Rate of convergence: Marcus-Lushnikov Process – Smoluchowski equation

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Introduction

System's Dynamics of evolution

- Set of cluster of particles labeled as x_i.
- "Mean - field models": detailed 3-dim geometry and particle's shape neglected.
- Memoryless evolution.
- x mass of a particle : $x \in \mathbb{N}$ or $x \in (0, \infty)$.

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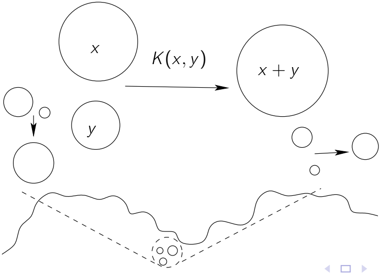
-$\mu_t(x)$:= average number of particles of mass x (discrete case).

Coalescence:



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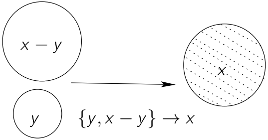

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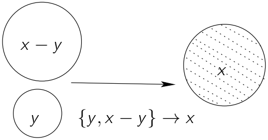

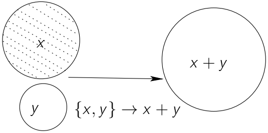

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Physical chemistry: Aerosols, phase separation in liquid mixtures, polymerization.

Astronomy: Formation of large-scale structure in the Universe.

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Each field uses an appropriate kernel. In most applications K is λ-homogeneous:

$$K(ux, uy) = u^\lambda K(x,y) \qquad u, x, y > 0.$$

$K(x,y)$	Comment
$(x^{1/3}+y^{1/3})(x^{-1/3}+y^{-1/3})$	Brownian motion (continuum regime)
$(x^{1/3}+y^{1/3})^3$	Shear (linear velocity profile)
$(x^{1/3}+y^{1/3})^2\lvert x^{1/3}-y^{1/3}\rvert$	Gravitational settling

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Weak Smoluchowski Coagulation Equation

"Infinite Volume Mean-Field Model"

Well-Posedness: Some Notation and Definitions

Notation

- $\mathcal{M}^+$: non-negative Radon measures on $(0, +\infty)$.
- μ measure and ϕ function: $\langle \mu(dx)\,,\, \phi(x)\rangle = \int_0^{+\infty} \phi(x)\mu(dx)$.
- For $\phi : (0, +\infty) \to \mathbb{R}$ measurable

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Definition (Moments and distance)

- For $\lambda \in (-\infty, 1] \setminus \{0\}$ and $\mu \in \mathcal{M}^+$:

$$M_\lambda(\mu) = \int_0^{+\infty} x^\lambda \mu(dx) \qquad \text{and} \qquad \mathcal{M}^+_\lambda = \{\nu \in \mathcal{M}^+ : M_\lambda(\nu) < +\infty\}.$$

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- For $\mu \in \mathcal{M}^+$ and $x \in (0, +\infty)$,

$$d_\lambda(\mu, \tilde{\mu}) = \int_0^{+\infty} x^{\lambda-1} \left| \int_x^{+\infty} (\mu - \tilde{\mu})(dy) \right| dx,$$

if $\lambda \in (0, 1]$. (If $\lambda < 0$ consider $\mathbb{1}_{(0,x]}(y)$)

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(AK) Assumptions on the kernel: $K : (0,+\infty) \times (0,+\infty) \to [0,+\infty)$.

- $K \in W^{1,\infty}\left((\varepsilon, 1/\varepsilon)^2\right) \forall \varepsilon \in (0,1)$.
- And $\exists \kappa_0, \kappa_1 > 0 \,\forall\, x, y > 0$:

$$\lambda \in (-\infty, 0), \quad K(x,y) \leq \kappa_0 \,(x+y)^\lambda \text{ and } \left(x^\lambda + y^\lambda\right) |\partial_x K(x,y)| \leq \kappa_1 x^{\lambda-1} y^\lambda, \tag{1}$$

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and embraces both equations: when $\mathrm{supp}(\mu_0) \subset \mathbb{N}$, and when $\mu_0(dx) = \mu_0(x)dx$.

