Smoluchowski coagulation equation with a flux of dust particles

Marina Amado Ferreira

CNRS, University of Toulouse

Joint work with: Aleksis Vuoksenmaa (U. Helsinki)

Probability in Mathematical Physics Seminar, IST, Lisbon, 6 March 2025

 $f_t(x)$ density of clusters of size x > 0 at time $t \ge 0$

$$\partial_t f_t(x) = \mathbb{K}[f](x,t)$$

with

$$\mathbb{K}[f](x,t) := \frac{1}{2} \int_0^x K(x-y,y) f_t(x-y) f_t(y) dy - \int_0^\infty K(x,y) f_t(x) f_t(y) dy.$$

 $f_t(x)$ density of clusters of size x > 0 at time $t \ge 0$

$$\partial_t f_t(x) = \mathbb{K}[f](x,t)$$

with

$$\mathbb{K}[f](x,t) := \frac{1}{2} \int_0^x K(x-y,y) f_t(x-y) f_t(y) dy - \int_0^\infty K(x,y) f_t(x) f_t(y) dy.$$

mass-conserving solutions [Banasiak-Lamb-Laurençot 2019]

$$M_1(t) = M_1(0)$$
, with $M_1(t) := \int_0^\infty x f_t(x)$

loss of mass-conservation

 $f_t(x)$ density of clusters of size x > 0 at time $t \ge 0$

$$\partial_t f_t(x) = \mathbb{K}[f](x,t)$$

with

$$\mathbb{K}[f](x,t) := \frac{1}{2} \int_0^x K(x-y,y) f_t(x-y) f_t(y) dy - \int_0^\infty K(x,y) f_t(x) f_t(y) dy.$$

mass-conserving solutions [Banasiak-Lamb-Laurençot 2019]

$$M_1(t) = M_1(0)$$
, with $M_1(t) := \int_0^\infty x f_t(x)$

- loss of mass-conservation
 - gelling solutions (e.g. K(x, y) = xy)

$$M_1(t) < M_1(0), \quad t > t_*$$

flux solutions (with a constant flux of mass from zero)

$$M_1(t) > M_1(0), \quad t > 0$$

 $f_t(x)$ density of clusters of size x > 0 at time $t \ge 0$

$$\partial_t f_t(x) = \mathbb{K}[f](x,t)$$

with

$$\mathbb{K}[f](x,t) := \frac{1}{2} \int_0^x K(x-y,y) f_t(x-y) f_t(y) dy - \int_0^\infty K(x,y) f_t(x) f_t(y) dy.$$

mass-conserving solutions [Banasiak-Lamb-Laurençot 2019]

$$M_1(t) = M_1(0)$$
, with $M_1(t) := \int_0^\infty x f_t(x)$

- loss of mass-conservation
 - gelling solutions (e.g. K(x, y) = xy)

$$M_1(t) < M_1(0), \quad t > t_*$$

• flux solutions (with a constant flux of mass from zero)

$$M_1(t) > M_1(0), \quad t > 0$$

Applications: coagulation in open systems (input of dust), formation of soot, aerosol growth [Friedlander 2000]

Continuity equation for the mass variable

 $xf_t(x)$ mass variable satisfies the continuity equation (for sufficiently regular f)

$$\partial_t(xf_t(x)) + \partial_x J_{f_t}(x) = 0$$

with the mass flux defined by

$$J_{f_t}(x) = \int_0^x \int_{x-y}^\infty y \, K(y,z) \, f_t(y) \, f_t(z) \mathrm{d}z \mathrm{d}y$$

Continuity equation for the mass variable

 $xf_t(x)$ mass variable satisfies the continuity equation (for sufficiently regular f)

$$\partial_t(xf_t(x)) + \partial_x J_{f_t}(x) = 0$$

with the mass flux defined by

$$J_{f_t}(x) = \int_0^x \int_{x-y}^\infty y \, K(y,z) \, f_t(y) \, f_t(z) dz dy$$

mass-conserving solutions

$$J_{f_t}(x) o 0, \quad \text{ as } \quad x o 0 \quad \text{ and } \quad x o \infty$$



