Coagulation-Fragmentation equations with multiplicative coagulation kernel and constant fragmentation kernel

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Coagulation-Fragmentation Equation

Let $c(s,t) \geq 0$ be the density of clusters of particles of size $s \geq 0$ at time $t \geq 0$. We write the (continuous) Coagulation-Fragmentation equation as following

$$\partial_t c(s,t) = Q_c(c) + Q_f(c)\,. \tag{1}$$

Here, the equation has two main effects: the coagulation term Q_c and the fragmentation term Q_f.

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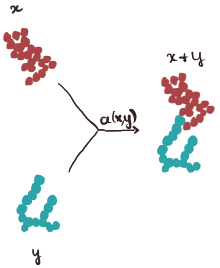
Here, the equation has two main effects: the coagulation term Q_c and the fragmentation term Q_f.

- Coagulation represents binary merging when two clusters of particles meet.
- Fragmentation represents binary splitting of a cluster.

Coagulation term

A cluster of size x meets a cluster of size y creates a cluster of size $x+y$.

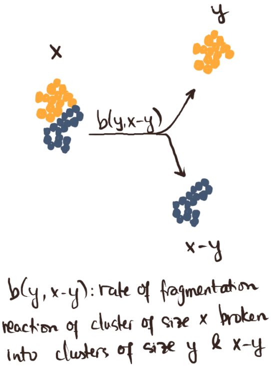


a(x,y): rate of coagulation reaction among an x-cluster and a y-cluster.

In the above, a denotes the coagulation kernel, which is a nonnegative and symmetric function defined on $(0,\infty)^2$.

Fragmentation term

A cluster of size x is broken into a cluster of size y and a cluster of size $x - y$ for some $y \in (0, x)$.



In the above, b denotes the fragmentation kernel, which is a nonnegative and symmetric function defined on $(0, \infty)^2$.

We can write that

$$Q_c(c)(s,t)$$
$$= \frac{1}{2}\int_0^s a(y, s-y)c(y,t)c(s-y,t)\,dy - c(s,t)\int_0^\infty a(s,y)c(y,t)\,dy\,,$$

and

$$Q_f(c)(s,t) = -\frac{1}{2}c(s,t)\int_0^s b(s-y,y)\,dy + \int_0^\infty b(s,y)c(y+s,t)\,dy\,.$$

And our C-F equation is

$$\partial_t c(s,t) = Q_c(c) + Q_f(c)\,.$$

Brief literature

When there is no fragmentation term Q_f, then C-F becomes the famous Smoluchowski equation. The Becker–Döring equations are special cases of C-F as well. Here is a very incomplete list of papers, surveys, and books in the literature.

Melzak (1957).
McLeod (1962).
Vigil–Ziff (1989).
Ball–Carr (1990).
Aldous (1999).
Escobedo–Mischler–Perthame (2002).
Escobedo–Laurencot–Mischler–Perthame (2003).
Menon–Pego (2004).
Bertoin (2006).
da Costa (2015).
Banasiak–Lamb–Laurencot (2019).

Our main focus and the critical case

A particularly interesting phenomenon of the C-F: the solution, while still physical, **does not conserve mass at all time.** There are two ways that this could happen in finite time.

- Formation of particles of infinite size: *gelation* phenomenon, which happens when the coagulation is strong enough.
- Formation of particles of size zero: *dust formation*, which happens when the fragmentation is strong enough.

These phenomena happen depending on the relative strengths between Q_c and Q_f. We here focus on a critical case where Q_c and Q_f have the same relative strength

$$a(s, \hat{s}) = s\hat{s} \quad \text{and} \quad b(s, \hat{s}) = 1 \quad \text{for all } s, \hat{s} > 0\,.$$

Weak solution to the critical C-F

We say that $c(s,t)$ is a solution to the critical C-F if for every test function $\phi \in BC([0,\infty)) \cap \mathrm{Lip}([0,\infty))$ with $\phi(0) = 0$, we have

$$\begin{aligned}
&\frac{d}{dt}\int_0^\infty \phi(s)c(s,t)\,ds \\
&= \frac{1}{2}\int_0^\infty \int_0^\infty (\phi(s+\hat{s}) - \phi(s) - \phi(\hat{s}))sc(s,t)\hat{s}c(\hat{s},t)\,d\hat{s}ds \\
&- \frac{1}{2}\int_0^\infty \int_0^s (\phi(s) - \phi(\hat{s}) - \phi(s-\hat{s}))\,d\hat{s}c(s,t)\,ds\,.
\end{aligned}$$

A natural idea from this weak formulation: Formally, take test function ϕ to be polynomials to read off information.

