be described as backward-in-time limits of eternal solutions scaled to preserve the $\gamma + 1$ st moment (if finite). E.g., for $K = x + y$ the measure H corresponding to an eternal solution ν_t satisfies

$$\int_{[0,x]} H(dy) = \lim_{t \rightarrow -\infty} \int_{[0,x]} y^2 \nu_t(e^t dy)$$

at each point of continuity.

- *Ultimate dynamics.* The Lévy-Khintchine representation *linearizes the dynamics on the attractor*. As a consequence of basic scaling properties of Smoluchowski's equation, nonlinear evolution on the attractor is conjugate

to a group of simple scaling transformations on the measures that generate the representation. E.g., for $K = x + y$, if a distribution F_0 on the scaling attractor evolves to F_t , then the corresponding measure H_0 evolves to

$$H_t(dx) = e^{2t} H_0(e^{-t} dx).$$

This representation makes precise the sensitive dependence of long-time dynamics on the tails of the initial size distribution—the ultimate dynamics on the scaling attractor is conjugate to a continuous dilation map.

- *Chaos.* We use the Lévy-Khintchine representation to construct orbits with complicated dynamics. The scaling attractor contains a dense family of scaling-periodic solutions. Furthermore, there are eternal solutions with trajectories *dense* in the scaling attractor — we call these *Doebelin solutions* by analogy with Doebelin’s universal laws in probability. And, for any given scaling trajectory, there is a dense set of initial data whose forward trajectories shadow the given one.

In addition, we find that Smoluchowski dynamics “compactifies” in a natural way that accounts for clusters of negligible and infinite size (dust and gel). Considering defective limits on $(0, \infty)$ that concentrate probability at 0 and ∞ yields a well-posed dynamics of “extended solutions” on $[0, \infty]$. Proper solutions remain fundamental, but considering extended solutions with dust and gel yields dynamics on a compact, metrizable space. We obtain an asymptotic shadowing result that for any two initial size distributions with the same large-tail behavior, under an arbitrary time-dependent scaling the distance between the rescaled solutions tends to zero as time grows.

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Convergence to self-similarity in addition models with input of monomers

FERNANDO PESTANA DA COSTA

(joint work with J.T. Pinto, R. Sasportes, H. van Roessel, J.A.D. Wattis)

We are interested in studying the large j and t limit of solutions to the system

$$(1) \quad \begin{cases} \dot{c}_1 &= J_1(t) - c_1^2 - c_1 \sum_{j=1}^{\infty} j^p c_j \\ \dot{c}_j &= j^{p-1} c_1 c_{j-1} - j^p c_1 c_j, \quad j \geq 2. \end{cases}$$

where $p < 1$, the input of monomers $J_1(t)$ satisfy $J_1(t) = (1 + \varepsilon(t))\alpha t^\omega$, and the continuous function $\varepsilon(t)$ converge to zero as $t \rightarrow +\infty$.

From now on we will consider only the case $p = 0$. We shall return to the more general case in the end. The main idea used in this study is the following: by defining a new variable $c_0 = \sum_{j=1}^{\infty} c_j$, we can decouple system (1) into a bidimensional system

$$(2) \quad \begin{cases} \dot{c}_0 &= J_1(t) - c_0 c_1 \\ \dot{c}_1 &= J_1(t) - c_0 c_1 - c_1^2, \end{cases}$$

and an infinite dimensional one that, upon the change in time scale $t \mapsto \varsigma(t) := \varsigma_0 + \int_{t_0}^t c_1(s) ds$, becomes the lower triangular linear system

$$(3) \quad \tilde{c}_j' = \tilde{c}_{j-1} - \tilde{c}_j, \quad j \geq 2,$$

where $\tilde{c}_j(\varsigma) := c_j(t(\varsigma))$.

Since (3) can be explicitly solved in terms of \tilde{c}_1 , namely

$$(4) \quad \tilde{c}_j(\varsigma) = e^{-\varsigma} \sum_{k=2}^j \frac{\varsigma^{j-k}}{(j-k)!} c_k(0) + \frac{1}{(j-2)!} \int_0^\varsigma \tilde{c}_1(\varsigma-s) s^{j-2} e^{-s} ds,$$

and the asymptotic behaviour of c_1 is determined by (2), our problem is reduced to that of determining the detailed asymptotic behaviour of solutions to the (generally non-autonomous) bidimensional ODE (2), and to the evaluation of an appropriate asymptotic behaviour of (4).

In all cases we have considered, the asymptotic evaluation of (4) follows essentially similar lines, that were first developed for the autonomous input case, $\omega = 0, \varepsilon(t) \equiv 0$, in [5]. The main differences between this one and the other, non-autonomous, cases are in the way the needed information about c_1 is extracted from (2).

In the autonomous case ($\omega = 0, \varepsilon(t) \equiv 0$) the main tools used were invariant regions, together with a compactification and a centre manifold argument [5], although the same result could be achieved using only invariant regions and monotonicity arguments [1].

Neither of these approaches work well in the non-autonomous cases. We start the study of these cases by making use of an ansatz about the behaviour of solutions

obtained by Wattis [7] by means of formal arguments. This ansatz suggests a change of variables to be applied to (2) in order to fix the prospective limit point (as $t \rightarrow +\infty$). Then, an analysis using differential inequalities and qualitative theory methods is applicable [2, 4]. The main is the following

Theorem. Let $p = 0$, $J_1(t) = (1 + \varepsilon(t))\alpha t^\omega$, where $\alpha > 0$, $\omega > -\frac{1}{2}$, and $\varepsilon(t)$ is a continuous function satisfying $\varepsilon(t) \rightarrow 0$ as $t \rightarrow +\infty$. Define $Q_0(\omega) := \left(\frac{3}{(1+2\omega)\alpha}\right)^{\frac{1}{2+\omega}} \left(\frac{2+\omega}{3}\right)^{r_0}$, where $r_0 := \frac{1-\omega}{2+\omega}$. Let (c_j) be any solution of (1) with initial data $c_j(0) \in \ell_1$. Let $\varsigma(t)$ and $\tilde{c}_j(\varsigma)$ be as above. Then

- (i): $\lim_{\substack{j, \varsigma \rightarrow +\infty \\ \eta = j/\varsigma \text{ fixed} \\ \eta \neq 1}} Q_0(\omega) \varsigma^{r_0} \tilde{c}_j(\varsigma) = \Phi_{1,\omega}(\eta) := \begin{cases} (1 - \eta)^{-r_0} & \text{if } \eta < 1 \\ 0 & \text{if } \eta > 1, \end{cases}$
- (ii): furthermore, if $c_j(0) = 0$ for $j \geq 2$,

$$\lim_{\substack{j, \varsigma \rightarrow +\infty \\ \xi = \frac{j-\varsigma}{\sqrt{\varsigma}} \text{ fixed} \\ \xi \in \mathbb{R}}} \left(\frac{\pi}{2}\right)^{\frac{1}{2}} Q_0(\omega) \varsigma^{\frac{1}{2}r_0} \tilde{c}_j(\varsigma) = \Phi_{2,\omega}(\xi) := e^{-\frac{1}{2}\xi^2} \int_0^{+\infty} y^{1-2r_0} e^{-\xi y^2 - \frac{1}{2}y^4} dy.$$

In Figure 1 we present plots of the similarity limits given in Theorem for several values of ω . Note that the profiles of $\Phi_{2,\omega}$ provide a kind of inner expansion of the jump discontinuities occurring in the profiles of $\Phi_{1,\omega}$ when $\omega \leq 1$.

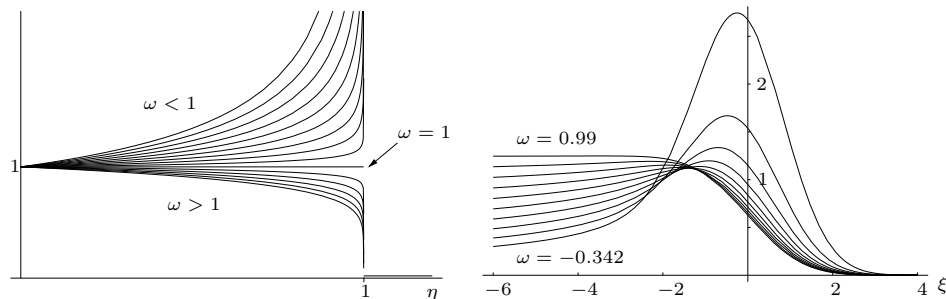


FIGURE 1. Graphs of the similarity limits in Theorem .
 Left: $\Phi_{1,\omega}$ for values of ω below and above 1 in steps of 0.1;
 Right: $\Phi_{2,\omega}$ for ω from -0.342 to 0.99 in steps of 0.148 .

The slow input cases ($\omega < -\frac{1}{2}$), as well as the borderline case $\omega = -\frac{1}{2}$, have also been studied, although a completely satisfactory understanding of what is going on is still missing [3, 6].

