Coagulation-Fragmentation Models

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Outline of the course

1. Motivation and modelling
2. The Smoluchowski equation : a model for coagulation
3. Coagulation-Fragmentation Models
   - The Becker-Döring model
   - Saturation phenomena and large-time asymptotics
4. Inhomogeneous coagulation-fragmentation models with diffusion
   - The existence theory of Laurençot and Mischler
   - A duality argument an entropy method
   - A fast reaction limit

Modelling

The Formation and the Break-up of Clusters/Polymers in

Physics aerosols, rainsdrops, smoke, sprays

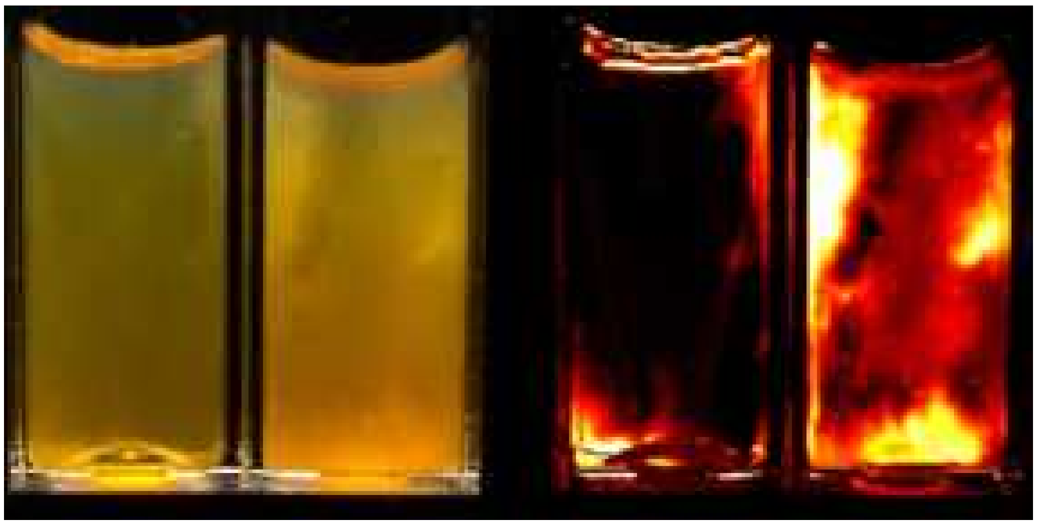
Chemistry monomers/polymers

Astronomy formation of galaxies

Biology hematology, animal grouping

Background

The Formation and the Break-up of Clusters/Polymers



assume particles fully described by mass/size $y \in Y$.

full/realistic models can quickly get very difficult

Introduction

Background

Levels of description:

Microscopic description $N \geq 1$ particles, stochastic events

Mesoscopic description density $f(t, y)$, mean-field equation

Macroscopic description physical observations

Linking limits

micro$\longrightarrow$meso Convergence of stochastic processes (Marcus-Lushnikov process), mean-field limits

meso$\longrightarrow$macro Fast-reaction-limits

The Smoluchowski coagulation equation [1916/17,1928]

mesoscopic density of clusters/polymers $f(t, y) \geq 0$, $y \in Y$:

$$\partial_t f(t, y) = Q_{coag}(f, f)(y) = Q_1(f, f) - Q_2(f, f)$$

$Q_1(f, f)$: gain of particles of size y

$$\{y'\} + \{y - y'\} \xrightarrow{a(y', y-y')} \{y\}, \qquad y' < y$$

Consider only binary interaction!

The Smoluchowski coagulation equation [1916/17,1928]

mesoscopic density of clusters/polymers $f(t,y) \geq 0$, $y \in Y$:

$$\partial_t f(t,y) = Q_{coag}(f,f)(y) = Q_1(f,f) - Q_2(f,f)$$

$Q_1(f,f)$: gain of particles of size y

$$\{y'\} + \{y-y'\} \xrightarrow{a(y',y-y')} \{y\}, \qquad y' < y$$

$Q_2(f,f)$: loss of particles of size y

$$\{y\} + \{y'\} \xrightarrow{a(y,y')} \{y+y'\}, \qquad y' \in Y$$

The Smoluchowski coagulation equation [1916/17,1928]

mesoscopic density of clusters/polymers $f(t,y) \geq 0$, $y \in Y$:

$$\partial_t f(t,y) = Q_{coag}(f,f)(y) = Q_1(f,f) - Q_2(f,f)$$

$Q_1(f,f)$: gain of particles of continuous size $y \in [0,\infty)$

$$Q_1(f,f) = \frac{1}{2}\int_0^y a(y', y-y') f(y-y') f(y') dy'$$

$Q_2(f,f)$: loss of particles of size y

$$\{y\} + \{y'\} \xrightarrow{a(y,y')} \{y+y'\}$$

The Smoluchowski coagulation equation [1916/17,1928]

mesoscopic density of clusters/polymers $f(t,y) \geq 0$, $y \in Y$:

$$\partial_t f(t,y) = Q_{coag}(f,f)(y) = Q_1(f,f) - Q_2(f,f)$$

$Q_1(f,f)$: gain of particles of continuous size $y \in [0,\infty)$

$$Q_1(f,f) = \frac{1}{2}\int_0^y a(y', y-y')\, f(y-y')\, f(y')\, dy'$$

$Q_2(f,f)$: loss of particles of continuous size $y \in [0,\infty)$

$$f(y)\int_0^\infty a(y,y')\, f(y')\, dy'$$

The continuous Smoluchowski coagulation equation

Evolution ($t \geq 0$) of mesoscopic density $f(t,y) \geq 0$ of clusters/polymers of size $y \in [0,\infty)$:

$$\partial_t f(t,y) = Q_{coag}(f,f)(y) = Q_1(f,f)(y) - Q_2(f,f)(y)$$

$$Q_{coag}(f,f)(y) = \frac{1}{2}\int_0^y a(y', y-y') f(y-y') f(y') dy' - f(y)\int_0^\infty a(y,y') f(y') dy'$$

coagulation coefficient/kernel/rate $0 \leq a(y,y') = a(y',y)$

The Smoluchowski equation

Examples of coagulation coefficients $0 \le a(y,y') = a(y',y)$

Colloidal particles: e.g. Smoluchowski $\alpha = \gamma = 1/3$, $\beta = 1$

$$a(y,y') = (y^\alpha + (y')^\alpha)^\beta (y^{-\gamma} + (y')^{-\gamma}), \qquad \alpha, \beta, \gamma \ge 0,\ \alpha\beta \le 1$$

Ballistic kernel:

$$a(y,y') = (y^\alpha + (y')^\alpha)^\beta |y^\gamma - (y')^\gamma|, \qquad \alpha, \beta, \gamma \ge 0,\ \alpha\beta + \gamma \le 1$$

Other kernels:

$$a(y,y') = y^\alpha (y')^\beta + (y')^\alpha (y)^\beta, \qquad \alpha, \beta \in [0,1]$$

e.g. Golovin kernel $(\alpha, \beta) = (0, 1)$ (cloud droplets)

e.g. Stockmeyer kernel $\alpha = \beta = 1$ (branched-chain polymers)

The continuous Smoluchowski coagulation equation

Weak formulation:

Multiplication with a testfunction $\varphi(y)$ and integration yields

$$\int_0^\infty Q_{coag}\,\varphi(y)\,dy = \frac{1}{2}\int_0^\infty\int_0^y a(y',y-y')f(y-y')f(y')\,\varphi(y)\,dy'dy - \int_0^\infty\int_0^\infty a(y,y')f(y)f(y')\,\varphi(y)\,dy'dy$$

The continuous Smoluchowski coagulation equation

Weak formulation:

Multiplication with a testfunction $\varphi(y)$ and integration yields (formally) with Fubini for $\int Q_1(y)\varphi(y)\,dy$

$$\int_0^\infty Q_{coag}\,\varphi(y)\,dy = \frac{1}{2}\int_{y'}^{\infty}\int_0^\infty a(y', y-y')f(y-y')f(y')\,\varphi(y)dy'dy$$
$$-\frac{1}{2}\int_0^\infty\int_0^\infty a(y, y')f(y)f(y')\,\varphi(y)\,dy'dy$$
$$-\frac{1}{2}\int_0^\infty\int_0^\infty a(y', y)f(y')f(y)\,\varphi(y')\,dydy'$$

The continuous Smoluchowski coagulation equation

Weak formulation:

Multiplication with a testfunction $\varphi(y)$ and integration yields with $y - y' = y''$ and $a(y, y') = a(y', y)$

$$\begin{aligned}\int_0^\infty Q_{coag}\,\varphi(y)\,dy = & \frac{1}{2}\int_0^\infty\int_0^\infty a(y', y'')f(y'')f(y')\,\varphi(y + y'')dy'dy'' \\ & - \frac{1}{2}\int_0^\infty\int_0^\infty a(y, y')f(y)f(y')\,\varphi(y)\,dy'dy \\ & - \frac{1}{2}\int_0^\infty\int_0^\infty a(y, y^{`})f(y)f(y')\,\varphi(y')\,dy'dy\end{aligned}$$

The continuous Smoluchowski coagulation equation

Weak formulation:

Multiplication with a testfunction $\varphi(y)$ and integration yields (formally) with Fubini for $\int Q_1(y)\varphi(y)\,dy$ to

$$\int_0^\infty Q_{coag}\,\varphi(y)\,dy = \frac{1}{2}\int_0^\infty\int_0^\infty a(y,y')f(y)f(y')(\varphi''-\varphi-\varphi')\,dydy'$$

Notation: $\varphi=\varphi(y)$, $\varphi'=\varphi(y')$, $\varphi''=\varphi(y+y')$

The Smoluchowski equation

Formal properties of the cont. Smoluchowski equation

Weak formulation: $\varphi(y)$, $\quad \varphi' = \varphi(y')$, $\quad \varphi'' = \varphi(y+y')$

$$\int_0^\infty Q_{coag}\, \varphi(y)\, dy = \frac{1}{2}\int_0^\infty\!\!\int_0^\infty a(y,y')f(y)f(y')(\varphi'' - \varphi - \varphi')\, dy dy'$$

Moments: $\varphi(y) = y^k$

From $\mathrm{sign}(\varphi'' - \varphi - \varphi') = \mathrm{sign}(k-1)$ follows

$$t \mapsto \int_0^\infty \varphi(y)\, f(t,y)\, dy = \begin{cases} \searrow & k<1 \\ \text{constant} & k=1 \\ \nearrow & k>1 \end{cases}$$

The Smoluchowski equation

Formal properties of the cont. Smoluchowski equation

Weak formulation: $\varphi(y)$, $\quad \varphi' = \varphi(y')$, $\quad \varphi'' = \varphi(y+y')$

$$\int_0^\infty Q_{coag}\,\varphi(y)\,dy = \frac{1}{2}\int_0^\infty\int_0^\infty a(y,y')f(y)f(y')(\varphi'' - \varphi - \varphi')\,dydy'$$

Decreasing number of particles: $\varphi = 1$
stoichiometric coefficients $\frac{1}{2}$,1

Formal conservation of mass: $\varphi(y) = y$

$$\frac{d}{dt}\int_0^\infty y\,f(t,y)\,dy = \int_0^\infty y\,Q_{coag}\,dy = 0$$

Formal properties of the cont. Smoluchowski equation

Weak formulation: $\varphi(y), \quad \varphi' = \varphi(y'), \quad \varphi'' = \varphi(y+y')$

$$\int_0^\infty Q_{coag}\,\varphi(y)\,dy = \frac{1}{2}\int_0^\infty\int_0^\infty a(y,y')f(y)f(y')(\varphi''-\varphi-\varphi')\,dydy'$$

Rigorous ?? Mass is non-increasing!

test-function $\varphi(y) = \min\{y,R\}$ with $\varphi''-\varphi-\varphi' \leq 0$ for $R > 0$

Then,

$$t \mapsto \int_0^\infty \min\{y,R\}\,f(t,y)\,dy \xrightarrow[\text{Fatou}]{R\to\infty} \int_0^\infty y\,f(t,y)\,dy$$

is non-increasing!

Formal properties of the cont. Smoluchowski equation

Weak formulation: $\varphi(y)$, $\quad \varphi' = \varphi(y')$, $\quad \varphi'' = \varphi(y+y')$

$$\int_0^\infty Q_{coag}\,\varphi(y)\,dy = \frac{1}{2}\int_0^\infty\!\!\int_0^\infty a(y,y')f(y)f(y')(\varphi''-\varphi-\varphi')\,dydy'$$

All the above kernels $a(y,y')$ satisfy

$$a(y,y') \leq a(y,y+y') + a(y',y+y'), \qquad y,y' \in Y$$

from which L^p-Norm: $\varphi(y) = pf(t,y)^{p-1}$

$$t \mapsto \|f(t,\cdot)\|_{L^p} \quad \text{non-increasing for} \quad p \geq 1$$