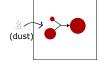
• gelling solutions (with mass flux leaving at infinity)

$$J_{f_t}(x) \to 1$$
, as $x \to \infty$



• flux solutions (with a constant mass flux from zero)

$$J_{f_t}(x) o 1$$
, as $x o 0$



Class of kernels: $K(x,y) \approx x^{\gamma+\lambda}y^{-\lambda} + x^{-\lambda}y^{\gamma+\lambda}$

- 1) Region where coagulation between similar sizes dominates: $|\gamma + 2\lambda| < 1$
 - stationary solutions: constant flux solutions
 [F., Lukkarinen, Nota, Velázquez 2024]

$$J_f(x)=1$$

(dust) (gel)

There is a power law constant flux solution $f(x) = cx^{-\frac{\gamma+3}{2}}$, but this solution is not always unique.

Class of kernels: $K(x,y) \approx x^{\gamma+\lambda}y^{-\lambda} + x^{-\lambda}y^{\gamma+\lambda}$

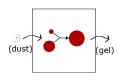
- 1) Region where coagulation between similar sizes dominates: $|\gamma+2\lambda|<1$
 - stationary solutions: constant flux solutions
 [F., Lukkarinen, Nota, Velázquez 2024]

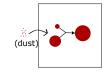
$$J_f(x)=1$$

There is a power law constant flux solution $f(x) = cx^{-\frac{\gamma+3}{2}}$, but this solution is not always unique.

• self-similar solution for homogeneous kernels $K(cx,cy)=c^{\gamma}K(x,y)$ with zero initial data ($\gamma<1$) [F., Franco, Velázquez 2022]

$$f_t(x) = \frac{t}{L(t)^2} \Phi\left(\frac{x}{L(t)}\right), \quad L(t) = t^{\frac{2}{1-\gamma}}$$





Class of kernels: $K(x, y) \approx x^{\gamma + \lambda} y^{-\lambda} + x^{-\lambda} y^{\gamma + \lambda}$

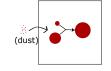
- 1) Region where coagulation between similar sizes dominates: $|\gamma+2\lambda|<1$
 - stationary solutions: constant flux solutions
 [F., Lukkarinen, Nota, Velázquez 2024]

$$J_f(x)=1$$

 $f(x) = cx^{-\frac{\gamma+3}{2}},$ (gel)

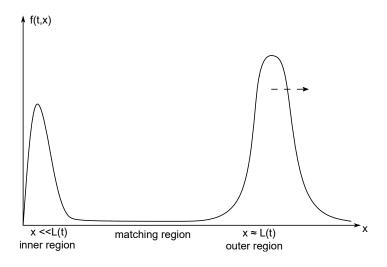
There is a power law constant flux solution $f(x) = cx^{-\frac{\gamma+3}{2}}$, but this solution is not always unique.

• self-similar solution for homogeneous kernels $K(cx,cy)=c^{\gamma}K(x,y)$ with zero initial data $(\gamma<1)$ [F., Franco, Velázquez 2022]



$$f_t(x) = \frac{t}{L(t)^2} \Phi\left(\frac{x}{L(t)}\right), \quad L(t) = t^{\frac{2}{1-\gamma}}$$

Expected long time behaviour: convergence towards a constant flux solution in a self-similar manner. [Davies, King, Wattis 1999]



Long time behaviour for flux solutions 2) different sizes

Class of kernels:
$$K(x,y) \approx x^{\gamma+\lambda}y^{-\lambda} + x^{-\lambda}y^{\gamma+\lambda}$$

- 2) Coagulation between particles of different sizes dominates: $|\gamma + 2\lambda| \ge 1$
 - No stationary solution exists [F., Lukkarinen, Nota, Velázquez 2021]
 - No flux solution is expected to exist

Long time behaviour for flux solutions 2) different sizes

Class of kernels: $K(x,y) \approx x^{\gamma+\lambda}y^{-\lambda} + x^{-\lambda}y^{\gamma+\lambda}$

- 2) Coagulation between particles of different sizes dominates: $|\gamma + 2\lambda| \ge 1$
 - No stationary solution exists [F., Lukkarinen, Nota, Velázquez 2021]
 - No flux solution is expected to exist