Well-Posedness: Existence and Unicity

Definition (Weak Solution of the Smoluchowski equation)

Let $\lambda \in (-\infty, 1] \setminus \{0\}$, K satisfying (AK), and $\mu^{in} \in \mathcal{M}_\lambda^+$.
$(\mu_t)_{t\geq 0}$ is a (μ^{in}, K, λ)-weak solution to Smoluchowski's equation if:

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- [FL06][3]: Well-posedness for λ-homogeneous-like kernels and existence and uniqueness hold in the class $\mathcal{M}_\lambda^+$.

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Marcus-Lushnikov Process

"Finite Volume Mean-Field Model"

(Intrinsically Stochastic)

Marcus-Lushnikov Process: Definition

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Example

N_t processus de Poisson:

$$\mathscr{G}(f) = [f(y+1) - f(y)]\lambda$$

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What if $f = Id$? N_t can be written as

$$N_t = \int_0^t \int_0^\infty \mathbb{1}_{z\leq\lambda} N(ds, dz) \quad = \quad \sum_n \mathbb{1}_{\tau_n \leq t}$$

Infinitesimal generator

$$N_t(n) = \frac{1}{n} N_{t/n} = \frac{1}{n} \int_0^t \int_0^\infty \mathbb{1}_{\{z \leq n\lambda\}} N(ds, dz)$$

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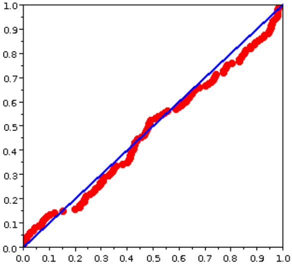

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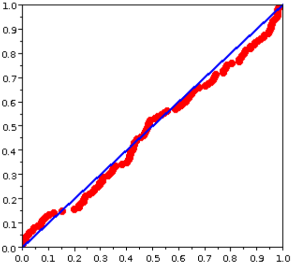

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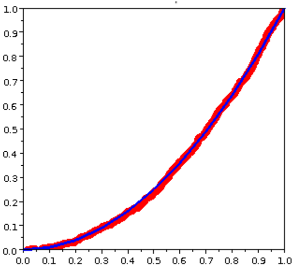

Poissonian representation (S.D.E.)

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$J(dt, d(i,j), dz)$ Poisson measure on $[0,+\infty) \times \{(i,j) \in \mathbb{N}^2, i<j\} \times [0,+\infty)$, for $\phi : (0,+\infty) \to \mathbb{R}$ and $\Psi(\mu) = \langle \mu(dx), \phi(x)\rangle$

$$\begin{aligned}\langle \mu_t^n(dx), \phi(x)\rangle &= \langle \mu_0^n(dx), \phi(x)\rangle \\ &+ \int_0^t \int_{i<j} \int_0^\infty \frac{1}{n}\left[\phi\left(X_{s-}^i + X_{s-}^j\right) - \phi\left(X_{s-}^i\right) - \phi\left(X_{s-}^j\right)\right] \\ &\qquad \mathbb{1}_{\left\{z \leq \frac{1}{n}K\left(X_{s-}^i, X_{s-}^j\right)\right\}} \mathbb{1}_{\{j \leq N(s-)\}} J(ds, d(i,j), dz).\end{aligned}$$

Results[4]

[4] E.C., N. Fournier, *Smoluchowski's equation: rate of convergence of the Marcus-Lushnikov process*. SPA 2011 vol. 6.

