Mathematisches Forschungsinstitut Oberwolfach

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# Stochastic models for coagulation processes

August 19th – August 25th, 2001

The mini-workshop was organized by James Norris, Cambridge, and Wolfgang Wagner, Berlin. On the first day, each of the 14 participants gave a short presentation introducing his or her main topics of interest. On the other days there were only morning sessions with four longer talks each, leaving the afternoons free for informal discussions.

The workshop was intended to bring together people working on various aspects of coagulation processes. The main subjects were

- Spatially inhomogeneous models
- Gelation phenomena
- Other models related to coagulation
- Approximation and numerics

All participants appreciated the excellent working conditions and the pleasant atmosphere, for which we thank both the administration and the staff of the MFO. We found the mini-workshop idea to be excellent: fifteen participants is large enough to be stimulating and small enough to encourage openness and collaboration within the whole group. We would strongly support further such workshops.

# Abstracts

### Number preserving simulation of Smoluchowski's coagulation equation

Hans Babovsky (Ilmenau Technical University)

One way of *numerically* simulating solutions of Smoluchowski's coagulation equation (SCE) is to follow physical intuition and to reproduce in finite particle systems stochastic realizations of the Marcus-Lushnikov process which imitates the behaviour of real particles.

This ansatz can be generalized. First, a mass-flow algorithm is discussed (introduced in [*Monte Carlo Methods and Applications*, 5:1–18, 1999]), which exhibits improved statistical properties.

Discretizing the *continuous* SCE by projecting onto an appropriate FE- or wavelet space leads to a finite discrete system in which each "particle" represents some Finite Element or some element of the wavelet basis. Such an approach may be used for an efficient adaptive discretization of the continuous SCE (see [Preprint No. M 26/99, Institute of Mathematics, TU Ilmenau; submitted]).

Finally, the techniques introduced above may be used for studying *gelation phenomena* by investigating truncated finite systems and passing to the limit of removing the truncation. We report on some recent results (see [Preprint No. M 11/01, Institute of Mathematics, TU Ilmenau; submitted]).

### Parking and the additive coalescent

Philippe Chassaing (Nancy)

Consider a parking lot with $n$ places $\{0, 1, 2, \dots, n-1\}$ and $\ell$ empty places, in which cars arrive at rate $\ell - 1$. Each car $c_i$ tries to park first on a random uniform place $p_i$, and actually parks there if $p_i$ is empty. Else $c_i$ tries successively $p_i + 1, p_i + 2, \dots$ until it finds an empty place, and parks there.

It turns out that the additive Marcus–Lushnikov process is embedded in this parking process as follows: if no place is empty in the set $\{i-1, i, i+1, \dots, j\}$, *but places* $i-1$ and $j$, then $\{i, i+1, \dots, j\}$ is called a *block of cars* with size $j - i + 1$ (assuming $i \leq j$). As a special case, if $i-1$ and $i$ are empty places, $\{i\}$ is a size-1 block. Blocks play the rôle of particles, so we can see the initial configuration, with $n$ empty places, as monodisperse. Finally, one checks easily that the probability that a size-$i$ and a size-$j$ block ("particle") merge is

$$\frac{i+j}{n(\ell-1)},$$

as would be the case for the additive Marcus–Lushnikov process.

These parking schemes are tightly related with hashing tables (a fundamental topic in computer science) and also to labeled trees and random graphs. Thus knowledge about the additive Marcus–Lushnikov process is useful for analysis of algorithms, or combinatorics, and conversely.

Let us give four examples:

- the convergence of the additive Marcus–Lushnikov process at time $t$ to solutions of the Smoluchowski equation (Jeon, Norris), gives the limit distribution of the individual displacement of a car in the *sparse* case, i.e. when $m/n \sim \alpha = e^{-t}$. This individual displacement is also the time needed to find an random item in a sparse hashing table;