The extension of these results to non-constant coagulation kernels $p \neq 0$ was obtained at a formal level [8], but attempts to turn it rigorous have, so far, been marred by a number of difficulties. We believe the following holds:

Conjecture 1. Let $p < 1$, $J_1(t) = \alpha t^\omega$, where $\alpha > 0$, and $\omega > -\frac{1}{2}$. For every solution (c_j) of (1) with initial data satisfying $\exists \rho > 0, \mu > r + p : \forall j, c_j(0) \leq \rho/j^\mu$, consider $\tilde{c}_j(\zeta)$ as previously defined, where now $\zeta(t) = \left(\frac{Q_p(\omega)(3-2p)}{2+\omega}\right)^{\frac{1}{1-p}} t^{\frac{2+\omega}{3-2p}}$, where $Q_p(\omega)$ is a known function of ω . Then, there exist constants $A(\omega, p)$ such that, with $r_p = \frac{1-\omega(1-p)}{(2+\omega)(1-p)}$, the following holds true:

$$\lim_{\substack{j, \zeta \rightarrow +\infty \\ \eta = j/\zeta \text{ fixed} \\ \eta \neq 1}} A(\omega, p) \zeta^{r_p} \tilde{c}_j(\zeta) = \Phi_{1, \omega, p}(\eta) := \begin{cases} \eta^{-p} (1 - \eta^{1-p})^{-r_p} & \text{if } \eta < 1, \\ 0 & \text{if } \eta > 1. \end{cases}$$

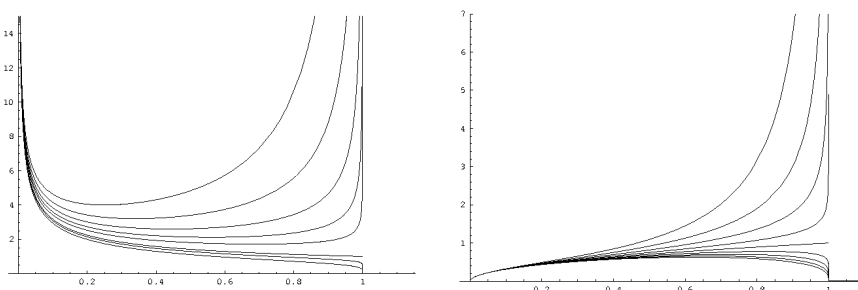


FIGURE 2. Graphs of $\Phi_{1, \omega, p}$ for $p > 0$ (left) and $p < 0$ (right), for several values of ω . Since $\Phi_{1, \omega, 0} \equiv \Phi_{1, \omega}$, the $p = 0$ case is in Figure 1.

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Some exact solutions to the coagulation equation with product kernel

HENRY VAN ROESSEL

(joint work with Mazi Shirvani, Claudia Calin)

1. INTRODUCTION

We consider the continuous version of the coagulation equation

$$(1) \quad \frac{\partial c}{\partial t}(\lambda, t) = \frac{1}{2} \int_0^\lambda K(\lambda - \mu, \mu) c(\lambda - \mu, t) c(\mu, t) d\mu - c(\lambda, t) \int_0^\infty K(\lambda, \mu) c(\mu, t) d\mu,$$

$$c(\lambda, 0) = c_0(\lambda),$$

with a non-homogeneous coagulation kernel of the form

$$(2) \quad K(\lambda, \mu) = \theta(\lambda)\theta(\mu), \quad \theta(\lambda) = \alpha + \beta\lambda, \quad \alpha, \beta \geq 0,$$

where $c(\lambda, t)$ represents the concentration of particles of size λ at time t . The vast majority of the literature on coagulation equations, with a some notable exceptions [3, 7, 10], deal with coagulation kernels that are homogeneous. The kernel in Eq. (2) contains both the constant kernel and the homogeneous product kernel as special cases. For this kernel it is well known that gelation occurs in finite time if and only if $\beta > 0$. Various models of gelation formation have been proposed. The one adopted here assumes that after a critical time (the gelation time), the coagulation process transfers large particles to a “super particle” or “gel” and that this gel does not interact with the pre-gel (or sol) particles. This model of gelation is usually referred to as the Stockmayer [8] model. See Ziff and Stell [10] and Lushnikov [4, 5, 6] for a discussion of other gelation models.

We use Laplace transforms to analyse the coagulation equation. While transforming (1) to a PDE by means of Laplace transforms is not new (see Leyvraz [2] for a review), it has recently been shown [9] that such a formulation can be used to reduce the problem for the post-gelation mass to an ordinary differential equation depending only on α, β and on the initial data. In some instances, this ODE can be solved explicitly, and, in a few rare cases, the solution of the post-gelation mass can then be used to obtain the explicit solution to (1).

2. FORMULATION AS A PDE

We will use Laplace transforms to convert Eq. (1) to a first-order quasilinear partial differential equation. Before doing so, however, it is convenient to make a change of variables and to re-write the equation in a slightly different form. Let us define

$$N(t) := \int_0^\infty \theta(\lambda) c(\lambda, t) d\lambda = \alpha M_0(t) + \beta M_1(t),$$

where $M_n(t) := \int_0^\infty \lambda^n c(\lambda, t) d\lambda$ represents the n^{th} moment of the solution. Now change variables from $c(\lambda, t)$ to $f(\lambda, t)$ as follows:

$$f(\lambda, t) := e^{\theta(\lambda)Q(t)} c(\lambda, t), \quad \text{where} \quad Q(t) := \int_0^t N(s) ds.$$

Then equation (1) becomes:

$$(3) \quad \frac{\partial f}{\partial t}(\lambda, t) = \frac{1}{2} e^{-\alpha Q(t)} \int_0^\lambda \theta(\lambda - \mu) \theta(\mu) f(\lambda - \mu, t) f(\mu, t) d\mu, \quad f(\lambda, 0) = c_0(\lambda).$$

Define the following Laplace transforms:

$$F(x, t) := \mathfrak{L}[\theta(\lambda) f(\lambda, t)] := \int_0^\infty e^{-\lambda x} \theta(\lambda) f(\lambda, t) d\lambda; \quad h(x) := \mathfrak{L}[\theta(\lambda) c_0(\lambda)].$$

Multiply Eq. (3) by $e^{-\lambda x}$ and integrate to obtain the following first-order, quasi-linear PDE for the transform function F :

$$(4) \quad e^{\alpha Q(t)} \frac{\partial F}{\partial t} + \beta F \frac{\partial F}{\partial x} = \frac{\alpha}{2} F^2, \quad F(x, 0) = h(x).$$

Equation (4) is unusual in that the function Q that appears in the first coefficient is itself unknown and must be determined as part of the solution. From the definition of Q one may easily show that it must satisfy the following ‘‘compatibility condition:’’

$$(5) \quad Q'(t) = e^{-\alpha Q(t)} F(\beta Q(t), t), \quad Q(0) = 0.$$

The coupled system of equations (4) and (5) must be solved simultaneously.

For $\beta > 0$, Eq. (4) will exhibit a shock, which is known to coincide with the occurrence of gelation. In the pre-shock (or pre-gelation) regime, analysis of the problem is straight forward and the moments M_0 and M_1 are easily computed. To compute these moments in the post-gelation regime is more problematic. However, one can show that the problem of computing the moments in the post-gelation regime can be reduced to the following ODE:

$$(6) \quad r' = \frac{\beta^2 h'^2(r)}{\beta h''(r) - \frac{\alpha}{2} h'(r)} e^{-\alpha r/\beta}, \quad r(t_0) = 0,$$

where t_0 is the gelation time. The post-gelation moments (i.e. for $t \geq t_0$) are explicitly given in terms of the solution to Eq. (6):

$$(7) \quad M_0(t) = \frac{\beta C_0(r(t)) C_0''(r(t)) - \frac{1}{2} [\alpha C_0(r(t)) + \beta C_0'(r(t))] C_0'(r(t))}{\frac{\alpha^2}{2} C_0(r(t)) - \frac{3}{2} \alpha \beta C_0'(r(t)) + \beta^2 C_0''(r(t))} \beta e^{-\frac{\alpha}{\beta} r(t)},$$

$$(8) \quad M_1(t) = -C_0'(r(t)) e^{-\frac{\alpha}{\beta} r(t)},$$

where $C_0(x) = \mathfrak{L}[c_0(\lambda)]$. For the case $\alpha = 0$, Eqs. (7) and (8) reduce to

$$M_0(t) = C_0(r(t)) - \frac{1}{2} \beta^2 t C_0'^2(r(t)), \quad M_1(t) = -C_0'(r(t)).$$

Lushnikov [6] has obtained an analogous formula for M_0 for the discrete, homogeneous kernel $K_{ij} = 2ij$.

3. EXACT SOLUTIONS

Having determined the post-gelation moments M_0 and M_1 of the solution, the next step is to determine F and then to take inverse Laplace transforms to get a solution to Eq. (1). This is not easily done. Only for $\alpha = 0$ have we managed to obtain exact solutions. Two examples follow, in both cases we take $\beta = 1$. In first example we recover the solution obtained by Ernst et al [1]. The solution in the second example is, as far as we know, new and has not appeared before in the literature.

Example 1. For $c_0(\lambda) = \frac{e^{-\lambda}}{\lambda}$ we get $h(x) = \mathfrak{L}[\lambda c_0(\lambda)] = \frac{1}{1+x}$, which leads to

$$M_1(t) = \begin{cases} 1, & 0 \leq t < 1 \\ \frac{1}{\sqrt{t}}, & t \geq 1 \end{cases}, \quad F(x, t) = \frac{2}{1+x+\sqrt{(1+x)^2-4t}},$$

and finally to the exact solution obtain by Ernst et al [1].

$$c(\lambda, t) = \frac{e^{-(1+Q(t))\lambda}}{\lambda^2 \sqrt{t}} I_1(2\lambda\sqrt{t}),$$

where I_1 is the modified Bessel function of order 1.