Theorem

Theorem ($\lambda < 0$)

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Then for any $T > 0$,

$$\mathbb{E}\left[\sup_{t\in[0,T]} d_\lambda(\mu_t^n,\mu_t)\right] \le \left[d_\lambda(\mu_0^n,\mu_0) + \frac{C_1}{\sqrt{n}}\right] \times e^{[TC_2]},$$

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$$\sup_{t\in[0,T]} \mathbb{E}\left[d_\lambda(\mu_t^n, \mu_t)\right] \leq \left[d_\lambda(\mu_0^n, \mu_0) + \frac{C_1}{\sqrt{n}}\right] \times e^{[TC_2]},$$

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Proof Positive Case ($\lambda \in (0, 1]$)

Proof (Sketch) Positive Case

M-L process, compensated Poisson measure related to J:

$$\begin{aligned}\langle \mu_t^n(dx), \phi(x)\rangle &= \langle \mu_0^n(dx), \phi(x)\rangle + \frac{1}{2}\int_0^t \langle \mu_s^n(dx)\mu_s^n(dy), (A\phi)(x,y)K(x,y)\rangle ds \\ &- \frac{1}{2n}\int_0^t \langle \mu_s^n(dx), (A\phi)(x,x)K(x,x)\rangle ds \\ &+ \int_0^t \int_{i<j} \int_0^{+\infty} \frac{1}{n} (A\phi)\left(X_{s-}^i, X_{s-}^j\right) \mathbb{1}_{\left\{z \le \frac{1}{n}K\left(X_{s-}^i, X_{s-}^j\right)\right\}} \\ &\qquad \mathbb{1}_{\{j \le N(s-)\}} \times \tilde{J},\end{aligned} \tag{5}$$

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$$\langle \mu_t(dx), \phi(x)\rangle = \langle \mu_0(dx), \phi(x)\rangle + \frac{1}{2}\int_0^t \langle \mu_s(dx)\mu_s(dy), (A\phi)(x,y)K(x,y)\rangle, \tag{6}$$

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Objective:

$$\begin{aligned}\mathbb{E}\left[d_\lambda(\mu_t^n, \mu_t)\right] &= \mathbb{E}\left[\int_0^{+\infty} x^{\lambda-1} \left|\langle (\mu_t^n - \mu_t)(dx), \mathbb{1}_{[x,+\infty)}\rangle\right| dx\right] \\ &\le d_\lambda(\mu_0^n, \mu_0) + \frac{C_1}{\sqrt{n}} + C_2 M_\lambda(\mu_0^n, \mu_0) \int_0^t \mathbb{E}\left[d_\lambda(\mu_s^n, \mu_s)\right] ds.\end{aligned}$$

and conclude with Gronwall.

Proof (Sketch) Positive Case

Using the notation:

$$
\begin{aligned}
\Psi(\mu,\phi) &= \langle \mu(dx), \phi(x)\rangle \\
\Lambda\left(\mu_1\mu_2, A\phi\right) &= \langle \mu_1(dx)\mu_2(dy), \left(A\phi\right)(x,y)K(x,y)\rangle.
\end{aligned}
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Recall:

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d_\lambda(\mu_t^n,\mu_t) &= \int_0^{+\infty} x^{\lambda-1}\left|\Psi\left((\mu_t^n-\mu_t),\mathbb{1}_{[x,+\infty)}\right)\right| dx \\
&:= \int_0^{+\infty} x^{\lambda-1}\left|E_n(t,x)\right| dx.
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Computing the difference, and since K is symmetric:

$$E_n(t,x) = E_n(0,x) + \frac{1}{2} \int_0^t \Lambda\left((\mu_s^n - \mu_s)(\mu_s^n + \mu_s), A\mathbb{1}_{(x,+\infty)}\right) ds - D(t,x) + \tilde{M}_t$$

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After integration by parts on the first integral (Lemma A.2.):

$$E_n(t,x) = E_n(0,x) + \frac{1}{2}\int_0^t \overline{B}(s,x)ds + \tilde{M}_t$$

Proof (Sketch) Positive Case

Finally,

$$\begin{aligned}\mathbb{E}\left[d_\lambda(\mu_t^n, \mu_t)\right] \quad &\leq \quad d_\lambda(\mu_0^n, \mu_0) + (1+t)\frac{C_\lambda}{\sqrt{n}}\left(1 + [M_0(\mu_0^n + \mu_0)]^2 + [M_\gamma(\mu_0^n + \mu_0)]^2\right) \\ &\times \exp\left[t\, C_\lambda M_\lambda(\mu_0^n + \mu_0)\right] + C_\lambda M_\lambda(\mu_0^n + \mu_0)\int_0^t \mathbb{E}\left[d_\lambda(\mu_s^n, \mu_s)\right] ds,\end{aligned}$$

we conclude using the Gronwall Lemma.