The Smoluchowski equation

The kernel $a(y,y') = y\,y'$

Coagulation kernel: $a(y,y') = y\,y'$

Testing with $\varphi(y) = 1$ and for $T > 0$,

$$\frac{d}{dt}\int_0^\infty f(t,y)\,\varphi(y)\,dy =$$

$$\frac{1}{2}\int_0^\infty\int_0^\infty yy' f(y) f(y')(\varphi'' - \varphi - \varphi')\,dy' dy$$

The Smoluchowski equation

The kernel $a(y, y') = y\,y'$

Coagulation kernel: $a(y, y') = y\,y'$

Testing with $\varphi(y) = 1$ and for $T > 0$,

and introducing the moments:

$$M_0(t) = \int_0^\infty f(t,y)\,dy, \qquad M_1(t) = \int_0^\infty y\,f(t,y)\,dy$$

yields

$$\frac{d}{dt} M_0(t) = -\frac{1}{2}\int_0^\infty \int_0^\infty yy' f(y) f(y')\,dy'dy = -\frac{1}{2} M_1^2(t)$$

The Smoluchowski equation

The kernel $a(y, y') = y\, y'$

Coagulation kernel: $a(y, y') = y\, y'$

Testing with $\varphi(y) = 1$ and for $T > 0$,

Moments: $M_0(t) = \int_0^\infty f(t,y)\, dy,$ $\quad M_1(t) = \int_0^\infty y\, f(t,y)\, dy.$

$$M_0(T) + \frac{1}{2} \int_0^T M_1^2\, dt = M_0(0)$$

$M_0 \geq 0$ implies $M_1 \in L^2((0, \infty))$!

Gelation: $M_1(t) < M_1(0)$ for some finite $t \geq 0$

Formation of clusters of infinite size, Phase separation

More gelation for other examples of kernels

Kernel

$$a(y, y') = y^{\alpha}(y')^{\beta} + (y')^{\alpha}(y)^{\beta}, \qquad \alpha, \beta \in [0, 1]$$

For $\lambda = \alpha + \beta \in (1, 2]$:

$$M_k = \int_0^{\infty} y^k \, f(t, y) \, dy \in L^2((0, \infty)) \quad \text{for} \quad k \in \left(\frac{\lambda}{2}, \frac{1+\lambda}{2} \right)$$

Gelation: have $M_1 \in L^2((0, \infty)$ for $\lambda > 1$

The Smoluchowski equation

The kernel $a(y, y') = y\, y'$

Gelation time:

$$T_g := \inf\{t \geq 0 : M_1(t) < M_1(0)\}$$

Second moment $M_2 = \int_0^\infty y^2\, f(t, y)\, dy$. Then,

$$\frac{d}{dt}\int_0^\infty f(t, y)\, y^2\, dy =$$

$$\frac{1}{2}\int_0^\infty\int_0^\infty yy' f(y) f(y') \left((y + y')^2 - y^2 - (y')^2\right) dy' dy$$

The Smoluchowski equation

The kernel $a(y, y') = y\, y'$

Gelation time:

$$T_g := \inf\{t \geq 0 : M_1(t) < M_1(0)\}$$

Second moment $M_2 = \int_0^\infty y^2 \, f(t, y) \, dy$. Then,

$$\frac{d}{dt} M_2(t) = \int_0^\infty \int_0^\infty y^2 (y')^2 f(y) f(y') \, dy' dy$$

The Smoluchowski equation

The kernel $a(y, y') = y\, y'$

Gelation time:

$$T_g := \inf\{t \geq 0 : M_1(t) < M_1(0)\}$$

Second moment $M_2 = \int_0^\infty y^2 \, f(t, y) \, dy$. Then,

$$\frac{d}{dt} M_2(t) = M_2^2(t)$$

blows-up at time $T_2 = \frac{1}{M_2(0)}$ (recall $M_2(t) = \frac{1}{\frac{1}{M_2(0)} - t}$)

Is this the gelation time $T_g = T_2$?

Yes, for $a(y, y') = y\, y'$. In general open problem!