Example 2. Let $a > b \geq 0$ and $k := \sqrt{a^2 - b^2}$. Then for $c_0(\lambda) = \frac{ke^{-a\lambda}}{\lambda^2} I_1(k\lambda)$ we get $h(x) = x + a - \sqrt{(x+a)^2 - k^2}$, which leads to

$$M_1(t) = \begin{cases} a-b, & 0 \leq t < \frac{b}{a-b}, \\ \frac{k}{\sqrt{1+2t}}, & t \geq \frac{b}{a-b}, \end{cases}, \quad F(x, t) = \frac{x+a-\sqrt{(x+a)^2-k^2(1+2t)}}{1+2t},$$

and finally to the exact solution:

$$c(\lambda, t) = \frac{ke^{-(a+Q(t))\lambda}}{\lambda^2 \sqrt{1+2t}} I_1(k\lambda\sqrt{1+2t}).$$

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Similarity Solutions for Coagulation Equations

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(joint work with Henry J. van Roessel, Mazi Shirvani)

We perform an analysis for investigating the symmetry groups for the Smoluchowski coagulation equation where the rate of production of particles is a bilinear, separable function of the form $K(\lambda, \mu) = (\alpha + \beta \lambda)(\alpha + \beta \mu)$, with $\alpha, \beta \geq 0$ arbitrary constants, under the assumption that new particle source terms are included into the coagulating system in the form of a nonnegative function $g(\lambda, t) \geq 0$ satisfying certain integrability conditions:

$$\begin{aligned} \frac{\partial c}{\partial t}(\lambda, t) &= \frac{1}{2} \int_0^\lambda K(\lambda - \mu, \mu) c(\lambda - \mu, t) c(\mu, t) d\mu - c(\lambda, t) \int_0^\infty K(\lambda, \mu) c(\mu, t) d\mu \\ &\quad + g(\lambda, t) \\ c(\lambda, 0) &= c_0(\lambda), \quad \text{where the size and time variables range in } \lambda, t \in [0, \infty). \end{aligned}$$

The study related to the symmetry groups for the coagulation equation has not received much attention in the literature. The main difficulty for developing such a study is related to the existence of the integral terms in these equations, in particular the nonlinear convolution integral. We are interested in modeling a key aspect of the coagulation theory, namely the asymptotic behavior of solutions to the coagulation equation with particle source terms for large particle sizes $\lambda \rightarrow \infty$ and all times $t \geq 0$ and also the long time behavior of such solutions and the total mass.

We present two methods that provide us with similarity solutions for the coagulation equation in the presence of particle source terms. Similarity solutions have played an important role in the analysis of qualitative properties of solutions of nonlinear problems. These two methods provide a new family of exact and asymptotic solutions to the coagulation equations which can be further used for numerical studies.

The first method is an indirect method applied to a partial differential equation associated to a new modified form of the coagulation equation and determines a local Lie group of transformations that leaves the PDE invariant. This method is based on the classical technique for investigating Lie symmetry groups of differential equations that were introduced by Sophus Lie. The advantage over previous methods is that in some special cases the expression of the total mass does not need to be known in advance. Based on this method we verified the previous solution obtained by Ernst et al [3] and also obtained new exact and asymptotic solutions for the case when new particle source terms are included in the coagulating system. The method that we provide is more general and its applicability is by far preferred.

To illustrate the first method we present two examples of new exact and asymptotic solutions for the coagulation equation (see below).

Example 1. If the coagulation kernel $K(\lambda, \mu) = \lambda \mu$, the initial condition

$$c_0(\lambda) = \frac{q e^{-a\lambda}}{p\lambda^2} \cdot I_1(p\lambda) \quad \text{and} \quad g(\lambda, t) = 0$$

then the solution $c(\lambda, t)$ to the coagulation equation

$$c(\lambda, t) = \frac{q e^{-(a+Q(t))\lambda}}{\lambda^2 \sqrt{2qt + p^2}} \cdot I_1(\lambda \sqrt{2qt + p^2})$$

where $a, q, p > 0$ are arbitrary constants and

$$Q(t) = \int_0^t M_1(\tau) d\tau = \begin{cases} \frac{q}{p^2} (a - m) t & \text{for } 0 \leq t < T_{gel} \\ \sqrt{2qt + p^2} - a & \text{for } t \geq T_{gel} \end{cases}$$

Here $T_{gel} = \frac{mp^2}{q(a-m)}$ represents the gelation time (see e.g. [4] for the definition of the gel-time), where $m = \sqrt{a^2 - p^2}$ and $a > p > 0$.

Example 2. If the coagulation kernel $K(\lambda, \mu) = \lambda \mu$, the initial condition

$$\lambda c_0(\lambda) = \frac{2b}{a} \cdot \mathcal{L}^{-1} \left\{ 1 - \sqrt{1 - \frac{a^4}{2b^2} \cdot e^{-x}} \right\}(\lambda) \quad \text{or} \quad c_0(\lambda) \approx \frac{b}{a\sqrt{\pi}} \lambda^{-5/2}$$

and the source term

$$\lambda g(\lambda, t) = a^2 e^{\frac{2b}{a}t} e^{-\lambda Q(t)} \delta(\lambda - 1)$$

where a, b are some arbitrary constants such that $a \cdot b > 0$ and $\frac{a^4}{2b^2} \leq 1$ then the asymptotic behavior of the solution is given by

$$c(\lambda, t) \approx e^{-\lambda Q(t)} \frac{b}{a\sqrt{\pi}} \lambda^{-5/2} \text{ as } \lambda \rightarrow \infty, \text{ and } \forall t \geq 0$$

where $\gamma := \frac{a^4}{2b^2}$, $A := 1 + \sqrt{1 - \gamma}$ and $Q(t) = \int_0^t M_1(\tau) d\tau$.

The total mass is given by

$$M_1(t) := \begin{cases} \frac{4b\gamma}{a} \cdot \frac{e^{\frac{b}{a}t}}{A^2 e^{-\frac{b}{a}t} + \gamma e^{\frac{b}{a}t}} & \text{if } 0 \leq t < T_{gel} \\ \frac{2b}{a} & \text{if } t \geq T_{gel} \end{cases}$$

if $\gamma < 1$, where $T_{gel} = \frac{a}{2b} \ln(\frac{A^2}{\gamma})$ represents the gelation time. If $\gamma = 1$ then the gelation occurs instantaneously.

The second method is a new generalized version of the direct methods that determine the symmetry group of the point transformations to integro-differential equations. The existence of symmetry groups for integro-differential equations with non-local structure has been developed only recently in the work of Akhieiev et al. [1] and Zawistowski [5]. Applications of this method are currently provided for a few classes of IDEs such as, Vlasov-Maxwell equations, Collisionless-Boltzmann equations and fragmentation equation. The study of existence of symmetry groups

for the coagulation equations with a general kernel has not been provided in the literature.

Our purpose is to extend the direct methods proposed by Akhieiev et al. [1] that determine the symmetry group of the point transformations to IDEs to a modified form of the coagulation equation. We have obtained a more general method for determining the symmetry groups for the coagulation equation. The advantage of this method over the previous methods used in the self-similarity theory is that new similarity solutions can be obtained for a general coagulation kernel, no special ansatz and structure of the scaling solutions to the coagulation equation being assumed a priori. Based on this method we obtained new similarity solutions to the coagulation equation for the constant and product kernels for the case when particle source terms have a similarity form. In addition, we considered the case when α and β are nonnegative, time dependent functions. Moreover, we also applied this second method directly to the original, unmodified version of the coagulation equation.

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Coagulation, Fragmentation and Growth Processes in Size Structured Population

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(joint work with W. Lamb)

Phytoplankton can be studied at different levels. Individual-based models, which can be thought of providing ‘microscopic’ models, track random motion and division of individual particles, see e.g. [3, 9, 10]. A ‘macroscopic’ description is provided by advection-diffusion-reaction equations describing concentrations (densities) of individual particles, see [8]. The model which we study can be considered to be in between, on a ‘mesoscopic’ scale, in that it recognizes the role played by the phytoplankton aggregates which are individual building blocks labelled by their size. Thus, we describe the phytoplankton using the aggregate density function $u(x, t)$ which gives the number density of aggregates of size x satisfying $0 \leq x_0 \leq x \leq x_1 \leq \infty$; that is, ‘consisting’ of x individual building blocks (we consider here x to be a continuous variable) at time t . Such a model,

fitting into a broad coagulation-fragmentation theory, can be obtained from the individual-based by appropriate limit passage (see e.g., [9, 10]) or derived from first principles, as in e.g. [7, 4, 1, 2]. In this model the aggregates grow due to division of single cells, can split and coalesce. Furthermore, drawing on some earlier works, the authors assume that all daughter cells fall off the aggregates and, joining the single cell population, enter the system as new aggregates. This results in the model described by the classical fragmentation-coagulation equation coupled with the McKendrick-von Foerster renewal model:

$$\begin{aligned}
 \partial_t u(x, t) &= -\partial_x(r(x)u(x, t)) - \mu(x)u(x, t) \\
 &\quad - a(x)u(x, t) - \int_x^{x_1} a(y)b(x|y)u(y, t)dy \\
 &\quad + u(x, t) \int_{x_0}^{x_1} k(x, y)u(y, t)dy + \frac{1}{2} \int_{x_0}^{x-x_0} k(x-y, y)u(x-y, t)u(y, t)dy, \\
 r(x_0)u(x_0, t) &= \int_{x_0}^{x_1} \beta(y)u(y, t)dy, \\
 (1) \quad u(x, 0) &= u_0(x).
 \end{aligned}$$

The functions β , r and μ represent, respectively, the rate at which daughter cells enter the single cell population, the rate of the increase of size x aggregate due to daughter cells remaining in the aggregate and, finally, the rate of the removal of cells due to death of cells or sinking. The ‘stickiness function’ $k(x, y)$ represents the likelihood of an aggregate of size x sticking to an aggregate of size y ; we assume that $k \in L_\infty([x_0, x_1] \times [x_0, x_1])$. Further, we assume that the number of daughter particles is bounded and that the processes conserve mass. In our considerations the function μ is bounded, and r and a are sublinear with $1/r$ integrable close to x_0 . The analysis is carried out in the space $X = L_1([x_0, x_1], (1+x)dx)$, which keeps track of both the number of aggregates and the total number of cells in the ensemble.