Some formal computations

1. The first moment (total mass) of all particles at time $t \geq 0$ is

$$m_1(t) = \int_0^\infty sc(s,t)\,ds.$$

Let $\phi(s) = s$ be a test function, we see right away that

$$m_1'(t) = \frac{d}{dt}\int_0^\infty sc(s,t)\,ds = 0 \quad \Rightarrow \quad \text{conservation of mass.}$$

But again, this is just a formal argument as $\phi(s) = s$ is not a bounded test function.

2. For $k \geq 0$, the k-th moment is

$$m_k(t) = \int_0^\infty s^k c(s,t)\,ds.$$

Some formal computations

The zeroth moment $m_0(t)$ represent the total number of clusters at time $t \geq 0$. Let $\phi(s) = 1$ be a test function. Then,

$$\begin{aligned} m_0'(t) &= \frac{d}{dt}\int_0^\infty c(s,t)\,ds \\ &= -\frac{1}{2}\int_0^\infty \int_0^\infty sc(s,t)\hat{s}c(\hat{s},t)\,d\hat{s}ds + \frac{1}{2}\int_0^\infty sc(s,t)\,ds \\ &= \frac{1}{2}m_1(t)(1 - m_1(t))\,. \end{aligned}$$

Suppose now $m_1(t) = m_1(0)$ **holds (conservation of mass).** Then,

- if $m_1(0) > 1$, $m_0(t)$ will be negative in finite time;
- on the other hand, $m_0(t)$ remains positive if $0 \leq m_1(0) \leq 1$.

Therefore, $m_1(0) = 1$ is believed to be the critical mass.

A conjecture

Conjecture. $m_1(0) = 1$ is the critical mass. Moreover,

1. If $0 \le m_1(0) \le 1$, then the critical C-F has a unique mass-conserving solution.
2. If $m_1(0) > 1$, then there is no global mass-conserving solution to the critical C-F.

This kind of formal computation and reasoning were discussed in
Vigil–Ziff (1989),
Escobedo–Mischler–Perthame (2002),
Escobedo–Laurencot–Mischler–Perthame (2003).

Some partial progress were done for this conjecture in the literature (to be described) by using the moment bound method.

Earlier progress toward resolving this conjecture

1. **Banasiak–Lamb–Laurencot (2019)** showed that if $m_1(0) > 1$ and $m_0(0) < \infty$, then there is no global mass-conserving solution to the critical C-F.
2. **Laurencot (2019)** obtained existence and uniqueness of mass-conserving solutions to C-F provided that c_0 has $0 < m_1(0) < \frac{1}{4 \log 2}$ and c_0 satisfies some further moment conditions.

Bernstein's transform

Another natural candidate for test functions is a combination of polynomials as described above, and let

$$\phi(s) = 1 - e^{-sx}$$

be a test function for each fixed $x \geq 0$. Denote by

$$F(x,t) = \int_0^\infty (1 - e^{-sx}) c(s,t)\, ds.$$

There is one key/magic point here

$$\phi(s+\hat{s}) - \phi(s) - \phi(\hat{s}) = -1 - e^{-(s+\hat{s})x} + e^{-sx} + e^{-\hat{s}x} = -\phi(s)\phi(\hat{s}).$$

And this helps to write down an equation for F.

A singular Hamilton-Jacobi equation

By using the key point above and some computations, we arrive at

$$\partial_t F(x,t) = -\frac{1}{2}(m_1(t) - \partial_x F(x,t))(m_1(t) - \partial_x F(x,t) + 1) - \frac{F}{x} + m_1(t)\,.$$

The key point is to transform a seemingly hopeless nonlocal equation to a somewhat more tractable nonlinear PDE, which enjoys some major developments in the past few decades. If conservation of mass holds, then we can assume $m_1(t) = m > 0$ for all $t \geq 0$ for some $m \in (0,\infty)$.

$$\partial_t F + \frac{1}{2}(\partial_x F - m)(\partial_x F - m - 1) + \frac{F}{x} - m = 0 \quad \text{in } (0,\infty)^2\,, \tag{2a}$$

$$0 \leq F(x,t) \leq mx \quad \text{on } [0,\infty)^2\,, \tag{2b}$$

$$F(x,0) = F_0(x) \quad \text{on } [0,\infty)\,. \tag{2c}$$

A singular Hamilton-Jacobi equation

One then can study wellposedness and properties of solutions of (2) to deduce back information of C-F. Indeed, this is our main goal.
Note that the condition (2b) implies that $F(0,t) = 0$ and that it comes directly from the Bernstein transform. Indeed, as $c \geq 0$, it is clear that $F \geq 0$. Besides, the inequality $1 - e^{-sx} \leq sx$ for $s, x \geq 0$ gives

$$F(x,t) = \int_0^\infty (1 - e^{-sx}) c(s,t)\, ds \leq \int_0^\infty sxc(s,t)\, ds = mx\,.$$