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Proposition (Construction of μ_0^n, control of moments and propagation)

- $t \mapsto M_\gamma(\mu_t)$ *is a.s. non-increasing for* $\gamma \leq 1$, *(both)*
- $\mathbb{E}[M_\gamma(\mu_t)] \leq M_\gamma(\mu_0)\exp\left[t\, C_{\lambda,\gamma} M_\lambda(\mu_0)\right]$ *for* $\gamma > 1$ *(both).*

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$$\mathbb{E}\left[d_\lambda(\mu_t^n,\mu_t)\right] \leq d_\lambda(\mu_0^n,\mu_0) + (1+t)\frac{C_\lambda}{\sqrt{n}}\left(1 + [M_0(\mu_0^n+\mu_0)]^2 + [M_\gamma(\mu_0^n+\mu_0)]^2\right)$$
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- $M_\gamma(\mu_0^n) \leq M_\gamma(\mu_0)$.

Let $\lambda \in (-\infty, 1] \setminus \{0\}$, $n \in \mathbb{N}$ *and* $\mu_0 \in \mathcal{M}_\lambda^+ \cap \mathcal{M}_{2\lambda}^+$, *supposed to be either atomless or discrete. Then there exists a positive measure* μ_0^n *of the form* $\frac{1}{n}\sum_{i=1}^{N_n}\delta_{x_i}$ *such that:*

$$d_\lambda(\mu_0^n,\mu_0) \leq \frac{C_\lambda}{\sqrt{n}},$$

where C_λ *depends on* λ *and* $M_{2\lambda}(\mu_0)$.

Result

Corollary

Under the assumptions of the Theorem, together with the Proposition, we deduce:

- *Under (1), for any* $T > 0$,
$$\mathbb{E}\left[\sup_{t\in[0,T]} d_\lambda(\mu_t^n, \mu_t)\right] \leq \frac{C_T}{\sqrt{n}};$$
- *Under (2), for any* $T > 0$,
$$\sup_{t\in[0,T]} \mathbb{E}\left[d_\lambda(\mu_t^n, \mu_t)\right] \leq \frac{C_T}{\sqrt{n}},$$

where C_T *is a positive constant depending only on* T, λ, κ_0, κ_1 *and* μ_0.

Numerical Tests

Simulation continuous and discret cases

$$K(x, y) = x + y \quad (\lambda = 1)$$

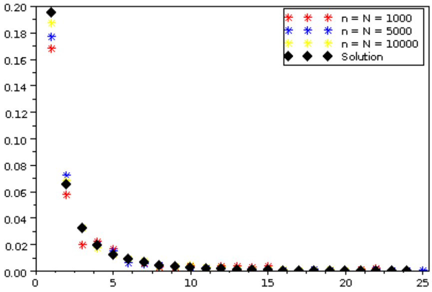
Continuous	Discret
$\mu_0(x) = \frac{1}{\sqrt{2\pi}} \frac{1}{x^{3/2}} e^{-x/2}$	$\mu_0(k) = \delta_1$
$\mu_t(x) = \frac{1}{\sqrt{2\pi}} \frac{e^{-t}}{x^{3/2}} e^{-e^{-2t}x/2}$	$\mu_t(k) = e^{-t} B(1 - e^{-t}, k)$

where $B(\lambda, k) = \frac{(\lambda k)^{k-1}}{k!} e^{-\lambda k}$.