Main goals:

- To construct a flux solution for general initial data for $|\gamma + 2\lambda| < 1$ and $\gamma < 1$.
- ullet To show non-existence of flux solutions if $|\gamma+2\lambda|>1$. (under construction)

Coagulation kernels

We assume that $K \in C(\mathbb{R}^2_*)$ satisfies

$$K(x,y) \ge 0$$
, $K(x,y) = K(y,x)$

$$c_1\left(x^{\gamma+\lambda}y^{-\lambda}+y^{\gamma+\lambda}x^{-\lambda}\right) \leq K\left(x,y\right) \leq c_2\left(x^{\gamma+\lambda}y^{-\lambda}+y^{\gamma+\lambda}x^{-\lambda}\right)$$

$$\gamma, \lambda \in \mathbb{R}, \quad c_1, c_2 > 0.$$

Coagulation kernels

We assume that $K \in C(\mathbb{R}^2_*)$ satisfies

$$K(x,y) \ge 0$$
, $K(x,y) = K(y,x)$

$$c_1\left(x^{\gamma+\lambda}y^{-\lambda}+y^{\gamma+\lambda}x^{-\lambda}\right) \leq K\left(x,y\right) \leq c_2\left(x^{\gamma+\lambda}y^{-\lambda}+y^{\gamma+\lambda}x^{-\lambda}\right)$$

$$\gamma, \lambda \in \mathbb{R}, \quad c_1, c_2 > 0.$$

ullet $\gamma < 1$, (and $\gamma + \lambda, -\lambda < 1$) no gelation, hence

$$M_1(t) = M_1(0) + t$$

- $|\gamma + 2\lambda| < 1$ ensures existence of a constant flux solution, $J_f(x) = 1$
- $|\gamma + 2\lambda| \ge 1$, no constant flux solution exists

Coagulation kernels

We assume that $K \in C(\mathbb{R}^2_*)$ satisfies

$$K(x,y) \ge 0$$
, $K(x,y) = K(y,x)$

$$c_1\left(x^{\gamma+\lambda}y^{-\lambda}+y^{\gamma+\lambda}x^{-\lambda}\right) \leq K\left(x,y\right) \leq c_2\left(x^{\gamma+\lambda}y^{-\lambda}+y^{\gamma+\lambda}x^{-\lambda}\right)$$

$$\gamma, \lambda \in \mathbb{R}, \quad c_1, c_2 > 0.$$

• $\gamma < 1$, (and $\gamma + \lambda, -\lambda < 1$) no gelation, hence

$$M_1(t) = M_1(0) + t$$

- $|\gamma + 2\lambda| < 1$ ensures existence of a constant flux solution, $J_f(x) = 1$
- $|\gamma + 2\lambda| \ge 1$, no constant flux solution exists

Motivation:

- nm scale: free molecular kernel ($\lambda = 1/2$, $\gamma = 1/6$) \rightarrow non-existence
- μm scale: **diffusion kernel** ($\lambda = 1/3, \gamma = 0$) \rightarrow existence

Definition (Flux solution, weak formulation)

A time-dependent measure $f \in C([0,T],\mathcal{M}_+(\mathbb{R}_*))$ is a weak flux solution with initial data $f_0 \in \mathcal{M}_+(\mathbb{R}_*)$ such that $xf_0 \in \mathcal{M}_{+,b}(\mathbb{R}_*)$, in case

(ii) for almost every
$$(t,z) \in [0,T] \times \mathbb{R}_*$$

(ii) for almost every
$$(t,z) \in [0,T] \times \mathbb{R}_*$$

$$\int \mathsf{vf}(\mathsf{d}\mathsf{v}) = \int \mathsf{v}$$

$$\int_{(0,z]} x f_t(\mathrm{d}x) - \int_{(0,z]} x f_0(\mathrm{d}x) = -\int_0^t J_{f_s}(z) \mathrm{d}s + t$$

$$\int_{(0,z]} x f_t(\mathrm{d} x) - \int_{(0,z]} x$$

where

) for almost every
$$(t,z)\in [0,T] imes \mathbb{R}_*$$

is finite for all $t \in [0, T]$ and all $z \in \mathbb{R}_*$, with $\Omega_{\tau} := \{(x, y) \in \mathbb{R}^2_* : 0 < x \le z, z - x < y\}.$