Moreover, the dominated convergence theorem gives

$$\lim_{x\to\infty} \frac{F(x,t)}{x} = \lim_{x\to\infty} \int_0^\infty \frac{1 - e^{-sx}}{x} c(s,t)\, ds = 0\,,$$

which means that $F(x,t)$ is sublinear in x. **It is therefore natural to search for solutions of (2) that are sublinear in x.**

A singular Hamilton-Jacobi equation

A quick look at our singular Hamilton-Jacobi equation

$$\partial_t F + \frac{1}{2}(\partial_x F - m)(\partial_x F - m - 1) + \frac{F}{x} - m = 0.$$

1. The Hamiltonian

$$H(p,z,x) = \frac{1}{2}(p-m)(p-m-1)+\frac{z}{x}-m \quad \text{for all } (p,z,x) \in \mathbb{R}\times\mathbb{R}\times(0,\infty)\,,$$

which is of course singular at $x = 0$.

2. This singular HJ equation admits two special solutions $F(x,t) = mx$, $F(x,t) = (m-1)x$. Both special solutions have linear growth at infinity except when $m = 1$.

Our main results

Theorem (T.-Van (2019))

Assume that $0 < m \leq 1$. *Assume further that* F_0 *is Lipschitz, sublinear, and* $0 \leq F_0(x) \leq mx$. *Then, HJ has a unique Lipschitz, sublinear solution* F.

Corollary

Assume that $m_1(0) = m \in (0, 1]$. *Then, C-F has at most one mass-conserving solution.*

We have obtained uniqueness result for the full range for $0 < m \leq 1$.

Our main results

Theorem (T.-Van (2019))

Suppose $m > 1$. *Assume that* F_0 *is smooth, sublinear, and* $0 \leq F_0(x) \leq mx$. *Then equation* (2) *does NOT admit a solution* $F \in C^1([0,\infty)^2)$ *which is sublinear in* x.

Corollary

Assume that $m_1(0) = m > 1$. *Then, there is no mass-conserving solution to C-F equation.*

We here obtain non-existence of mass-conserving solutions under the minimal assumption, that is, $m_1(0) > 1$. We do not need to impose that the zeroth moment, number of clusters, is finite as in **Banasiak–Lamb–Laurencot (2019)**.

Our main results

Next is our existence result for C-F when $0 < m < \frac{1}{2}$.

Theorem (T.-Van (2019))

Assume that F_0 is the Bernstein transform of $c_0 = c(\cdot, 0)$, where c_0 has $m_1(0) = m \in (0, \frac{1}{2})$ and also bounded second moment, that is,

$$m_2(0) = \int_0^\infty s^2 c(s, 0)\, ds \leq C\,.$$

Then C-F has a mass-conserving weak solution in the measure sense.

We have obtained existence result in the range of $0 < m < \frac{1}{2}$.

Why is it hard to obtain existence result?

Recall the Bernstein transform

$$F(x,t) = \int_0^\infty (1 - e^{-sx}) c(s,t)\, ds.$$

It is clear that F is smooth in x, and, in fact, for $n \geq 1$,

$$\partial_x^n F(x,t) = \int_0^\infty (-1)^{n+1} s^n e^{-sx} c(s,t)\, ds.$$

In particular, $(-1)^{n+1} \partial_x^n F(x,t) \geq 0$ always.

Therefore, to obtain an existence result, we need to show that the viscosity solution F to HJ satisfies that

$$F \in C^\infty((0,\infty)^2) \quad \text{and } (-1)^{n+1} \partial_x^n F \geq 0.$$

Our strategy when $0 < m < 1/2$ – Step 1

First step: Show that $F \in C^{1,1}((0,\infty)^2) \cap C^1([0,\infty) \times (0,\infty))$.

Let $a \in C^\infty([0,\infty))$ be a nondecreasing and concave function such that

$$a(x) = \begin{cases} x\,, & x \in [0,1]\,, \\ 2\,, & x \in [3,\infty)\,. \end{cases} \tag{3}$$

For $\epsilon > 0$, we consider

$$\begin{cases} \partial_t F + \frac{1}{2}(\partial_x F - m)(\partial_x F - m - 1) + \frac{F}{x} - m & = \epsilon a(x) \partial_{xx} F\,, \\ F(x,0) & = F_0(x)\,, \\ F(0,t) & = 0\,. \end{cases} \tag{4}$$

It is not hard to prove the solution to the above, F^ϵ satisfies

$$0 \leq \partial_x F^\epsilon \leq m \quad \text{and} \quad \partial_x^2 F^\epsilon \leq 0.$$

What's really hard is to get a lower bound of $\partial_x^2 F^\epsilon$.

