Some mathematical properties of coagulation and coagulation-fragmentation equations.

Juan J. L. Velázquez (University of Bonn).

The model. (Smoluchowski, 1917).

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

$c_n = c_n(t) =$ concentration of clusters of size n

$K_{n,j} =$ coagulation rate $(n,j) \to (n+j)$

$\Gamma_{n,j} =$ fragmentation rate $(n) \to (j, n-j)$

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.

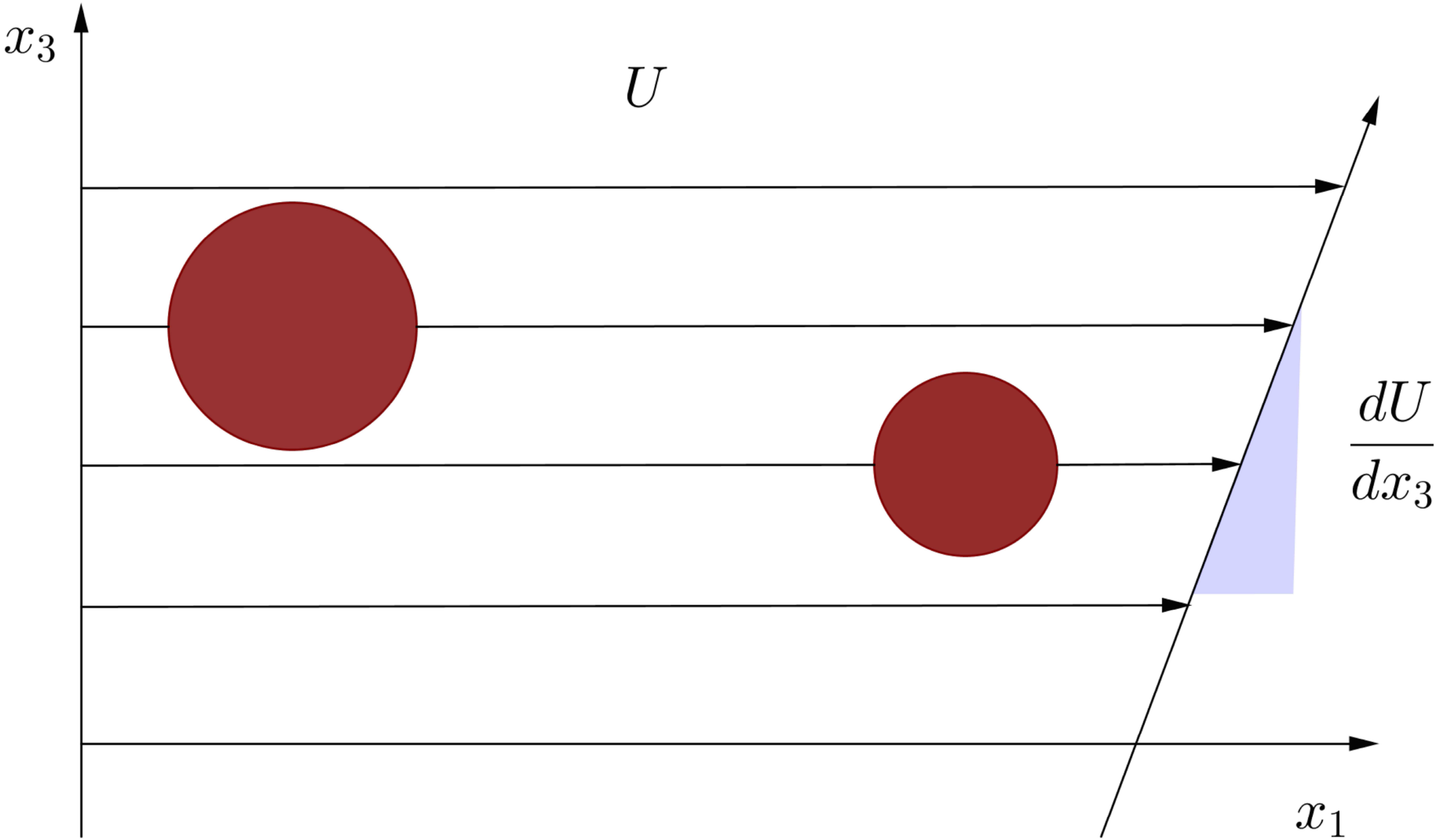
Coagulation rates:

- Aggregation of Brownian particles:

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

- Coagulation of particles in laminar shear flows:

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



x_3
U
$\frac{dU}{dx_3}$
x_1

Coagulation rates:

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

$$K(v_1, v_2) = 1.3\sqrt{\frac{\epsilon_d}{\nu}}(a_1 + a_2)^3 \ , \ \sqrt{\overline{\left(\frac{\partial v_\ell}{\partial x_m}\right)^2}} = \frac{2}{15}\sqrt{\frac{\epsilon_d}{\nu}}$$

where ϵ_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):

$$K(v_1, v_1) = \left(\frac{3}{4\pi}\right)^{\frac{1}{6}}\left(\frac{6k_BT}{\rho_p}\right)^{\frac{1}{2}}\left(\frac{1}{v_1} + \frac{1}{v_2}\right)^{\frac{1}{2}}\left(v_1^{\frac{1}{3}} + v_2^{\frac{1}{3}}\right)^2$$

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:

$$K_I(v,w) = 1 \ , \ K_{II}(v,w) = v + w \ , \ K_{III}(v,w) = v \cdot w$$

The equations are solvable using Laplace transforms:

$$\tilde{c}(z) = \int_0^\infty c(v)e^{-zv}dv$$

(Flory, Stockmeyer, Mc Leod, van Dongen-Ernst, 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),
  $K = 1 + \varepsilon[(\frac{v}{w})^{\mu} + (\frac{w}{v})^{\mu}]$, $\varepsilon > 0$ small (Niethammer-Throm-V).
- Stability of self-similar solutions for general kernels largely open.

Coagulation-fragmentation models.

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

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

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

for some free energy functional ΔE_n.

$(n,j) \rightleftarrows n+j$ (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).

$$\partial_t c_1 = -J_1 - \sum_{\ell=1}^{\infty} J_\ell \ , \ \partial_t c_n = J_{n-1} - J_n \ , \ 2 \leq n < \infty$$

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

with $a_n \simeq n^{\frac{1}{3}}, \ b_n \simeq n^{\frac{1}{3}}$ as $n \to \infty$. Conservation of the number of monomers yields:

$$\partial_t \left(\sum_{n=1}^{\infty} n c_n \right) = 0$$

The Becker-Döring model: Detailed balance is assumed. Steady states:

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

Total number of monomers for unit of volume:

$$N = \sum_{n=1}^{\infty} n c_n^s(z)$$

Therefore, steady states exist for:

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

The Becker-Döring model:

Steady states exist if:

$$z \le 1 \text{ or } N \le N_* = \sum_{n=1}^{\infty} n c_n^s(1) < \infty$$

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

(Ball, Carr, Penrose):

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

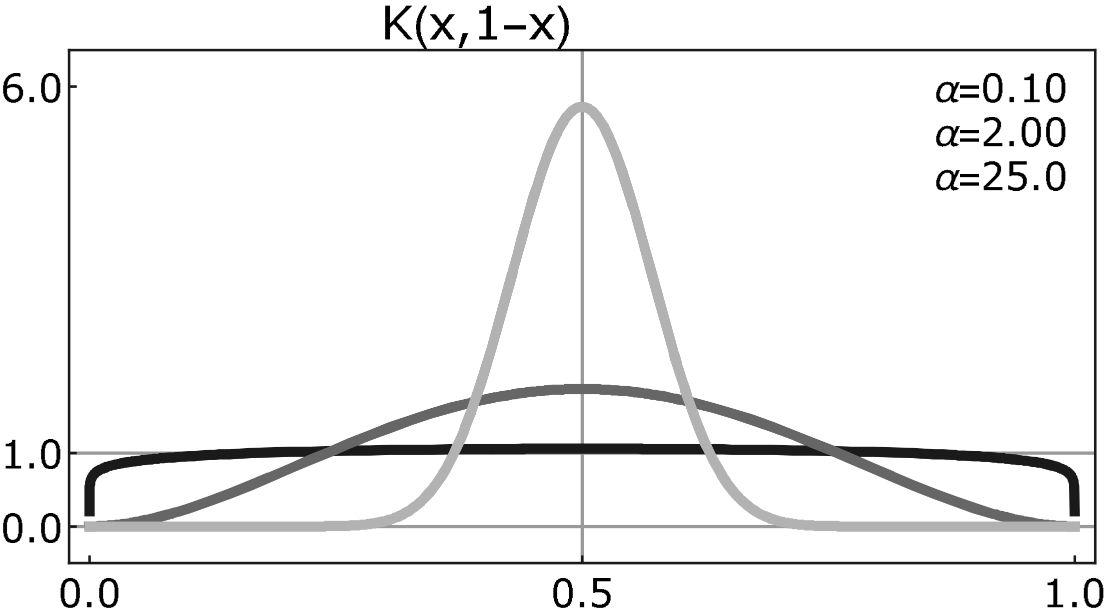
If $N_0 > N_*$ the excess of mass escapes to $n = \infty$ as $t \to \infty$ (Coarsening)

