Some mathematical properties of coagulation and coagulation-fragmentation equations.

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The model. (Smoluchowski, 1917).

\[ \partial_t c_n = \frac{1}{2} \sum_{j=1}^{n-1} K_{n-j,j} c_{n-j} c_j - \sum_{j=1}^\infty K_{n,j} c_n c_j - \frac{1}{2} \sum_{j=1}^{n-1} \Gamma_{n,j} c_j + \sum_{j=1}^\infty \Gamma_{n+j,n} c_{n+j} \]

\[ c_n = c_n(t) = \text{concentration of clusters of size } n \]

\[ K_{n,j} = \text{coagulation rate } (n,j) \rightarrow (n+j) \]

\[ \Gamma_{n,j} = \text{fragmentation rate } (n) \rightarrow (j,n-j) \]

Continuous version:

\[ \partial_t c(v) = \frac{1}{2} \int_0^v K(v-w,w)c(v-w)c(w)dw - \int_0^\infty K(v,w)c(v)c(w)dw \]

\[ -\frac{1}{2} \int_0^v \Gamma(v,w)c(w)dw + \int_0^\infty \Gamma(v+w,w)c(v+w)dw \]

where \( v \) is the particle size.
Derivation of the model: Smoluchowski (1917).

The collision kernel depends on the specific coagulation fragmentation mechanism.

Coagulation rates:

- Aggregation of Brownian particles:

\[ K(v_1, v_1) = \frac{2k_B T}{3\mu} \left( \frac{1}{v_1^3} + \frac{1}{v_2^3} \right) \left( v_1^{\frac{1}{3}} + v_2^{\frac{1}{3}} \right) \]

- Coagulation of particles in laminar shear flows:

\[ K(v_1, v_2) = \frac{4}{3} (a_1 + a_2)^3 \frac{du}{dx}, \quad \frac{4\pi}{3} (a_j)^3 = v_j, \quad j = 1, 2 \]
Coagulation rates:

- Turbulent shear coagulation (Saffman-Turner, 1956):

\[ K(v_1, v_2) = 1.3 \sqrt{\frac{\varepsilon_d}{V}} (a_1 + a_2)^3, \quad \sqrt{\left( \frac{\partial v}{\partial x_m} \right)^2} = \frac{2}{15} \sqrt{\frac{\varepsilon_d}{V}} \]

where \( \varepsilon_d \) is the rate of dissipation of energy for unit of volume in a turbulent flow.

- Ballistic coagulation. (Particles in a gas much smaller than the mean free path):

\[ K(v_1, v_1) = \left( \frac{3}{4\pi} \right)^{\frac{1}{6}} \left( \frac{6k_B T}{\rho_p} \right)^{\frac{1}{2}} \left( \frac{1}{v_1} + \frac{1}{v_2} \right)^{\frac{1}{2}} \left( v_1^3 + v_2^3 \right)^{\frac{1}{2}} \]
Coagulation equation: Qualitative behaviour of the solutions.

\[ \partial_t c(v) = \frac{1}{2} \int_0^v K(v - w, w)c(v - w)c(w)dw - \int_0^\infty K(v, w)c(v)c(w)dw \]

Explicitly solvable kernels:
\[ K_I(v, w) = 1, \quad K_{II}(v, w) = v + w, \quad K_{III}(v, w) = v \cdot w \]

The equations are solvable using Laplace transforms:
\[ \tilde{c}(z) = \int_0^\infty c(v)e^{-zv}dv \]

(Flory, Stockmeyer, Mc Leod, van Dongen-Ernest, Menon-Pego,...).
Coagulation equation: **Self-similar behaviour.**

Homogeneous kernels $K(\lambda v, \lambda w) = \lambda^\mu K(v, w), \; \mu \leq 1$.

Mass conserving solutions:

$$\partial_t \left( \int_0^\infty vc(v, t) dv \right) = 0 \; , \; c(v, t) = \frac{1}{t^{2\alpha}} F\left( \frac{v}{t^\alpha} \right)$$

Power law behaviour (fat tails):

$$c(v, t) \simeq \frac{1}{v^\beta} \; \text{as} \; v \to \infty, \; \beta \in (1, 2), \; c(v, t) = \frac{1}{t^{\alpha\beta}} F\left( \frac{v}{t^\alpha} \right)$$

The average radius increases as a power law:

$$\langle v \rangle = Ct^\alpha$$
Coagulation equation: Self-similar behaviour.
Kernels $K_I = 1$, $K_{II} = v + w$: Explicit formulas.

General kernels. Existence of self-similar solutions:
- Mass conserving case (Escobedo-Mischler, Fournier-Laurencot).
- Fat tails (Niethammer-V, Niethammer-Throm-V).