(i) $xf \in C([0,T], \mathcal{M}_{+b}(\mathbb{R}_*))$

me-dependent measure
$$f \in C([0,T],\mathcal{M}_+(\mathbb{R}_*))$$

 $\int_0^t J_{f_s}(z) \mathrm{d}s := \int_0^t \iint_{\Omega} x K(x, y) f_s(\mathrm{d}x) f_s(\mathrm{d}y) \mathrm{d}s$

(1)

(2)

Proposition

Let $\gamma < 1$. Then f satisfies the weak coagulation equation

$$\int_{(0,\infty)} x\varphi(t,x)f_t(dx) = \int_{(0,\infty)} x\varphi(0,x)f_0(dx) + \int_0^t \int_{(0,\infty)} x\partial_s\varphi(s,x)f_s(dx)ds$$

$$+ \frac{1}{2} \int_0^t \int_{(0,\infty)} \int_{(0,\infty)} K(x,y)[(x+y)\varphi(s,x+y) - x\varphi(s,x) - y\varphi(s,y)]f_s(dx)f_s(dy)ds$$

for every $\varphi \in C^1_c([0,T] \times \mathbb{R}_*)$ and almost every $t \in [0,T]$, together with the flux boundary condition (in some weak sense),

$$\int_0^t J_{f_s}(z) \mathrm{d}s o t, ext{ as } z o 0, ext{ a.e. } t \in [0,T].$$

Proposition (Mass is linearly increasing)

Let $\gamma < 1$ and $|\gamma + 2\lambda| < 1$. Then,

$$\textit{M}_1(t) = \textit{M}_1(0) + t, \quad \text{ a.e. } t \in [0, T].$$

Proposition (Mass is linearly increasing)

Let $\gamma < 1$ and $|\gamma + 2\lambda| < 1$. Then,

$$M_1(t) = M_1(0) + t$$
, a.e. $t \in [0, T]$.

Fix $\varepsilon > 0$ arbitrarily. Since $|\gamma + 2\lambda| < 1$, there is a small positive δ such that

$$J_{f_t}^1(z;\delta) + J_{f_t}^3(z;\delta) \leq \varepsilon C_T.$$

On the other hand, using the upper bound of the kernel, it holds

$$J_{f_t}^2(z;\delta) \leq C \int_{\left[\frac{\delta}{1+\delta}z,\infty\right)} x^{\gamma} f_t(dx) \int_{\left[\frac{\delta}{1+\delta}z,\infty\right)} x f_t(dx)$$

Since $M_1(f_t) < \infty$, for all $t \in [0, T]$, and $\gamma < 1$, there is a large enough z_* , depending on ε and δ , such that, for all $z > z_*$,

$$J_{f_t}^2(z;\delta) \leq \varepsilon C_T$$
.

- $\rightarrow f$ behaves like a constant flux solution near zero
 - Upper bound

$$f_t(\mathrm{d}x)\lesssim rac{1}{x^{rac{\gamma+3}{2}}}C_t(t+M_1(f_0)),\quad x>0$$

Asymptotic lower bound

For each t there is a constant $\delta > 0$ and a constant b, satisfying 0 < b < 1, such that,

$$f_t(x) \gtrsim \frac{1}{x^{\frac{\gamma+3}{2}}} C_{t,b}, \quad x \in \left(0, \frac{\delta}{\sqrt{b}}\right)$$

- $\rightarrow f$ behaves like a constant flux solution near zero
 - Upper bound

$$f_t(\mathrm{d}x)\lesssim rac{1}{x^{rac{\gamma+3}{2}}}C_t(t+M_1(f_0)),\quad x>0$$

Asymptotic lower bound

For each t there is a constant $\delta > 0$ and a constant b, satisfying 0 < b < 1, such that.