Simulation discret case

Distances $d_1(\mu_1, \mu_1^n)$

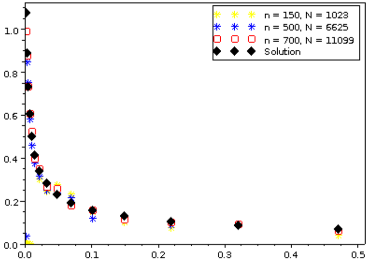
	N		$distance$	
n	$t=0$	$t=1$	$t=0$	$t=1$
1000	1000	330	0	0.1265
5000	5000	1775	0	0.0467
10000	10000	3626	0	0.0413



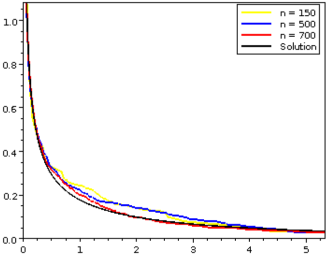
Distances $d_1(\mu_1, \mu_1^n)$

	N		distance	
n	$t=0$	$t=1$	$t=0$	$t=1$
150	1023	397	0.0961	0.3127
500	6625	2402	0.0551	0.2681
700	11099	4107	0.0437	0.1034

Distributions: $\mu_1^n([x_i, x_{i+1}))$



Tails: $\mu_1^n([x_i, \infty))$



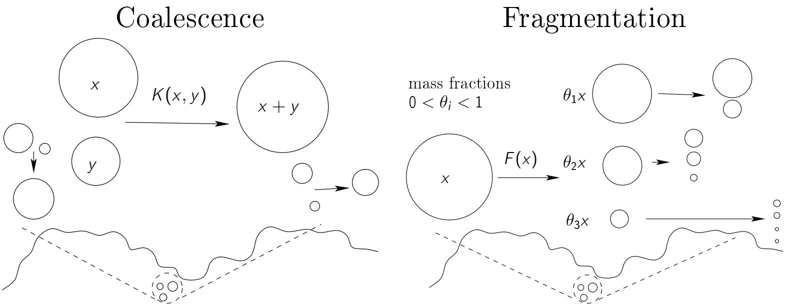
Merci pour votre attention !

Current Research

(Extension of [FL09][5])

[5] N. Fournier and E. Löcherbach. *Stochastic coalescence with homogeneous-like interaction rates*. Stoch. Proc. Appl., 2009.

Description



- Let $\mathcal{S}^{\downarrow}$ the set of non-increasing sequences $m = (m_n)_{n\geq 1}$ with $m_n \geq 0$.
- For the splitting mechanism :

$$\Theta = \left\{ \theta = (\theta_k)_{k\geq 1} : \theta_1 \geq \cdots \geq 0, \sum_{k=1}^{n} \theta_k = 1 \right\} \quad .$$

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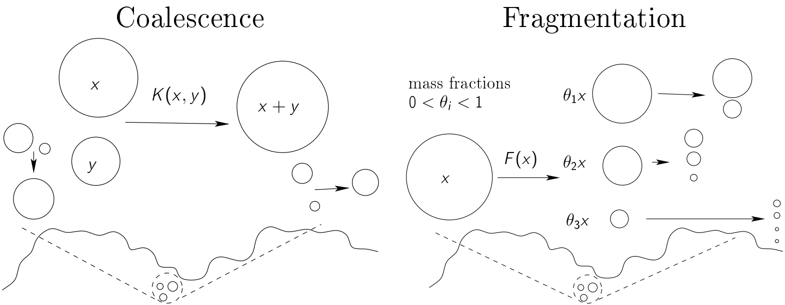

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- At t, m_i fragments at $F(m_i)$ or coalesces with m_j at $K(m_i, m_j)$, described by the maps $c_{ij}, f_{i\theta} : \ell_\lambda \mapsto \ell_\lambda$, with

$$\begin{aligned} c_{ij}(m) &= \text{reorder}(m_1, \cdots, m_{i-1}, m_i + m_j, m_{i+1}, \cdots, m_{j-1}, m_{j+1}, \cdots), \\ f_{i\theta}(m) &= \text{reorder}(m_1, \cdots, m_{i-1}, \theta \cdot m_i, m_{i+1}, \cdots). \end{aligned}$$

Objectifs

Roughly: Given K and F coagulation and fragmentation kernels. We study an infine particle process $(M(t))_{t\geq 0}$ as the limit process of a finite particle process $(M^n(t))_{t\geq 0}$.