- through discussions with A. Lushnikov during the mini–workshop, it seems that the analysis of the generating function of the total displacement in hashing tables, by Flajolet, Viola, & Poblete, Louchard, Knuth, Kreweras ... , is an important ingredient in the study of coalescence kernels $xf(y) + yf(x)$;
- The additive Marcus–Lushnikov process at time $t + 1/2\ \log n$ converges to the standard additive coalescent, as explained by Aldous & Pitman (1999). The embedding in a parking process translates, in the limit, in an embedding, also discovered by Bertoin, of the standard additive coalescent in the Brownian excursion, yielding a simple construction of the standard additive coalescent;
- the study of the standard additive coalescent leads to the answer to an old problem of Meir and Moon: how many random cuts are needed to destroy a random size-$n$ labeled tree ? The answer being $\sqrt{n}$ times a random variable that converges weakly to

$$X = \int_0^{+\infty} \frac{da}{1 + T_a}$$

in which $T_a$ is the stable subordinator with index $1/2$. It turns out that $X$ is Rayleigh-distributed.

Some of these correspondences were revealed to me due to the very opportune organization of this mini workshop in Oberwolfach, so I am pleased to thank the organizers for their invitation!

## A Hierarchical Cluster System Based on Strahler's Rules for River Networks

F.P. da Costa (I.S.T., Lisboa)

Partially supported by Fundação Calouste Gulbenkian and by FCT (Portugal) through program POCTI and project POCTI/32931/MAT/2000.

By the 1940's and 1950's, geologist's attempts to give a quantitative description to the morphology of river networks led to the introduction of several notions of "order" of a river. In Strahler's version of this concept the order of a river channel is a positive integer with the following operative behaviour: when two river channels with orders $i$ and $k$ meet the order of the resulting river channel is given by $\bigvee\big(i, k, ((i \wedge k) + 1)\big)$.

We consider clusters (rivers ... ) characterized by two parameters: an "order" $i$, following Strahler's rules, and a "mass" $j$ following the usual additive rule. Denoting by $c_{i,j}(t)$ the concentration of clusters of order $i$ and mass $j$ at time $t$, we derive a coagulation-like ordinary differential system for the time dynamics of these clusters. Results about existence and the behaviour of solutions as $t \to \infty$ are obtained, in particular we prove that $c_{i,j}(t) \to 0$ and $N_i(c(t)) \to 0$ as $t \to \infty$, where the Lyapunov functional $N_i(\cdot)$ measures the total amount of clusters of a given fixed order $i$. Exact and approximate equations for the time evolution of these functionals are derived. We also present numerical results that suggest the existence of self-similar solutions to these approximate equations and discuss its possible relevance for an interpretation of Horton's law of river numbers.

This is joint work with M. Grinfeld (Glasgow) and J. Wattis (Nottingham).

### Pure Jump Markov Process associated with Smoluchowski's coagulation equation

Madalina Deaconu (Nancy)

The solution of the Smoluchowski's coagulation equation is associated with a nonlinear pure jump Markov process. This interpretation in terms of stochastic processes is helpful because it describes clearly the time evolution of the coagulation in the Smoluchowski's model. Jumps in the Markov process are equivalent to instants where coalescence phenomena occur.

We use the corresponding interacting particle system in order to get rid of the non linearity in the Markov process. This furnishes an approximation scheme for the law of the process and also for the solution to the Smoluchowski's coagulation equation, more precisely, the empirical probability measure of the system converges, as the number of particles goes to infinity, to the solution of the Smoluchowski's coagulation equation.

Under quite stringent hypothesis, we obtain a central limit theorem for our Monte Carlo method.

The more natural model, including the position of particles, the so-called coagulation equation with diffusion, can also be studied via a couple of stochastic processes $(X_t, Z_t)$, where $X$ denotes the position of the particle and $Z$ its mass. The component $X$ is mainly a Brownian diffusion while $Z$ is as in the homogeneous case, a pure jump Markov process.

This is a common work with N. Fournier and E. Tanré.

### Stochastic algorithms for the Coagulation Equation

Andreas Eibeck (Berlin)

Two different stochastic particle systems are considered: The first one is the probabilistic counterpart to Smoluchowski's coagulation equation which describes the time evolution of concentrations $c(t,k)$ of clusters of size $k$. The second one arises from the probabilistic interpretation of a modified equation which is obtained from the coagulation equation by means of the transformation $\tilde{c}(t,k) = k\,c(t,k)$. Under suitable assumptions on the coagulation kernel and on the initial distribution, convergence theorems are given which provide the basis for numerical investigations. Introducing fictitious jumps and using acception-rejection methods, algorithms for an efficient realization of both particle systems are derived. A numerical comparison shows that the modified process provides smaller systematic errors and strong variance reduction features and leads to a larger efficiency.