Our strategy when $0 < m < 1/2$ – Step 1

To get a lower bound of $\partial_x^2 F^\epsilon$, we use maximum principle to show that

$$x\partial_x^2 F^\epsilon \geq -1.$$

Here is a quick sketch. Assume that, for some $(x_0, T) \in (0, \infty)^2$,

$$\min_{[0,\infty)\times[0,T]} x\partial_x^2 F^\epsilon(x,t) = x_0\partial_x^2 F^\epsilon(x_0, T) = \alpha\,.$$

Then,

$$\alpha^2 + A\alpha + B \geq 0\,,$$

$$A = m + \frac{3}{2} - 2\epsilon - \partial_x F^\epsilon(x_0, T), \quad B = \frac{2(F^\epsilon(x_0, T) - x_0\partial_x F^\epsilon(x_0, T))}{x_0}\,.$$

From this and the continuity method, we yield

$$\alpha \geq \frac{-A + \sqrt{A^2 - 4B}}{2} \geq -1\,.$$

Here, $\kappa = m - \partial_x F^\epsilon(x_0, T) \in (0, m)$,

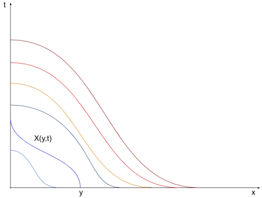
$$A^2 - 4B \geq (\frac{3}{2} + \kappa - 2\epsilon)^2 - 8\kappa \geq (\frac{1}{2} - \kappa)(\frac{9}{2} - \kappa) - 8\epsilon > 0.$$

Our strategy when $0 < m < 1/2$ – Step 2

Second step: Show that $F \in C^\infty((0,\infty)^2)$.

Denote by $X(x,t)$ the characteristic starting from x, that is, $X(x,0) = x$. Set $P(x,t) = \partial_x F(X(x,t),t))$, and $Z(t) = F(X(x,t),t)$ for all $t \geq 0$. We have the following Hamiltonian system

$$\begin{cases} \dot{X} = \partial_p H(P(t),Z(t),X(t)) = P(t) - \left(m + \frac{1}{2}\right) , \\ \dot{P} = -\partial_x H - (\partial_z H)P = \frac{Z(t)}{X(t)^2} - \frac{P(t)}{X(t)} , \\ \dot{Z} = P \cdot \partial_p H - H = \frac{P(t)^2}{2} - \frac{Z(t)}{X(t)} + \frac{m(1-m)}{2} . \end{cases}$$



Our strategy when $0 < m < 1/2$ – Step 3

Third step: Show that $(-1)^{n+1}\partial_x^n F \geq 0$ in $(0,\infty)^2$ by induction.

Let $W(x,t) = x^{k-1}\partial_x^k F$, and we have

$$\partial_t W - \left(m + \frac{1}{2} - \partial_x F\right)\left(\partial_x W - (k-1)\frac{W}{x}\right) + \frac{W}{x} - \frac{k}{x^2}\int_0^x W(z,t)\,dz$$
$$= -k(\partial_x^2 F)W - x^{k-1}\sum_{i=2}^{k-2}\frac{k!(\partial_x^{i+1}F)(\partial_x^{k+1-i}F)}{i!(k-i)!}.$$

We use the analysis along characteristics and localization arguments to conclude.

Why choose $x\partial_x^2 F$?

1. Recall that

$$\partial_x^2 F(x,t) = \int_0^\infty (-1)s^2 e^{-sx} c(s,t)\, ds.$$

So,

$$x\partial_x^2 F(x,t) = -\int_0^\infty [(sx)e^{-sx}] sc(s,t)\, ds,$$

which gives a correct scaling as we have $m_1(t) = \int_0^\infty sc(s,t)\, ds = m$.

2. This is also the reason why we deal with $W(x,t) = x^{k-1}\partial_x^k F$ as in the above slide.

Concluding remarks

This is just the beginning. There are many more interesting questions to be studied.

1. Open problem: Existence of solution when $1/2 \leq m \leq 1$.
2. Deeper connection to the optimal control theory.
3. Large time behavior results. Recent result **Mitake-T.-Van (2020)**.

THANK YOU FOR YOUR ATTENTION!