The Smoluchowski equation

The kernel $a(y,y') = y\,y'$

Formal Laplace-type-transform:

$$E(t,p) = \int_0^\infty e^{-py}\, y f(t,y)\, dy, \quad \partial_p E(t,p) = \int_0^\infty -e^{-py}\, y^2 f(t,y) dy$$

Note that $E(t,0) = M_1(t)$ and $\partial_p E(t,0) = -M_2(t)$.

Testing with $\varphi(y) = e^{-py} y$ for $p \in [0,\infty)$

$$\frac{d}{dt}\int_0^\infty f(t,y)\,\varphi(y)\,dy =$$

$$\frac{1}{2}\int_0^\infty\int_0^\infty yy' f(y) f(y')\,(\varphi'' - \varphi - \varphi')\,dy'dy$$

The Smoluchowski equation

The kernel $a(y, y') = y\, y'$

Formal Laplace-type-transform:

$$E(t,p) = \int_0^\infty e^{-py}\, y f(t,y)\, dy, \quad \partial_p E(t,p) = \int_0^\infty -e^{-py}\, y^2 f(t,y) dy$$

Note that $E(t,0) = M_1(t)$ and $\partial_p E(t,0) = -M_2(t)$.

$$\frac{d}{dt} E(t,p) = \frac{1}{2} \int_0^\infty \int_0^\infty y y' f(y) f(y') \times \left(e^{-py} e^{-py'} (y + y') - e^{-py} y - e^{-py'} y' \right) dy' dy$$

The Smoluchowski equation

The kernel $a(y,y') = y\,y'$

Formal Laplace-type-transform:

$$E(t,p) = \int_0^\infty e^{-py}\, y f(t,y)\,dy, \quad \partial_p E(t,p) = \int_0^\infty -e^{-py}\, y^2 f(t,y) dy$$

Note that $E(t,0) = M_1(t)$ and $\partial_p E(t,0) = -M_2(t)$.

$$\frac{d}{dt}E(t,p) = \int_0^\infty e^{-py} y^2 f(y)\,dy \int_0^\infty e^{-py'} y' f(y')\,dy' - \int_0^\infty e^{-py} y^2 f(y)\,dy \int_0^\infty y' f(y')\,dy'$$

The Smoluchowski equation

The kernel $a(y, y') = y\, y'$

Formal Laplace-type-transform:

$$E(t,p) = \int_0^\infty e^{-py}\, y f(t,y)\, dy, \quad \partial_p E(t,p) = \int_0^\infty -e^{-py}\, y^2 f(t,y) dy$$

Note that $E(t,0) = M_1(t)$ and $\partial_p E(t,0) = -M_2(t)$.

Thus,

$$\partial_t E(t,p) + (E(p) - E(0))\, \partial_p E(t,p) = 0$$

Note also $\partial_p E(t,p) \geq \partial_p E(t,0) = -M_2(t)$ and the above Burgers equation develops a first shock at $p = 0$ and gelation occurs at $T_g = T_2$:

$$E(t,0) = M_1(t) < M_1(0), \qquad t > T_g = T_2$$

Subcritical kernels

Absence of gelation, Conservation of mass

- $a(y, y') \leq C(1 + y + y')$
- $a(y, y') = y^\alpha (y')^\beta + (y')^\alpha (y)^\beta$ and $\lambda = \alpha + \beta \leq 1$

See below

The Smoluchowski equation

Loss of mass in infinite time

Number of particles is reduced by coagulation.

Rigorous: Assume $a(y,y')>0$ for $(y,y')\in Y\times Y$. Then,

$$M_k(t)=\int_0^\infty y^k\, f(t,y)\, dy \to 0 \quad \text{as} \quad t\to\infty, \qquad k\in[0,1)$$

Loss of mass in infinite time (even if M_1 is conserved)

Speed: Assume $\lambda\in[0,1)$ such that $a(y,y')\geq (yy')^\lambda$ and $f^{in}\equiv 0$ a.e. on $(0,\delta>0)$. Then, $M_k(t)\leq C_k t^k$ for all $k\in(0,1)$.

J. Carr, F.P. da Costa *Asymptotic behaviour of solutions to the coagulation-fragmentation equations. II. Weak fragmentation* J. Stat. Phys. **77** (1994) pp. 89-123.