This is joint work with W. Wagner.

### Spatially inhomogeneous models for coagulation-fragmentation processes

Flavius Guias (Dortmund)

We construct a stochastic model for coagulation-fragmentation processes and analyze its convergence properties toward the solution of the deterministic spatially inhomogeneous coagulation-fragmentation equation. The model can be described as follows: we approximate a bounded domain $\Omega$ by cubic cells of size $\epsilon$ and consider particles of sizes $1, 2, \ldots, k, \ldots, N$. Inside each cell can occur one of the following reactions: a particle of size $i$ can coagulate with a particle of size $j$ and form a new particle of size $i+j$, or a particle of size $i$ can split into a particle of size $j$ and a particle of size $i-j$. The diffusion is approximated by random walks performed between the cells by the $k$-fold clusters, $k = 1, 2, \ldots, N$. Under the hypothesis of bounded coagulation coefficients and bounded diffusion coefficients, we prove a result of convergence in probability toward the solution of the deterministic equation, by using the martingale characterization of the Markov process restated in a form corresponding to the mild semigroup formulation of the dynamics.

### Stochastic Fragmentation and Shattering Phenomena

Intae Jeon (Catholic University of Korea)

We investigate the fragmentation process developed by Kolmogorov and Filippov, which has been studied extensively by many physicists (independently for some time). One of the most interesting phenomena is the shattering (or disintegration of mass)transition which is considered a counterpart of the well known gelation phenomenon in the coagulation process. Though masses are subtracted from the system during the break-up process, the total mass decreases in finite time. The occurrence of shattering transition is explained as due to the decomposition of the mass into an infinite number of particles of zero mass.

Considering the n-particle system of stochastic fragmentation processes and a tagged particle of the system, we find general conditions of the rates which guarantee the occurrence of the shattering transition.

We also consider the crash models of stock price. We show that a simple coagulation type model can be used to explain the endogenous model of bubble-crash. We explain how we generalize this model to study market microstructure.

### On general models of interacting particle systems that include coagulation

V.N. Kolokol'tsov (Nottingham)

The generators of the general transition probability semigroups acting on the spaces with the variable (or random) number of interacting particles are characterised in terms of (a nonlinear version of) the property of conditional positive definiteness of their generating functionals. The class of models include both fragmentation and coagulation of particles moving in real space-time of arbitrary dimension. The general kinetic equation (of Boltzmann type) is given that describes the limit density of the distribution of particles as their average number tends to infinity.

### Coagulation-fragmentation models with diffusion

Ph. Laurençot (Toulouse)

In this talk are presented some joint works with S. Mischler (Université de Versailles-Saint Quentin) on the existence of global weak solutions to the discrete and continuous coagulation-fragmentation equations with diffusion. The approach used relies on weak compactness arguments in $L^1$ in the spirit of the ones developed by R.J. Di Perna and P.-L. Lions (1989) in their proof of the existence of renormalized solutions to the spatially inhomogeneous Boltzmann equations. In the discrete case, fairly general assumptions on the kinetic coefficients are made and the assumption of weak fragmentation usually required in previous works is removed. In the continuous case, stronger assumptions are needed : in particular, we consider the cases where either the kinetic coefficients satisfy a detailed balance condition or the coagulation coefficient enjoys a monotonicity condition.

### Occurrence of gelation and temporal decay estimates for the coagulation equation

Ph. Laurençot (Toulouse)

The occurrence of gelation in the coagulation equation for some classes of kinetic coefficients is known for a long time but a rigorous mathematical proof was only supplied recently by Jeon (1998), using a probabilistic approach. The aim of this talk is to present a deterministic proof of the occurrence of gelation recently obtained by M. Escobedo, S. Mischler & B. Perthame (2001) which is much more elementary. Temporal decay estimates of the total density and extensions to the coagulation-fragmentation equations are also discussed.