Analysis of the linear part of the problem, consisting of the growth term with the renewal boundary conditions and the fragmentation term, is only non-trivial if $x_1 = \infty$ and a is unbounded. It can be proved that the introduced assumptions allow to reduce the linear part so that it fits into the framework of the substochastic semigroup theory [6] and to show that its’ appropriate realization generates a positive semigroup in X .

The nonlinear part is treated as a semilinear perturbation of the linear problem. Due to quadratic character, the coagulation term is Frechét differentiable which ensures strong local solvability of (1). In the next step, by rescaling, we are able to prove that the solution is nonnegative on its interval of existence. This allows to control the norm of the solution and, consequently, prove the existence and uniqueness of a global in time strong positive solution to (1), see [5].

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Some applications of spinal decompositions of fragmentation trees

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(joint work with Grégory Miermont, Jim Pitman, Matthias Winkel)

Self-similar fragmentation trees are Continuum Random Trees (\mathcal{T}, μ) that naturally arise ([5]) as genealogical trees of self-similar fragmentation processes, as introduced by Bertoin ([1],[2]). Given a sample of labeled leaves according to μ , we call *spine* the path from the root to the leaf labeled 1. Deleting each edge along this spine defines a graph whose connected components define the (coarse) spinal decomposition of the tree. We give two examples of applications we obtain by studying some properties of this spinal decomposition.

- (1) **Asymptotics of consistent families of Markov branching models** [6]. Let $(T_n, n \geq 1)$ be a family of rooted combinatorial trees with n leaves labeled $\{1, 2, \dots, n\}$. This family is said to be *consistent* if the restricted tree obtained from T_n by considering the leaves $\{1, 2, \dots, n-1\}$ and the root is distributed as T_{n-1} . It possesses the *Markov branching property* if given that the unique branchpoint neighboring the root connects $r \geq 2$ subtrees, say τ_1, \dots, τ_r with, respectively, k_1, \dots, k_r leaves, the subtrees τ_1, \dots, τ_r are independent and distributed, respectively, as T_{k_1}, \dots, T_{k_r} . Under some additional assumptions of regular variation type, we identify some self-similar fragmentation trees as scaling limits of consistent Markov branching models, where the discrete trees have been endowed with edge-lengths 1.

- (2) **Invariance under uniform re-rooting** [7]. It has been shown by Miermont [8] that the stable trees of Duquesne and Le Gall [3] belong to the family of self-similar fragmentation trees. These stable trees are also known to possess an interesting symmetry property of *invariance under uniform re-rooting* (cf. [4]). Informally, this means that taking a leaf at random according to μ and considering \mathcal{T} rooted at this random leaf, gives a CRT with the same distribution as the original CRT with its original root. Using the spinal decomposition, we show that, up to a scaling factor, stable trees are the only self-similar fragmentation trees that are invariant under uniform re-rooting.

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The size of random fragmentation trees

SVANTE JANSON

(joint work with Ralph Neininger)

We consider the random fragmentation process introduced by Kolmogorov, where a particle having some mass is broken into pieces and the mass is distributed among the pieces at random in such a way that the proportions of the mass shared among different daughters are specified by some given probability distribution (the dislocation law); this is repeated recursively for all pieces. More precisely, we consider a version where the fragmentation stops when the mass of a fragment is below some given threshold, and we study the associated random tree. Dean and Majumdar found a phase transition for this process: the number of fragmentations is asymptotically normal for some dislocation laws but not for others, depending on the position of roots of a certain characteristic equation. This parallels the

behaviour of discrete analogues with various random trees that have been studied in computer science. We give rigorous proofs of this phase transition, and add further details.

The proof uses the contraction method. We extend some previous results for recursive sequences of random variables to families of random variables with a continuous parameter; we believe that this extension has independent interest.

Details will appear in a paper accepted for publication in *Probability Theory and Related Fields*.

Random search trees as fragmentation trees

ALAIN ROUAULT

(joint work with J. Bertoin, B. Chauvin, J-F. Marckert, Th. Klein)

The binary search tree (BST) is a very popular model in computer science (see [7]). We consider it as a Yule fragmentation tree stopped at the successive times $(\tau_n)_n$ of appearance of a new fragment. The size of a fragment of generation k is just 2^{-k} . The "additive" martingale used in the study of branching random walks by Biggins ([2]), and extended in the case of fragmentations in [1], can then be stopped at $(\tau_n)_n$. We obtain a martingale in discrete time which is a product of two martingales: one connected with the jump times, and the other connected with the successive shapes of the BST. This latter was known before as the Jabbour martingale ([6]).

This allows to capture the profile of the BST (i.e. the collection of number of leaves of each generation) and its asymptotic behavior ([4]), in the whole range of presence of leaves, extending the results obtained by previous methods ([3]).

Besides, with the help of the two other natural stopping lines (fixed time / fixed generation), we get three families of additive martingales. A fourth one (the bisection martingale) can be extracted from the Yule tree by considering right and left subtrees issued from vertices ([5]). Thanks to a convenient adjustment of the parameters, we establish strong links between these martingales and their limits. There are only two different limits (a.s.) in the domain of L^1 convergence. On the boundary of this domain, we obtain identification by taking derivatives.

The branching property leads to remarkable identities in law, seen here as identities between random variables built on the same probability space.

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Trees and random maps

GRÉGORIE MIERMONT

A map is a cell complex of a compact oriented surface without boundary, considered up to homeomorphisms of the surface, and can be considered as a graph embedded in the surface. Random maps are used in physics, in the field of 2-dimensional quantum gravity, as discretized versions of an ill-defined random surface [2]. Important progress has been made towards a mathematical understanding of this approach thanks to bijective approaches initiated in Schaeffer's work [14], and allowing to encode geometric properties of maps with simpler combinatorial objects, namely labeled tree-like objects. This allowed Chassaing and Schaeffer [5] to obtain the scaling limits for the radius and profile of a uniform rooted planar quadrangulation with n faces, considered as a metric space by endowing its vertices with the usual graph distance. Generalizations of this result have been obtained for much more general families of random maps by Marckert, Weill and the author in [9, 12, 15, 13], by relying on generalizations of Schaeffer's bijection by Bouttier, Di Francesco and Guitter [4].

Marckert and Mokkadem [10] proved convergence of random planar quadrangulations towards a limiting object they called the *Brownian map*, using the convergence of encoding functions of the underlying labeled trees. Another important step was accomplished by Le Gall [7], who showed that scaling limits of these random quadrangulations, considered in the Gromov-Hausdorff sense [6], must be a topological quotient of the Brownian Continuum Random Tree of Aldous [1]. This allowed Le Gall and Paulin [8] to infer that these limits must be homeomorphic to the two-dimensional sphere. At the present stage, it is however not known whether the metric structure of the scaling limit is uniquely determined, which would lead to a nice mathematical understanding of approximating random surfaces by random maps.

While most the articles on the topic have focused on scaling limits as $n \rightarrow \infty$ of random maps with n faces, we rather draw our attention to natural probability measures on quadrangulations, called Boltzmann measures (the term being inspired from [3], see also [9, 12]), and that are obtained by assigning a weight to the faces. In the Physics terminology, these measures correspond to the so-called *grand-canonical* measures, while the measures with fixed number of faces are the *microcanonical* measures.

It turns out that a simple variant of Schaeffer's bijection allows to treat geometric properties of certain Voronoi-like tessellations of maps. By making a proper

use of this bijection, we prove that the Gromov-Hausdorff limits of Boltzmann-distributed random quadrangulations are path metric spaces endowed with a natural mass measure, such that almost-every pair of points are joined by a unique geodesic segment. We do not restrict ourselves to the planar case, as the most natural framework for our bijection is to consider maps of arbitrary (but fixed) genus g . Thus, our bijection is really a variant of the Marcus-Schaeffer bijection in arbitrary genus [11].

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A stratified sampling simulation of coagulation processes and application to crystal growth.

KARL SABELFELD

We develop a new version of the direct simulation Monte Carlo method (e.g., see [2], [5], [1]) for coagulation processes governed by homogeneous Smoluchowsky equations. The method is based on a subdivision of the set of particle pairs into classes, and on an efficient algorithm for sampling from a discrete distribution, the so-called Walker's alias method [3]. The efficiency of the new method is drastically increased compared to the conventional methods, especially when the coagulation kernel is strongly varying. The method is applied to solving a problem of islands formation on a surface due to a diffusion controlled coagulation [4].