$$f_t(x) \gtrsim \frac{1}{x^{\frac{\gamma+3}{2}}} C_{t,b}, \quad x \in \left(0, \frac{\delta}{\sqrt{b}}\right)$$

 \rightarrow no dust in the system

$$\int_0^t \int_{(0,x_0]} x f_s(\mathrm{d}x) \mathrm{d}s \leq C_T x_0^{\frac{1-\gamma}{2}}.$$

Existence of flux solutions

Theorem

Assume that $|\gamma+2\lambda|<1$ and $\gamma<1$. Given an initial data $f_0\in\mathcal{M}_+(\mathbb{R}_*)$ such that the mass measure satisfies $xf_0\in\mathcal{M}_{+,b}(\mathbb{R}_*)$, there exists a weak flux solution in the sense of the Definition.

Existence of flux solutions

Theorem

Assume that $|\gamma+2\lambda|<1$ and $\gamma<1$. Given an initial data $f_0\in\mathcal{M}_+(\mathbb{R}_*)$ such that the mass measure satisfies $xf_0\in\mathcal{M}_{+,b}(\mathbb{R}_*)$, there exists a weak flux solution in the sense of the Definition.

Proposition (Coagulation equation with constant-in-time source term)

Assume that $-\lambda, \gamma + \lambda < 1$. Let $f_0 \in \mathcal{M}_+(\mathbb{R}_*)$ be the initial data, with $\operatorname{spt}(f_0) \subset [a, +\infty)$ for some a > 0 and $xf_0 \in \mathcal{M}_{+,b}(\mathbb{R}_*)$. Assume that $\eta \in \mathcal{M}_{+,b}(\mathbb{R}_*)$ is a source term with $\operatorname{spt}(\eta) \subset [a, +\infty)$. Then, for every T > 0, there exists a weak solution $f \in C([0, T], \mathcal{M}_+(\mathbb{R}_*))$ to

$$\partial_t f_t = \frac{1}{2} \int_0^x K(x-y,y) f_t(x-y) f_t(y) dy + \int_0^\infty K(x,y) f_t(x) f_t(y) dy + \eta(x).$$

[Escobedo, Mishler 2006] time-dependent source, homogeneous kernels with $\gamma \in [0,1)$

Remark: Interestingly, solutions with source also exist for $|\gamma + 2\lambda| \ge 1$.

[Cristian, F., Franco, Nota, Lukkarinen, Velázquez 2023]

Construction of a flux solution

- For each $\varepsilon \in (0,1)$, let f^{ε} be a solution to the coagulation equation with source $\eta_{\varepsilon} = \frac{1}{\varepsilon} \delta_{\varepsilon}$ and initial data $f_0|_{[\varepsilon,+\infty)}$
- For each $M \in \mathbb{N}$, consider the family of the solutions restricted to the closed interval $I_M = [2^{-M}, 2^M]$.

Construction of a flux solution

- For each $\varepsilon \in (0,1)$, let f^{ε} be a solution to the coagulation equation with source $\eta_{\varepsilon} = \frac{1}{\varepsilon} \delta_{\varepsilon}$ and initial data $f_0|_{[\varepsilon,+\infty)}$
- For each $M \in \mathbb{N}$, consider the family of the solutions restricted to the closed interval $I_M = [2^{-M}, 2^M]$.

Construction of a diagonal sequence

- M=1, by compactness we find a limit point F^1 and a sequence $(\varepsilon_i)_{i=1}^{\infty}$ such that $xf^{\varepsilon_i}|_{I_1} \to F^1$.
- M=2, by compactness we find a limit point F^2 and a subsequence $(\varepsilon_{i_k})_{k=1}^{\infty}$ such that $xf^{\varepsilon_{i_k}}|_{I_2} \to F^2$. Moreover, $F^2|_{I_1} = F^1$.
- ...