### Sol-gel transition: problems and approaches

A.A. Lushnikov (Moscow)

Two approaches are proposed for considering the sol–gel transition in coagulating systems. The first approach relies upon the evolution equation for the generating functional of the probability to have in the system a given mass spectrum. The exact solutions to this equation are found for linear models. The analytic results are shown can be obtained for the gelling model with the coagulating kernel proportional to the product of the mass of colliding particles. The critical behaviour of this model is studied. Another interesting model considers the time evolution of the random bipartite graph. It is shown that this problem is also exactly soluble. The full solution of this problem is found below the critical point. A new approximate evolution equation conserving the total mass of the system is formulated.

The second approach assumes introducing a sharp cutoff in the Smoluchowski equation corresponding to the instant sink of the particles with the masses exceeding $G$. Although such models do not display the sol–gel transition the behaviour of the particle mass spectra is different for gelling and non-gelling coagulating kernels. In the former case the total mass sharply drops down during the time proportional to negative powers of $G$. So these models can be used for the diagnostics of the phase transitions in coagulating systems.

### A Tagged Particle in Coagulation Processes

Peter March (Ohio State University)

Consider $n$ particles undergoing a coagulation (Marcus-Lushnikov) process $X^n$ with rates $K(i,j)$. We are interested in the class of rates $K$ for which gelation is known to occur in the corresponding Smoluchowski equations, eg, $K(i,j) = (ij)^\alpha$ for $1/2 < \alpha \leq 1$. More specifically, we are interested in understanding how gelation occurs. To this end we tag one of the particles and keep track of the size of the cluster which contains it. Formally this amounts to augmenting the Marcus-Lushnikov chain to include an extra integer state $(X^n, Y^n)$. We show that under the usual Euler scaling, $(X^n, Y^n)$, $n \geq 1$ is tight, that under any limit point $P$ the first coordinate of the coordinate process $(X, Y)$ is almost surely a solution of the Smoluchowski equations and that conditional on the first coordinate, the second coordinate is a Markov chain. We then show that gelation for the first coordinate $X$ is equivalent to explosion of the second coordinate $Y$.

We report on joint work in progress with Intae Jeon.

**Existence and uniqueness in the spatially inhomogeneous coagulation equation**

James Norris (Cambridge)

The equation is formulated in a weak sense, allowing particles to assume types in a general measurable space according to some distribution, and to have spatial positions according to some density. We prove existence and uniqueness under some general conditions which include the case of Brownian coagulation, where particles of radius $r$ diffuse at speed $1/r$ and coagulate with other particles, of radius $r'$ and at the same spatial location, at rate (r+r')((1/r)+(1/r')).

The methods combine ideas used previously by the author in the spatially homogeneous case, with new estimates expressing that, even if large particles diffuse more slowly and coagulate rapidly with small particles, they do not pile up uncontrollably around one spatial location.

**Self-attracting reinforced random walks and their continuous approximations**

Angela Stevens (MPI for Mathematics in the Sciences, Leipzig)

Conditions for global existence and finite time blowup of a system of PDE are discussed, which is formally related to a one dimensional edge reinforced self-attracting random walk. The condition for the particle in the random walk to visit a finite number of sites only is strongly related to the condition for the continuous system to show finite time blowup.

This part is joint work with Yin Yang (Huazhong University, Wuhan).

More general systems of PDE of this type (so-called chemotaxis systems) can rigorously be derived from stochastic interacting many particle systems under the assumption that the particles interact moderately. These models are well known to describe aggregation phenomena in self organizing micro-biological populations.

**Gelation phenomena: Conjectures and numerical observations**

Wolfgang Wagner (Berlin)

In this talk we present and discuss numerical results for Smoluchowski's coagulation equation. These results were obtained using two different algorithms based on stochastic particle systems. The algorithms were applied in situations where the phenomenon of gelation occurs - the loss of mass in finite time. Several old conjectures for different classes of coagulation kernels are compared with the numerical observations. Some new conjectures are stated, in particular, concerning the relationship of gelation with some explosion behaviour in one of the stochastic algorithms.

This is joint work with A. Eibeck.

# Participants

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