Formation of clusters and their growth through aggregation is the main feature of many physical processes, from polymerization and gelation in polymer science, flocculation and coagulation in aerosol and colloidal chemistry, percolation and coarsening in phase transitions and critical phenomena, formation of aerosol particles in combustion processes, agglutination and cell adhesion in biology, to island nucleation and thin film growth in material science we developed in [6] and [4].

To explain the main idea behind the new method, let us suppose we have an extremely efficient method (EEM) of sampling from an arbitrary discrete distribution. Then we could imagine that we keep the table of the pair collision probabilities and sample the collision pairs from this table using the above mentioned method, EEM. Bad news is that after each coagulation event, we have to recalculate the table of probabilities. The crucial point of our new method is that the change in the table can be done quite rarely, and the choice of the class of pair particles is done by the method suggested by Walker [3]. Thus instead of using the rejection method where the coagulation event happens with small probabilities, we turn to a stratified sampling which ends up with a coagulation having large probability, so we call the method shortly SLP (stratified sampling with large probabilities).

Summarizing, the general scheme for solving Smoluchowski equation can be described as follows:

First step: we choose the current particle distribution as a given initial distribution $L(t_0, l)$.

Second step: take N particles according to the current distribution, choose a subdivision of the set of all particle pairs into (many) classes; this subdivision is generated by a subdivision of the whole sizes into a set of size bins; the random index of the class is sampled by EEM, while inside the sampled class the von Neumann rejection method is applied. The majorant of the rejection method is fixed: Each coagulation event $\{i\} + \{j\} = \{k\}$ leads to the corresponding change in the arrays containing the clusters $\{i\}, \{j\}, \{k\}$; sample the time step Δt according to the exponential distribution. The process simulations proceed till the number of particles in the size bins is twice decreased or increased. After that we go to step 2.

Becker–Döring equations

The number of atoms n in a cluster increases or decreases by one when an atom is attached to the cluster or detached from it. Let J_n be the net rate of transformation of n mers into $(n + 1)$ mers. The number c_n of n mers increases due to the transformation of $(n - 1)$ mers into n mers and decreases because of the transformation of n mers into $(n + 1)$ mers:

$$(1) \quad dc_n/dt = J_{n-1} - J_n.$$

This equation is valid for $n \geq 2$. The equation describing the number of monomers c_1 is obtained by requiring that the total number of atoms in the system

$$(2) \quad N = \sum_{n=1}^{\infty} nc_n$$

does not change in time. The condition $dN/dt = 0$ gives, after substitution of Eqs. (1) and rearrangement of the terms,

$$(3) \quad dc_1/dt = -2J_1 - \sum_{n=2}^{\infty} J_n.$$

This equation takes into account that each transformation of an n mer into an $(n + 1)$ mer decreases the number of monomers by one, except in the case $n = 1$, where two monomers form a dimer.

The net rate J_n is a result of two processes. First, an n mer catches a monomer. The rate of this process is proportional to the densities of the n mers and the monomers and can be written as $a_n c_1 c_n$, where a_n is a time-independent coefficient that remains to be determined. The second process is a spontaneous detachment of a monomer from a $(n + 1)$ mer. It is proportional to the density of $(n + 1)$ mers solely and can be written as $b_n c_{n+1}$, where b_n is another time-independent coefficient to be specified. Hence, we obtain

$$(4) \quad J_n = a_n c_1 c_n - b_{n+1} c_{n+1}.$$

Equations (1), (3), and (4) are the Becker–Döring equations.

If the time limiting process is the adatom diffusion between clusters, the attachment and detachment coefficients a_n and b_n for the 3D problem are calculated, for large n , as follows. The cluster of n atoms is considered as a sphere of radius r_n , so that $n = 4\pi r_n^3/3$. To calculate the attachment coefficient, we solve the steady-state diffusion equation $\nabla^2 c(r) = 0$ with two boundary conditions: the concentration of the monomers far away from the cluster is equal to their mean concentration, $c(r)|_{r=\infty} = c_1$, while the concentration of the monomers at the cluster surface is zero, $c(r)|_{r=r_n} = 0$, since the monomers are attached to the cluster as soon as they reach it. The solution is $c(r) = (1 - r_n/r)c_1$. The total atom flux at the cluster surface

$$(5) \quad j_n = 4\pi r_n^2 D \nabla c(r)|_{r=r_n},$$

where D is the diffusion coefficient of the monomers, is equal to $4\pi Dr_n c_1$, and hence the attachment coefficient is

$$(6) \quad a_n = 4\pi Dr_n.$$

The detachment coefficient is calculated assuming that the concentration of the monomers at the cluster surface is equal to the equilibrium monomer concentration c_{neq} , while there is an ideal sink for monomers at infinity, $c(r)|_{r=\infty} = 0$. The solution of the steady-state diffusion equation with these boundary conditions is $c(r) = c_{neq} r_n / r$, and the corresponding detachment flux of the monomers is $b_{n+1} = 4\pi Dr_n c_{neq}$. Here we take into account that this flux refers to the detachment from the $(n+1)$ mer. The ratio of the detachment and the attachment coefficients is then

$$(7) \quad b_{n+1}/a_n = c_{neq}.$$

The equilibrium density of monomers at the surface of a cluster is given by the Gibbs–Thomson formula

$$(8) \quad c_{neq} = c_{\infty eq} \exp(\gamma/r_n) \approx c_{\infty eq} (1 + \gamma/r_n),$$

where γ is a constant proportional to the surface tension. A correction to Eq. (8) for small clusters consisting of very few atoms, while being important for the nucleation theory, is not essential for the Ostwald ripening problem. Then, equations (1)–(8) form a complete set that describes the process of Ostwald ripening.

When the clusters are large enough, n can be treated as a continuous variable. It can be verified (e.g., see [4]) that the continuous equations derived from the set of equations above are the Lifshitz–Slyozov equations. The results of numerical simulations of the crystall growth based on the described method can be seen in [4].

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Computing likelihoods under Λ -coalescents (in the infinitely-many-sites model)

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(joint work with Jochen Blath and Matthias Steinrücken, TU Berlin)

We derive a recursion for the probability of sequence observations in a situation where the underlying genealogy is described by a Λ -coalescent, extending earlier work by Griffiths and Tavaré [3], [4] for Kingman's coalescent, and use this to implement a Monte Carlo scheme to estimate these probabilities. We illustrate resulting likelihood surfaces for the family of Beta($2 - \alpha, \alpha$)-coalescents with simulated datasets and a subsample from a cod dataset taken from Árnason [1].

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Coagulation and Fragmentation Models in Chemical Engineering

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(joint work with Computational Modelling Group in Cambridge)

Three different applications for coagulation and fragmentation processes appearing in chemical engineering are presented. For each application a stochastic model is formulated, numerically solved by a direct simulation Monte Carlo method (DSMC) and the simulation results are discussed. In case of Titania flame synthesis the particle type space is given by the mass, surface area, and number of primary particles which comprise an aggregate. The particles are subject to inception, coagulation, growth, and sintering and coupled to a gas-phase kinetic model using an operator splitting technique. The model is used to simulate a heated furnace laboratory reactor and an industrial production facility. Using the primary particle information, transmission electron microscopy (TEM) style images of the particles are generated. The stochastic model for the synthesis of soot is an extension of the Titania model in as much as the positions of the primary particles to each other are included. Numerical simulations are presented and the formation mechanism of primary particles is illustrated. Finally, a model for the granulation of powders is introduced. The model is also given in terms of a stochastic jump process in which the stochastic particles are assumed to be spherical and have five characteristic properties: solid material, binder on solid, pores, binder in pores, and reaction products. The results of a DSMC scheme are presented and

the influence of the rate of the chemical reaction of the binder turning into solid is investigated.

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Fragmentation problem in mining

SERVET MARTÍNEZ

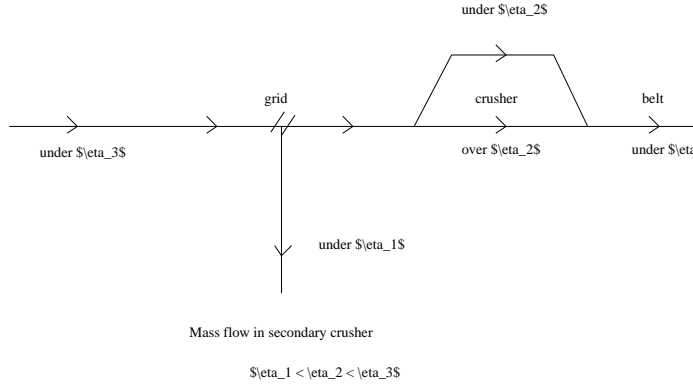
(joint work with Jean Bertoin)

The objective of the mining activity is to liberate, via fragmentation, the metal associated particles and then separate these from its non valued content. An idea of the magnitudes involved in fragmentation in the mining process is given by Chuquicamata, the biggest open pit copper mine on earth, one blasts and transports nearly 600.000 of tons material per day. Out of this, 200.0000 tons are defined as mineral and the average grade of copper content of this mineral is around 1 per cent.