Candidate solution as the limit of a diagonal subsequence

• Take a diagonal subsequence $(\varepsilon(i))_{i=1}^{\infty}$ and a limiting function F_t , defined pointwise in time by

$$\langle \varphi, F_t \rangle = \lim_{i \to \infty} \left\langle \varphi, x f^{\varepsilon(i)}|_{I_i} \right\rangle, \quad \varphi \in C_c(\mathbb{R}_*)$$

- $t \mapsto F_t$ is continuous
- canditate solution: $f \in C([0,T], \mathcal{M}_{+,b}(\mathbb{R}_*))$, such that xf = F.
- Final step: Show that f verifies the flux equation in the sense of the Definition.

Long time behaviour for the constant kernel

Theorem

If the coagulation kernel is constant, $K(x,y)\equiv 2$, there exists a unique solution f_t to the flux equation with the initial data $f_0=0$. This solution converges weakly as a measure on \mathbb{R}_* to the stationary solution of the flux equation, i.e.,

$$f_t(\mathrm{d}x) \to \frac{1}{\sqrt{2\pi}} x^{-\frac{3}{2}} \mathrm{d}x, \quad t \to \infty.$$

The proof relies on the use of the Bernstein transform $B_{f_t}(\lambda) = \int_{\mathbb{R}_*} (1 - e^{-\lambda x}) f_t(dx)$.

Non-existence (under construction)

Theorem

If $\gamma+2\lambda>1$ then there are no flux solutions in the sense of the definition satisfying the pointwise in time upper bound

$$\frac{1}{R} \int_{[R/2,R]} f_t(\mathrm{d}x) \le \frac{1}{R^{\frac{\gamma+3}{2}}} C_T, \quad R > 0$$
 (3)

Non-existence (under construction)

Theorem

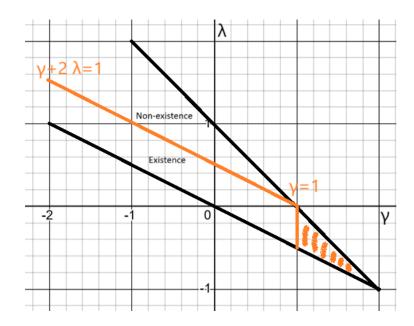
If $\gamma + 2\lambda > 1$ then there are no flux solutions in the sense of the definition satisfying the pointwise in time upper bound

$$\frac{1}{R} \int_{[R/2,R]} f_t(\mathrm{d}x) \le \frac{1}{R^{\frac{\gamma+3}{2}}} C_T, \quad R > 0$$
 (3)

The idea is to use the boundedness of the flux to obtain a bound for the moment $1-\lambda$ near the origin. Then the upper estimate (3) allow to conclude that (in some weak sense)

$$\int_0^t \int_{(0,z]} \int_{(z-x,\infty)} x K(x,y) f_s(dy) f_s(dx) ds \leq C_T z^{\frac{\gamma+2\lambda-1}{2}}.$$

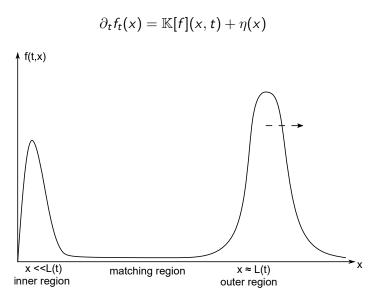
Therefore, taking $z \to 0$ and using $\gamma + 2\lambda > 1$, yields $\int_0^t Jds \to 0$ as $z \to 0$, which is a contradiction.



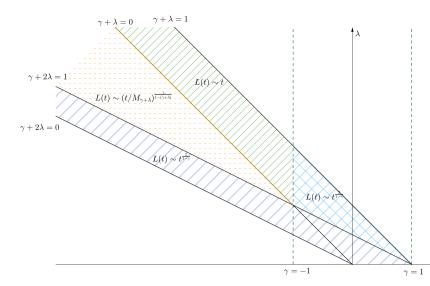
Coagulation equation with a source term $\gamma + 2\lambda > 1$

$$\partial_t f_t(x) = \mathbb{K}[f](x,t) + \eta(x)$$

Coagulation equation with a source term $\gamma + 2\lambda > 1$



Anomalous self-similarity



[F., Franco, Velázquez 2022], [Cristian, F., Franco, Velázquez 2023], [F., Franco, Nota, Lukkarinen, Velázquez 2023]