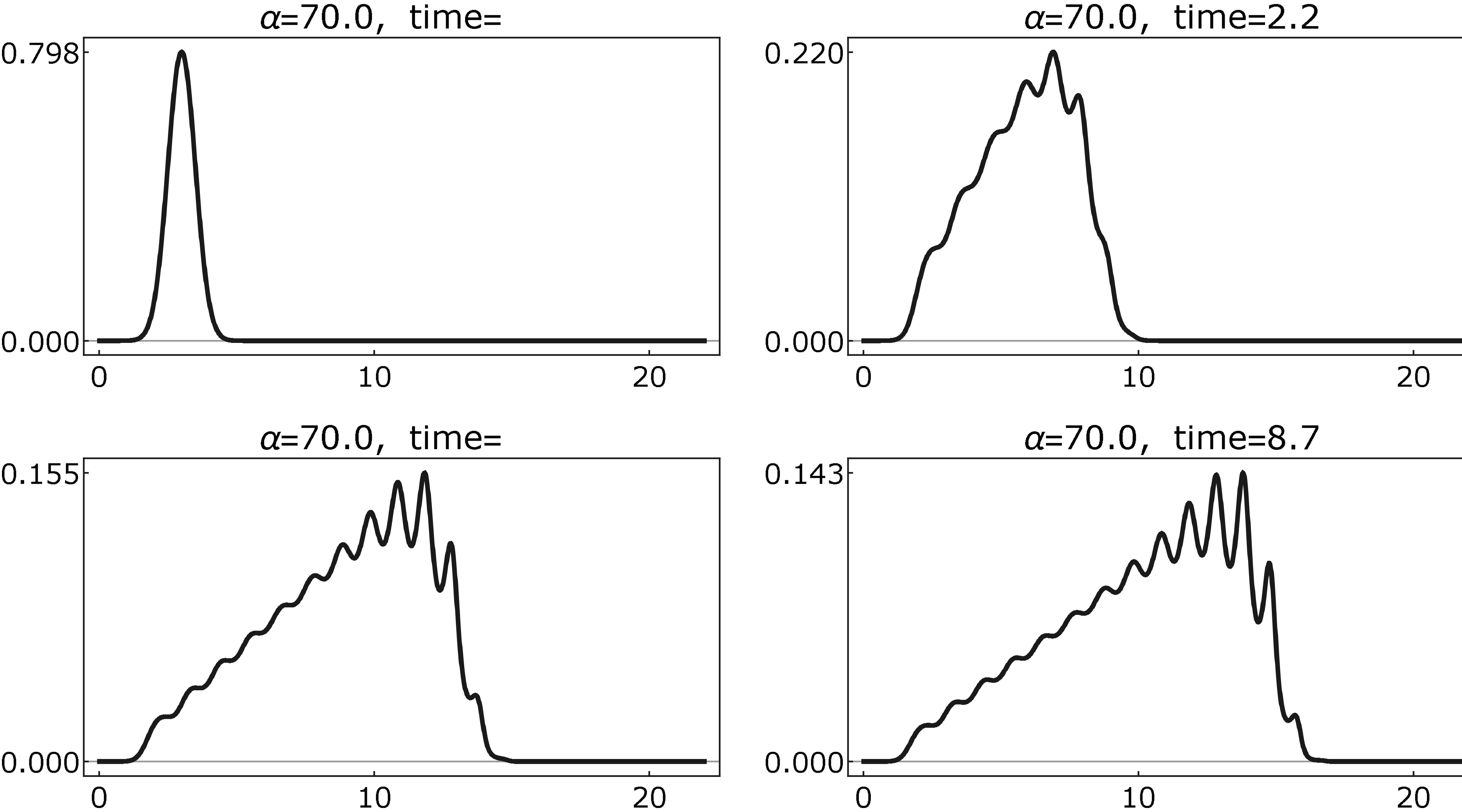
Formal asymptotics of the mass escaping. (Self-similar behaviour as $n \simeq t^3$).

Oscillatory behaviours in coagulation and coagulation-fragmentation models.

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

$$K(v,w) = v^{\alpha} w^{\alpha} (v+w)^{1-2\alpha} \quad , \quad \alpha \text{ large.}$$


K(x,1−x)
6.0
1.0
0.0
α=0.10
α=2.00
α=25.0
0.0
0.5
1.0



α=70.0, time=
0.798
0.000
0
10
20
α=70.0, time=2.2
0.220
0.000
0
10
20
α=70.0, time=
0.155
0.000
0
10
20
α=70.0, time=8.7
0.143
0.000
0
10
20

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 a 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!