There, the fragmentation is carried out in a series of steps, the first one being blasting. After, there are two circuits for mechanically decrease the mineral size. The conventional process uses three types of crushers (primary, secondary and tertiary) and the particles are forwarded to the mills once they are smaller than 1/2 inches. The fragmentation process is stopped once the particles have a size smaller than $20\mu m$. In the other process the SAG mills are fed with particles of size smaller than 8 inches with a similar end product of $20\mu m$. At every step each particle is screened, so, if it is smaller than the diameter of the mesh of a grid, it is forwarded to the next step. As described, in crushers, grinders and mills the material is broken by a repetitive mechanism, finishing when the particles can go across the classifying-grid. The process finishes when the material attains a size sufficiently small for the mining purposes.

In the figure below it is drawn a secondary crusher fed with particles with diameter smaller than η_3 . The particles with diameter smaller than η_1 are forwarded directly to the mills. The other particles are segregated, those with a diameter bigger than η_2 proceed to the crushers and exit once its diameter is smaller that η_2 . After, in a sorting belt they join the particles whose diameter is smaller than η_2 (but bigger than η_1) and the material flow is forwarded to the next crusher. The hypothesis that particles break independently of each other, which is at the base of random fragmentation theory, is a reasonable assumption in the mining

process. Moreover, it can be also assumed that the fragmentation process happens in a self-similar way.



One of the problems that faces mining industry is to minimize the energy used in these processes. Let us assume that the energy required to break a block of size s into a set of smaller blocks of sizes (s_1, s_2, \dots) (in one unit of time in the discrete case, and instantaneously in the continuous case), is of the form $s^\beta \varphi(\Delta)$ where $\Delta = (s_1/s, s_2/s, \dots)$, φ is a cost function and $\beta > 0$ a fixed parameter. When $\varphi(s_1, s_2, \dots) = \sum_{n=1}^\infty s_n^\beta - 1$, the energy is potential, because the total energy needed to break a series of masses (m_1, m_2, \dots) summing up to 1 into a finer distribution (m'_1, m'_2, \dots) is given by $\sum_i m_i'^\beta - \sum_j m_j^\beta$, and this is independent of the fragmentation path leading from the initial configuration to the final one. The potential energy is one of the most used models in mining and corresponds to the laws of Charles, Walker and Bond.

The mining process inspired the study of the evolution of a fragmentation process until every fragment in the system has size less than a fixed bound η , so each fragment whose size is smaller than η is frozen in the system. Let $\mathbf{E}(\eta)$ be the energy needed to reduce a fragment of unit mass to the set of final fragments $(x_{\eta,j})$ resulting from the above process (so with size at most η).

Below one set the results already stated in the continuous case [2]. One uses the constructions and results developed by J. Bertoin, that can be found in [1]. Let us denote by $\mathbb{S} = \{S = (s_1, s_2, \dots) : s_1 \geq s_2 \geq \dots \geq 0, \sum_i s_i \leq 1\}$ and by ν the dislocation measure that satisfies $\int_{\mathbb{S}} (1 - s_1) \nu(dS) < \infty$. One assumes that there is no erosion. The energy is given by

$$\mathbf{E}(\eta) = \sum_{t \geq 0} \mathbf{1}_{X_{k(t)}(t^-) \geq \eta} X_{k(t)}^\beta(t^-) \varphi(\Delta(t))$$

where $k(t)$ is the index of the fragment that dislocates at time t and $X_{k(t)}(t^-) \Delta(t)$ is the sequence of fragments in which it dislocates.

An essential assumption is the existence of the Malthusian parameter $\alpha > \beta_c$ (see the definition of β_c in [1] or [2]), so it verifies

$$\int_{\mathbb{S}} \left(1 - \sum_n s_n^\alpha \right) \nu(dS) = 0.$$

Define $m(\alpha) = - \int_{\mathbb{S}} \sum_n s_n^\alpha \log s_n \nu(dS)$ and let W_∞ be the terminal values of the martingale $W_n = \sum_n X_n^\alpha(t)$. The main result in [2], under the condition $\varphi \in L^1(d\nu) \cap L^2(d\nu)$, shows that whenever $\beta \in (\beta_c, \alpha)$,

$$\lim_{\eta \rightarrow 0} \eta^{\beta-\alpha} \mathbf{E}(\eta) = \frac{W_\infty}{(\alpha - \beta)m(\alpha)} \int_{\mathbb{S}} \varphi(S) \nu(dS) \text{ in } L^2.$$

In [2] it is also obtained a limit theorem for the empirical distribution of fragments with size less than η which result from the process. Indeed, if ρ_η is the finite measure given by

$$\langle \rho_\eta, f \rangle = \sum_j x_{\eta,j}^\alpha f\left(\frac{x_{\eta,j}}{\eta}\right) \text{ for } f : [0, 1] \rightarrow \mathbb{R} \text{ measurable,}$$

then

$$\lim_{\eta \rightarrow 0} \langle \rho_\eta, f \rangle = W_\infty \langle \rho, f \rangle \text{ in } L^2, \text{ with } \langle \rho, f \rangle =$$

$$\frac{1}{m(\alpha)} \int_0^1 f(u) \left(\int_{\mathbb{S}} \sum_n \mathbf{1}_{u > s_n} s_n^\alpha \nu(dS) \right) \frac{du}{u}.$$

In the discrete framework no L^2 hypothesis is needed and above limits are in L^1 . This is shown by using Nerman results [4] on the CMP branching process.

In the mining process the mass of the rocks is preserved. Hence, if the size of a fragment corresponds to its mass, the Malthusian parameter is $\alpha = 1$ which is known as the conservative case. A problem appears because the bound η corresponds to the diameter of the fragment, and not to its mass. One can assume that the density of the material is constant, so the mass of the rock is proportional to its volume. But the volume is not a function of the diameter since there is no shape preserving. But it is reasonable to assume that the volume is a random function V of the diameter, that this function verifies $0 \leq V \leq 1$, and that it is independent of the fragment process. So, instead of stopping the fragmentation of a particle once its size is smaller than η , the problem turns into freezing the fragmentation of a particle once its size is smaller than ηV . When V is lower bounded by a strictly positive constant, analogous results as those already stated also hold.

Let us point out that the above results applies to the action of only one crusher (or mill) possessing a well-defined fragmentation mechanism. In [3], the behavior of the fragmentation process when the material flow crosses several machines acting in a sequential way as it happens in the mining process, is being studied.

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Scenarios of gelation in coagulating systems

ALEX A. LUSHNIKOV

The critical and post-critical behavior of coagulating systems, where the coagulation efficiency grows with the masses of colliding particles g and l as $K(g, l) = 0.5(g^\alpha l^\beta + g^\beta l^\alpha)$, $\lambda = \alpha + \beta > 1$, $\mu = |\alpha - \beta| < 1$ is studied. The instantaneous sink that removes the particles with masses exceeding G is introduced which allows one to describe the coagulation kinetics by a finite set of equations and define the gel as a deposit of particles with masses between $G + 1$ and $2G$. This system displays the critical behavior (the sol-gel transition) in the limit $G \rightarrow \infty$ if $\lambda = \alpha + \beta > 1$. The exact post-critical particle mass spectrum is shown to be an algebraic function of g times a *growing* exponent. All critical parameters of the systems are determined as the functions of α and β .

Three possible scenarios of gelation are reported.

- (1) Only one giant particle (gel) forms after the critical time t_c . This particle actively interacts with the sol part consuming the mass of the sol particles. Such scenario realizes when the coagulation kernel has a term linear in particle mass, $\alpha = 1$. In particular this scenario realizes in the exactly solvable model with $K = gl$. This scenario is referred to as active gelation.
- (2) Gelation is always passive at $\alpha, \beta < 1$, $\lambda > 1$, $\mu < 1$. This situation is well described by the truncated models. In this case there is a finite mass flux through the cutoff mass G (this flux is independent of G). The gel itself does not affect the sol spectrum.
- (3) Collapse in gelling systems occurs at $\lambda > 1$, $\mu \geq 1$. In collapsing systems the post-gelation sol spectrum contains the multiplier $G^{-1/2}$, i.e. it vanishes as $G \rightarrow \infty$. Nevertheless its mass remains finite and the mass flux from sol to gel remains finite as $G \rightarrow \infty$. Hence, in the limit of large G the sol disappears after the critical time. There are other examples of collapsing systems, where the gel appears right after the very beginning of the coagulation process.

Main results are published in [1, 2, 3]

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Numerical simulation of spatially inhomogeneous coagulation dynamics in the gelation regime

FLAVIUS GUIAŞ

We present a stochastic approach for the simulation of coagulation-diffusion dynamics in the gelation regime. The method couples the mass flow algorithm for coagulation processes with a stochastic variant of the diffusion-velocity method in a discretized framework. The simulation of the stochastic processes occurs according to an optimized implementation of the principle of grouping the possible events. A full simulation of a particle system driven by coagulation-diffusion dynamics is performed with a high degree of accuracy. This allows a qualitative and quantitative analysis of the behaviour of the system. The performance of the method becomes more evident especially in the gelation regime, where the computations become usually very time-consuming.

Our basic approach is to consider a discretization of a spatial domain into cells, which are considered as spatially homogeneous “reactors”. Inside each cell we simulate the population balance dynamics with a usual algorithm, e.g. the mass flow algorithm. In addition to this, we have to couple these reactions with a mechanism which allows exchange of mass between the cells.