Uniqueness of self-similar solutions:
- Perturbative results (mass conserving case),
  $K = 1 + \varepsilon\left[(\frac{v}{w})^\mu + (\frac{w}{v})^\mu\right]$, $\varepsilon > 0$ small (Niethammer-Throm-V).
- Stability of self-similar solutions for general kernels largely open.
Coagulation-fragmentation models.

\[
\frac{\partial_t c_n}{c_n} = \frac{1}{2} \sum_{j=1}^{n-1} K_{n-j,j} c_{n-j} c_j - \sum_{j=1}^{\infty} K_{n,j} c_n c_j - \frac{1}{2} \sum_{j=1}^{n-1} \Gamma_{n,j} c_j + \sum_{j=1}^{\infty} \Gamma_{n+j,n} c_{n+j}
\]

**Detailed balance condition.** The coagulation and fragmentation rates related as:

\[
\Gamma_{n+j,n} = K_{n,j} e^{[\Delta E_{n+j} - \Delta E_n - \Delta E_j]}
\]

for some free energy functional \( \Delta E_n \).

\((n,j) \succsim n + j\) (Equal rates at equilibrium)

Steady states: \( c_n^s = e^{-\beta \Delta E_n} (z)^n \), \( z = e^{\beta \mu} \).

Global stability using the entropy: \( S = \sum_{n=1}^{\infty} c_n \log \left( \frac{c_n}{c_n^s} \right) \)
The Becker-Döring model: A particular type of coagulation-fragmentation models. (Nucleation theory).
(Cluster sizes change only by means of addition or loss of monomers).

\[ \dot{c}_1 = -J_1 - \sum_{l=1}^{\infty} J_l, \quad \dot{c}_n = J_{n-1} - J_n, \quad 2 \leq n < \infty \]

\[ J_n = a_n c_n c_1 - b_n c_{n+1}, \quad 1 \leq n < \infty \]

with \( a_n \approx n^{\frac{1}{3}}, \quad b_n \approx n^{\frac{1}{3}} \) as \( n \to \infty \). Conservation of the number of monomers yields:

\[ \dot{\sum_{n=1}^{\infty} n c_n} = 0 \]
The Becker-Döring model: Detailed balance is assumed. Steady states:

\[ c_n^s(z) \simeq \frac{z^n}{(1 + n)^a} \text{ as } n \to \infty, \ a > 2 \]

Total number of monomers for unit of volume:

\[ N = \sum_{n=1}^{\infty} nc_n^s(z) \]

Therefore, steady states exist for:

\[ z \leq 1 \text{ or } N \leq N_* = \sum_{n=1}^{\infty} nc_n^s(1) < \infty \]
The Becker-Döring model:

Steady states exist if:

\[ z \leq 1 \text{ or } N \leq N_* = \sum_{n=1}^{\infty} nc_n^s(1) < \infty \]

What happens if \( N_0 = \sum_{n=1}^{\infty} nc_n(0) > N_* \)?

(Ball, Carr, Penrose):

If \( N_0 \leq N_* \) then \( c_n(t) \to c_n^s \text{ as } t \to \infty, \sum_{n=1}^{\infty} nc_n^s = N_0 \)

If \( N_0 > N_* \) the excess of mass escapes to \( n = \infty \) as \( t \to \infty \) (Coarsening)

Formal asymptotics of the mass escaping. (Self-similar behaviour as \( n \approx t^3 \)).
Oscillatory behaviours in coagulation and coagulation-fragmentation models.

- Coagulation equation. Kernels close to the diagonal kernel. (Homogeneity one):

\[ K(v,w) = v^\alpha w^\alpha (v + w)^{1-2\alpha} , \ \alpha \text{ large.} \]
Other phenomena:

- Gelation: Loss of mass in finite time for kernels with homogeneity larger than one. (Example $K_{III} = x \cdot y$).

- Solutions with fluxes of monomers.

- Oscillatory behaviour for coagulation-fragmentation models without detailed balance (Niethammer-Pego-V).
Concluding remarks:

- Coagulation and coagulation-fragmentation equations: A class of kinetic equations which describe aggregation phenomena in many physical situations. (Coagulation of particles in flows, polymerization, droplet merging in the atmosphere, planetesimals,...).
- The rigorous mathematical analysis of these equations has been restricted mostly to the study of problems in which the clusters described by just one parameter.
- A complete picture of the solutions for coagulation equation is available for some specific explicitly solvable kernels.
- In the case of the coagulation-fragmentation equation it is possible to derive stability results for steady states if the detailed balance condition holds and there are not phase transitions.
- For general kernels, the only general information available is the existence of self-similar solutions or steady states. Uniqueness and stability of these solutions is mostly open.
Thank you for your attention!