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- $\mathcal{S}^{\downarrow}$-valued Markov process $(M(t))_{t\geq 0}$, with $M(0) \in \mathcal{S}^{\downarrow}$. Generator $\mathcal{L}$ given, for any $\Psi : \mathcal{S}^{\downarrow} \mapsto \mathbb{R}$, any $m \in \mathcal{S}^{\downarrow}$ and $\theta \in \Theta_f$, by

$$\begin{aligned}\mathcal{L}\Psi &= \sum_{1\leq i<j<\infty} K(m_i, m_j)\left[\Psi\left((c_{ij}(m)\right) - \Psi(m)\right] \\ &\quad + \sum_{i\geq 1} F(m_i) \int_{\Theta} \left[\Psi\left((f_{i\theta}(m)\right) - \Psi(m)\right] \beta(d\theta).\end{aligned}$$

The fragmentation process is self-similar-like $F(x) \leq x^{\alpha}$, $\alpha \in \mathbb{R}$

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- For $\lambda\in\mathbb{R}\setminus\{0\}$ and m, $\tilde{m}\in\ell_{\lambda}$, we set

$$d_{\lambda}(m,\tilde{m})=\sum_{k\geq 1}|m_k^{\lambda}-\tilde{m}_k^{\lambda}|$$

Poisson-SDE representation

Definition

a) $J^c(dt, d(i,j), dz)$ Poisson measure on $[0,\infty) \times \{(i,j) \in \mathbb{N}^2, i < j\} \times [0,\infty)$, denote by $\{\mathcal{F}_t\}_{t \geq 0}$ the associated canonical filtration.

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b) $J^f(dt, d(i,j), \beta(\theta), dz)$ Poisson measure on $[0,\infty) \times \mathbb{N} \times \Theta_f \times [0,\infty)$, denote by $\{\mathcal{G}_t\}_{t\geq 0}$ the associated canonical filtration. J^f is independent of J^c.

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c) Let $M(0) \in \mathcal{S}^{\downarrow}$. A càdlàg $\{\mathcal{H}_t\}_{t\geq 0} = \{\sigma(\mathcal{F}_t, \mathcal{G}_t)\}_{t\geq 0}$-adapted $\mathcal{S}^{\downarrow}$-process $(M(t))_{t\geq 0}$ is said to be a solution to the equation $SDE(K, F, M(0), J^c, J^f)$ if a.s. for all $t \geq 0$,

$$M(t) = M(0) + \int_0^t \int_{i<j} \int_0^\infty \left[c_{ij}\left(M(s-)\right) - M(s-)\right] \mathbb{1}_{\{z \leq K(M_i(s-), M_j(s-))\}} J^c$$
$$+ \int_0^t \int_i \int_{\Theta_f} \int_0^\infty \left[f_{i\theta}\left(M(s-)\right) - M(s-)\right] \mathbb{1}_{\{z \leq F(M_i(s-))\}} J^f.$$

Results

Consider $\lambda \in (0,1]$ and $\alpha \in \mathbb{R}^+$. For kernels bounded on compacts and satisfying for all $((x,y) \in (0,a]^2$:

$$\begin{aligned} |K(x,y) - K(\tilde{x},\tilde{y})| &\leq \kappa_a \left[|x^\lambda - \tilde{x}^\lambda| + |y^\lambda - \tilde{y}^\lambda| \right] \\ |F(x) - F(y)| &\leq \mu_a |x^\alpha - y^\alpha|. \end{aligned}$$

and a fragmentation measure such that

$$\beta\left(\sum_{k\geq 1} > 1\right) = 0 \qquad \text{and} \qquad \int_\Theta \sum_{k\geq 2} \theta_k^\lambda \beta(d\theta) < \infty$$