In [1] the coupling of directly simulated coagulation-fragmentation dynamics with random walks was analyzed from a theoretical point of view. Conditions were given under which the corresponding deterministic equation has a unique solution and a convergence result of the family of stochastic particle models to this solution was proven. However, this approach turns out to be extremely inefficient from the numerical point of view.

In order to be able to perform numerical simulations for models of the type described above, one needs on the one hand to improve the efficiency of the existing algorithms for population balance dynamics and on the other hand to simulate the diffusive motion of particles by a method which surpasses significantly -concerning speed and accuracy- the performance of the random walk method.

The first step towards this goal is to work directly with approximations of the macroscopic quantities (like densities or mass corresponding to particles of a given size, at a given place) rather than treating each particle individually. We make therefore no distinction between particles located at the same point in the size space or in the physical space. The set of possible events of the Monte Carlo simulation decreases significantly, while the state of the system continues to change according to the same particle dynamics.

The second step towards higher speed is to group possible events. The basic idea is to divide the set of possible events into a number of groups, choose a group according to its probability and then select the transition event inside this group. The expected number of operations needed to compute one transition decreases in

this way significantly compared to the situation when we try to consider the whole set of events at once. Here, we use the method introduced in [3] to optimize the underlying grouping principle. The optimization is done by a simple method based on binary partitions of the groups. Usually the events to be computed correspond to a list which is ordered in a natural way (e.g. by size, in the case of coagulating particles). Having a given group, we choose from all possible splittings in two consecutive parts the one which minimizes the number of expected operations needed to compute an event (to be precise: an approximation of it). We call this division a *binary partition* of the original group. The algorithm which computes the optimized structure starts with a single group (which contains all possible events) and follows then the next procedure: having the current group structure, do successive binary partitions of the existing groups. If by replacing a group with the two parts the expected number of operations decreases, then we keep this binary partition and update the group structure. Otherwise, we reject it. We stop if the binary partition steps are rejected for all existing groups. For the present simulation, where the data has a two-dimensional spatial structure, we can perform a similar decomposition into rectangular patches. We take now binary partitions in both directions: horizontally and vertically.

In order to simulate particle diffusion, we use the method introduced in [2]. It is based on the idea of associating a velocity vector to the particles, which can be computed formally as $-\nabla u/u$, where u denotes the density of the quantity which diffuses. Unlike in the random walk method, where the particles can jump in all directions, we simulate here essentially only the flux between neighbouring cells. The jumps of the particles are oriented and the efficiency of the method increases significantly.

The numerical simulations of coagulation-diffusion dynamics in 2D are realized by applying the principles discussed before. The most important feature of these simulations is that they allow computations beyond the gelation time, i.e. where we have also particles of large size, or “giant clusters”. According to the mass flow algorithm, they are removed from the system and account for the gel phase. The computations in this regime are extremely time consuming, even in the spatially homogeneous setting, and were made possible by the optimization of the stochastic algorithms as described above and by the simulation of diffusion using a new scheme, instead of random walks. The results of these simulations are presented in [4].

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**Measurability of optimal transportation and convergence rate for
Landau type interacting particle systems**

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(joint work with Joaquin Fontbona, H el ene Gu erin)

We consider nonlinear diffusion processes driven by space-time white noises, which have an interpretation in terms of nonlinear partial differential equations. For a specific choice of coefficients, they correspond to Landau equations arising in kinetic theory. Our aim is to construct an easily simulable diffusive interacting particle system, converging towards this nonlinear process and to obtain an explicit pathwise rate. This requires to find a significant coupling between finitely many Brownian motions and the infinite dimensional white noise process. The key idea is to construct the right Brownian motions by pushing forward the white noise processes, through the Brenier map realizing the optimal transport between the law of the nonlinear process, and the empirical measure of independent copies of it. A striking problem then is to establish the joint measurability of this optimal transport map with respect to the space variable and the parameters (time and randomness) making the marginals vary. We prove a general measurability result for the mass transportation problem and for the support of the optimal transfert plans, in the sense of set-valued mappings. This allows us to construct the coupling and to obtain explicit convergence rates.

Asymptotic density for a variety of coalescing random walks model

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We study coalescing random walk models in \mathbb{Z}^d , for $d \geq 3$. For the basic model, where particles always coalesce when they meet, we know that the density $p(t)$ satisfies $p(t) \sim 1/(yt)$, as t tends to infinity, where y is the probability that a single random walk particle never returns to its starting point. Their proof relies heavily on the duality relation with the voter model. Van den Berg and Kesten (2000) introduced a more robust method with which several modifications of the model can be handled as well. Recently, it became clear that the method also applies to a seemingly quite different problem, namely the behaviour of the stationary state density for a coalescing random walk model in which new particles are spontaneously created at rate λ . We study the asymptotic density for this model as $\lambda \downarrow 0$.

The speed of coalescence when it comes down from infinity

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(joint work with Nathanaël Berestycki, Vlada Limic)

Exchangeable coalescent which allow multiple collisions but not simultaneously are called Λ -coalescent since their law is characterized by a finite measure Λ on $[0, 1]$. A coalescent is said to “come down from infinity” if the number of its clusters N_t is immediately finite for all positive time $t > 0$ (initially $N_t = \infty$ as each integer form a single block). In 2000 Schweinsberg [4] gave a criteria to determine whether a coalescent do comes down from infinity or not. The question of the speed of coalescence is that of determining the behavior of N_t as $t \searrow 0$. For instance it is known that in the case of Kingman’s coalescent $N_t/t \rightarrow 2$ almost surely as $t \searrow 0$. In 2006 Berestycki, Berestycki and Schweinsberg [1] (see also [2] for a result obtained independently in the same direction) showed that if $\Lambda(dx) = f(x)dx$ with $f(x) = Ax^{1-\alpha}$ for $\alpha \in (1, 2)$ then

$$\lim_{t \searrow 0} t^{1/(\alpha-1)} N_t = (\alpha / (A\Gamma(\alpha-2)))^{1/(\alpha-1)} \text{ a.s.}$$

We obtain the speed of coalescence, i.e. a function $t \mapsto v(t)$ such that $N_t/v(t) \rightarrow 1$ as $t \rightarrow 0$ almost surely, for general measures Λ . More precisely, define $\Psi(q) := \int_0^1 (e^{-qx} - 1 + qx)x^{-2} \Lambda(dx)$ and let $v(t) := \inf\{s : \int_s^\infty \frac{dq}{\Psi(q)} < t\}$. Call δ the lower-index of the Lévy process with Laplace exponent Ψ (see [3]). Then we have

Theorem. *Call $(\Pi(t), t \geq 0)$ the coalescent associated with the measure Λ . Then*

- $\Pi(\cdot)$ comes down from infinity if and only if $\int_s^\infty \frac{dq}{\Psi(q)} < \infty$.
- If it does, $\frac{N_t}{v(t)} \rightarrow 1$ almost surely as $t \rightarrow 0$ provided that $\delta \neq 1$

The first point had already been observed analytically by Bertoin and Le Gall in [2] who noted that Schweinsberg’s criteria can be reexpressed under this form which is also Grey’s criteria for a continuous branching process with mechanism Ψ to become extinct in finite time almost surely. However no probabilistic explanation of this fact was known. By shedding more light on the relations (which have been the focus of much attention lately) between Λ -coalescent, continuous-state branching processes and so-called generalized Fleming-Viot super-processes, we are able to give such an explanation. Then by combining this approach with martingale techniques we obtain the second part of the result.

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The central limit theorem for the Smoluchovski coagulation model

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We establish a central limit theorem (CLT) for the fluctuations of the Markus–Lushnikov process in the limit of large particle numbers thus giving a solution to problem 10 in the list of open problems in mathematical theory of coagulation from the well known review [1]. Analysis of CLT is of course a natural next step after the convergence of the Markus–Lushnikov process to the solution of Smoluchovski equation was established in [7]. Full exposition of our results is given in [5]. In case of bounded kernels and discrete mass distributions the corresponding CLT was established in [2]. Bounded kernels with not necessarily discrete mass was addressed in [3] in a much more general context including possible fragmentation and collisions. Here we develop further the approach from [3] using also some ideas and results from [4] and [6].

Consider the simplest case where coagulation rates are a function only of particle masses, so that any two particles, of masses $E(x) = x$ and $E(x') = x'$ say, coagulate to form a particle of mass $x + x'$ at a given rate $hK(x, x')$. Here, $N = 1/h$ is the number of initial particles and the coagulation rates are scaled to give the following law of large numbers. The process of empirical particle distributions $Z^h = (Z_t^h)_{t \geq 0}$ converges weakly, as $h \rightarrow 0$ (or equivalently $N \rightarrow \infty$), when Z_t^h converges weakly to μ_0 , to the solution $(\mu_t)_{t \geq 0}$ of Smoluchowski's coagulation equation

$$\mu_t = \mu_0 + \int_0^t K(\mu_s, \mu_s) ds.$$

Here, for suitable measures μ and μ' on $(0, \infty)$, $K(\mu, \mu')$ is the signed measure, given by

$$(f, K(\mu, \mu')) = \int_{(0, \infty)^2} (f(x + x') - f(x) - f(x')) \mu(dx) \mu'(dx'),$$

for suitable measurable functions f . Our result concerns the limiting distribution of the fluctuations

$$F_t^h = F_t^h(Z_0^h, \mu_0) = (Z_t^h - \mu_t) / \sqrt{h}.$$

This is of interest if we consider the Markus–Lushnikov model as representing a good mathematical description in some applied context and wish to understand, for large particle numbers, how this model deviates from the deterministic evolution given by Smoluchowski's equation. It is also important in quantifying the stochastic errors which may arise in a computational approach to Smoluchowski's equation using Monte–Carlo techniques.