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Consider $\lambda \in (0,1]$ and $\alpha \in \mathbb{R}^+$. For kernels bounded on compacts and satisfying for all $((x,y) \in (0,a]^2$:

$$\begin{aligned} |K(x,y) - K(\tilde{x},\tilde{y})| &\leq \kappa_a \left[|x^\lambda - \tilde{x}^\lambda| + |y^\lambda - \tilde{y}^\lambda| \right] \\ |F(x) - F(y)| &\leq \mu_a |x^\alpha - y^\alpha|. \end{aligned}$$

and a fragmentation measure such that

$$\beta\left(\sum_{k\geq 1} > 1\right) = 0 \qquad \text{and} \qquad \int_\Theta \sum_{k\geq 2} \theta_k^\lambda \beta(d\theta) < \infty$$

Theorem

Endow ℓ_λ with the distance d_λ.

i) *For any $m \in \ell_\lambda$, there exists a (unique in law) strong Markov process $(M(t))_{t\geq 0} \in \mathbb{D}([0,\infty), \ell_\lambda)$ solution to $SDE(K, F, m, J^c, J^f)$.*

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ii) *For all $m^n \in \ell_0^+$ such that $\lim_{n\to\infty} d_\lambda(m^n,m) = 0$, the sequence of Coagulation - Fragmentation processes $(M^n(t))_{t\geq 0}$ solutions to the equations $SDE(K,F,m^n,J^c,J^f)$ converges in law to $(M(t))_{t\geq 0}$.*

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iii) *The obtained process is **Feller**: for all $t \geq 0$, the map $m \mapsto Law\,(M(t))$ is continuous from ℓ_λ into $\mathcal{P}(\ell_\lambda)$.*

Results

Proposition

Consider K, F, β, J^c, J^f and the process M as before. Endow ℓ_λ with the distance d_λ, and $m \in \ell_\lambda$

- $t \mapsto ||M(m,t)||_1$ *is a.s. non-increasing and*

$$\mathbb{E}\left[\sup_{s\in[0,t]} ||M(s)||_\lambda\right] \leq ||m||_\lambda \, e^{\tilde{F} C_\theta^\lambda \ t}, \tag{7}$$

where $\tilde{F}$ is a positive constant depending on F.

- *We define, for all $x > 0$, $\tau(m,x) = \inf\{t \geq 0, ||M(m,t)||_\lambda \geq x\}$. Then for all $t \geq 0$ and all $x > 0$,*

$$\mathbb{E}\left[\sup_{s\in[0,t\wedge\tau(m,x)\wedge\tau(\tilde{m},x)]} d_\lambda\left(M(s), \tilde{M}(s)\right)\right] \leq d_\lambda\left(m, \tilde{m}\right) e^{C(x\vee 1\vee ||m||_1^\alpha \vee ||\tilde{m}||_1^\alpha)\, t}. \tag{8}$$

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We show the following:

- We build a finite process $M^n(t) := M(m^n,t)$. We control its intensities (truncating β, $m \in \ell_{0+}$).
- $M(m^n,t)$ is a Cauchy sequence in $\mathbb{D}([0,\infty),\ell_\lambda)$.
- The limit process $M(m,t)$ satisfies the SDE.

Conjectures

Consider $\lambda < 0$ and $\alpha < 0$. For kernels satisfying:

$$\boxed{K(x,y) \geq \kappa(x+y)^{\lambda} \qquad \text{and} \qquad F(x) \leq x^{\alpha} \quad x,y > 0}$$

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$$\boxed{\int_{\Theta} \left(\sum_{k} \theta_k^{\lambda} - 1 \right) \beta(d\theta) < +\infty \;\; a.s.}$$

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Conjectures

Endow ℓ_λ with the distance d_λ.

i) *For $\lambda < \alpha$ existence and uniqueness for $t \geq 0$. $||\cdot||_\lambda$ bounded.*

ii) *For $\alpha \geq \lambda < 0$, explosion in finite time.*

Merci pour votre attention !