Formal calculations of the limiting generator for the fluctuation process F_t^h are not difficult and yield for it the expression

$$(1) \quad \Lambda_t F(Y) = \frac{1}{2} \int \int \int (\delta F(Y), \delta_{z_1+z_2} - \delta_{z_1} - \delta_{z_2}) K(z_1, z_2) (Y(dz_1) \mu_t(dz_2) + \mu_t(dz_1) Y(dz_2)) \\ + \frac{1}{4} \int \int \int (\delta^2 F(Y), (\delta_{z_1+z_2} - \delta_{z_1} - \delta_{z_2})^{\otimes 2}) K(z_1, z_2; dy) \mu_t(dz_1) \mu_t(dz_2).$$

Hence the mathematical problem we are solving is in constructing a well defined infinite dimensional Gaussian Ornstein-Uhlenbeck (OU) process in an appropriate space of generalized functions (distributions) with a generator of this form and to prove the convergence of the fluctuations F_t^h to this OU process.

Assume K is non-decreasing in each argument 2-times continuously differentiable with all the first and second partial derivatives being bounded by a constant.

For a positive non-decreasing f we denote by $C_f^{1,0}$ the Banach space of continuously differentiable functions ϕ on \mathbf{R}_+ such that $\lim_{x \rightarrow 0} \phi(x) = 0$ with the norm

$$\|\phi\|_{C_f^{1,0}} = \sup_x |\phi'/f|(x)$$

and by \mathcal{M}_f^1 we denote its dual. This space seems to be natural for building the limiting OU process. However the norms are difficult to estimate in this space leading to a necessity (that one would of course expect here) to use Hilbert space methods. Having this in mind, we introduce further weighed spaces.

Define $L_{2,f}$ as the space of measurable functions g on \mathbf{R}_+ having finite norm $\|g\|_{L_{2,f}} = \|g/f\|_{L_2}$. Also let $L_{2,f}^{2,0}$ denote the spaces of absolutely continuous functions ϕ on \mathbf{R}_+ such that $\lim_{x \rightarrow 0} \phi(x) = 0$ with the norm respectively

$$\|\phi\|_{L_{2,f}^{2,0}(X)} = \|\phi'/f\|_{L_2} + \|(\phi'/f)'\|_{L_2},$$

Let $(L_{2,f}^{2,0})'$ denotes its dual.

From the Sobolev embedding lemma one deduces the inclusion $L_{2,f}^{2,0} \subset C^{1,0}$ and hence also $L_{2,f}^{2,0} \subset C_f^{1,0}$ implying by duality the inclusion $\mathcal{M}_f^1 \subset (L_{2,f}^{2,0})'$.

Theorem 1. *Suppose $k \geq 0$ and $h_0 > 0$ are given such that*

$$(2) \quad \sup_{h \leq h_0} (1 + E^{k+5}, Z_0^h + \mu_0) < \infty.$$

and $F_0^h \in (L_{2,1+E^{k+2}}^{2,0})'$ converge to some F_0 in $(L_{2,1+E^{k+2}}^{2,0})'$, as $h \rightarrow 0$. Then the processes of fluctuations $F_t^h(Z_0^h, \mu_0)$ converge in distributions on the Skorohod space of càdlàg functions $D([0, T]; (L_{2,1+E^{k+2}}^{2,0}(\mathbb{R}_+))')$ (with J_1 -topology), where $(L_{2,1+E^{k+2}}^{2,0}(\mathbb{R}_+))'$ is considered in its weak topology, to the finite-dimensional Gaussian Ornstein-Uhlenbeck process on $(L_{2,1+E^{k+2}}^{2,0}(\mathbb{R}_+))'$ specified by the (non-homogeneous) generator (1).

One can also estimate the rate of convergence. Say for linear functionals on measures the following holds.

Theorem 2.

$$(3) \quad \sup_{s \leq t} |\mathbb{E}(g, F_s^h(Z_0^h, \mu_0)) - (U^{0,s}g, F_0^h)| \leq \kappa(C, t, k, e_0, e_1)\sqrt{h}\|g\|_{C_{1+E^k}^{2,0}} (1 + E^{k+5}, Z_0^h + \mu_0)^3 \cdot \left(1 + \left\| \frac{Z_0^h - \mu_0}{\sqrt{h}} \right\|_{\mathcal{M}_{1+E^{k+1}}^1(X)}^2 \right)$$

for all $k \geq 0, g \in C_{1+E^k}^{2,0}(X)$, where the bald \mathbb{E} denotes the expectation with respect to the process Z_t^h and κ is a constant. Here $U^{t,r}$ is the backward propagator of the equation

$$(4) \quad \dot{g}(z) = -\Lambda_t g(z) = - \int \int (g(y) - g(x) - g(z))K(x, z; dy)\mu_t(dx)$$

(which as one shows is well defined in $C_{1+E^k}^{2,0}$).

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Fragmenting random permutations

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(joint work with Christina Goldschmidt, Dario Spanò)

Denote by $[n]$ the set $\{1, 2, \dots, n\}$.

Problem 1.5.7 from Pitman’s Saint-Flour lecture notes [4] asks: Does there exist a “fragmentation process” $(\Pi_1, \Pi_2, \dots, \Pi_n)$ such that: (i) for each k, Π_k has the same distribution as that of the partition generated by cycles of a uniform random permutation of $[n]$, conditioned to have k cycles, and (ii) for each k, Π_k is obtained from Π_{k-1} by splitting a block into two parts. (See also [1] and [3]).

We show that the answer to this question is yes.

Using the “Chinese restaurant process” construction of a uniform random permutation of $[n]$, we show that the result is implied by the following proposition:

Proposition 1. Let n be fixed and let $p_1, p_2, \dots, p_n \in [0, 1]$. Consider independent Bernoulli random variables B_i , $1 \leq i \leq n$, with $\mathbb{P}(B_i = 1) = 1 - \mathbb{P}(B_i = 0) = p_i$. Then there exists a collection of random variables B_i^k , $1 \leq k \leq n$, $1 \leq i \leq n$ with the following properties:

- (i) For all k , (B_1^k, \dots, B_n^k) has the distribution of (B_1, \dots, B_n) conditioned on the event $\sum_{i=1}^n B_i = k$;
- (ii) For all i and all k , $B_i^k \geq B_i^{k-1}$ with probability 1.

In the application to the random permutation question via the Chinese restaurant process, one has

$$(1) \quad B_i = I(i \text{ is the smallest element in its block}),$$

and $p_i = 1/i$.

Proposition 1 can be proved by applying a form of Strassen’s theorem on the existence of couplings with given marginals, which also manifests itself as a version of Hall’s Marriage Theorem or as a version of the max-flow min-cut theorem. One has to verify the following result:

Proposition 2. Let A_1, A_2, \dots, A_m be distinct k -subsets of $[n]$ and let

$$E_j = \{B_i = 1 \forall i \in A_j\}, \quad 1 \leq j \leq m.$$

Then for $0 \leq k \leq n - 1$,

$$\mathbb{P} \left(E_1 \cup E_2 \cup \dots \cup E_m \left| \sum_{i=1}^n B_i = k \right. \right) \leq \mathbb{P} \left(E_1 \cup E_2 \cup \dots \cup E_m \left| \sum_{i=1}^n B_i = k + 1 \right. \right).$$

This in turn is a corollary of the following result from Efron [2]:

Proposition 3. Let $\phi_n : \mathbb{Z}^n \rightarrow \mathbb{R}$ be a function which is increasing in all of its arguments. Let $I_i \sim \text{Bernoulli}(p_i)$, $1 \leq i \leq n$ independently. Then

$$\mathbb{E} \left(\phi_n(I_1, I_2, \dots, I_n) \left| \sum_{i=1}^n I_i = k \right. \right) \leq \mathbb{E} \left(\phi_n(I_1, I_2, \dots, I_n) \left| \sum_{i=1}^n I_i = k + 1 \right. \right),$$

for all $0 \leq k \leq n - 1$.

In general there are many possible distributions satisfying the conditions in Proposition 1, and hence many different fragmentation processes with the required properties. We give a particular example which has a consistency property as n varies and has a simple recursive construction. To construct the partition Π_n^k , one first conditions on whether the element k will be a singleton in the partition. If so, the partition is obtained by adding this singleton to the partition Π_{n-1}^{k-1} . If not, then instead the partition is obtained by adding the element k to one of the blocks of the partition Π_{n-1}^k . Using Proposition 2 it is not hard to verify that this construction can be carried out in such a way as to satisfy the fragmentation conditions.

The partition obtained from a random partition of $[n]$ has the so-called Poisson-Dirichlet(0, 1) distribution. We give a partial extension to the more general case of a Poisson-Dirichlet(α, θ) distribution. One can again define the variables B_i as at (1); now they are no longer independent. In this case, a log-concavity property of certain Stirling numbers of the second kind can be established, which implies an equivalent of Proposition 1 for the random variables B_i . However, the Chinese restaurant process representation no longer seems enough to show directly that the corresponding property for partitions holds.

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