Gelation profiles, many open problems

Conjecture:

For the kernel $a(y,y') = y^\alpha (y')^\beta + (y')^\alpha (y)^\beta$, $\alpha, \beta \in [0,1]$, if $\lambda = \alpha + \beta \in (1,2]$:

$$f(T_g, y) \sim y^{-3/2 - \lambda/2} \quad \text{as} \quad y \to \infty$$

Dynamical scaling hypothesis:

As mean particle size $s(t) \to \infty$ as $t \to T_*$

$$f(t,y) \sim \frac{1}{s(t)^\tau} \varphi\left(\frac{y}{s(t)}\right) \quad \text{as} \quad t \to T_*$$

If $a(\xi y, \xi y') = \xi^\lambda a(y,y')$ conjecture that $\frac{1}{s(t)^\tau} \varphi\left(\frac{y}{s(t)}\right)$ self-similar solution ($\tau = 2$ for $T_* = \infty$ and $\tau = (\lambda + 3)/2$ for $T_* = T_g$).

The beginning

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Absence of gelation and gelation time

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Discrete coagulation-fragmentation models

Discrete in size models

discrete size $y = i \in \mathbb{N} = Y$, $\quad f(t,y) = c_i(t) \geq 0$, $\quad c = (c_i)$

$$
\begin{aligned}
d_t c_i(t) &= Q_{coag}(c,c) + Q_{frag}(c) \\
&= Q_1(c,c) - Q_2(c,c) + Q_3(c) - Q_4(c)
\end{aligned}
$$

Binary coagulation:

$Q_1(c,c)$: gain of particles of size i

$$\{i-j\} + \{j\} \xrightarrow{a_{i-j,j}} \{i\}, \qquad j < i$$

$Q_2(c,c)$: loss of particles of size i

$$\{i\} + \{j\} \xrightarrow{a_{i,j}} \{i+j\}, \qquad j \geq 1$$

Discrete in size models

discrete size $y = i \in \mathbb{N} = Y$, $\quad f(t,y) = c_i(t) \geq 0$, $\quad c = (c_i)$

$$d_t c_i(t) = Q_{coag}(c,c) + Q_{frag}(c)$$
$$= Q_1(c,c) - Q_2(c,c) + Q_3(c) - Q_4(c)$$

Fragmentation:

$Q_3(c)$: gain of particles of size i

$$\{i+j\} \xrightarrow{B_{i+j}\beta_{i+j,i}} \{i\} + \{j\}, \qquad j > 1$$

$Q_4(c)$: loss of particles of size i

$\{i\} \xrightarrow{B_i}$ all pairs $\quad \{i-j\} + \{j\}$ with $\quad j < i$

Discrete in size models

discrete size $y = i \in \mathbb{N} = Y$, $c_i(0) \geq 0$, $c = (c_i)$

$$d_t c_i = Q_{coag}(c, c) + Q_{frag}(c)$$

$$= \frac{1}{2}\sum_{j=1}^{i-1} a_{i-j,j}\, c_{i-j} c_j - \sum_{j=1}^{\infty} a_{i,j}\, c_i c_j + \sum_{j=1}^{\infty} B_{i+j} \beta_{i+j,i}\, c_{i+j} - B_i c_i$$

coagulation-fragmentation coefficients

$$a_{i,j} = a_{j,i} \geq 0, \qquad \beta_{i,j} \geq 0, \qquad (i, j \in \mathbb{N}),$$

$$B_1 = 0 \qquad B_i \geq 0, \qquad (i \in \mathbb{N}),$$

(mass conservation) $\quad i = \sum_{j=1}^{i-1} j\, \beta_{i,j}, \qquad (i \in \mathbb{N}, i \geq 2).$

The Becker-Döring model

Interactions between monomers and polymers only

discrete size $i \in \mathbb{N}$, $c_i(t) \geq 0$, $c = (c_i)$

$$
\begin{aligned}
d_t c_i(t) &= Q_{coag}(c,c) + Q_{frag}(c) \\
&= Q_1(c,c) - Q_2(c,c) + Q_3(c) - Q_4(c)
\end{aligned}
$$

Binary coagulation between monomers and polymers

$Q_1(c,c)$: gain of particles of size i

$$\{i-1\} + \{1\} \xrightarrow{a_{i-1}} \{i\}, \qquad 1 < i$$

$Q_2(c,c)$: loss of particles of size i

$$\{i\} + \{1\} \xrightarrow{a_i} \{i+1\}, \qquad 1 \leq i$$

The Becker-Döring model

Interactions between monomers and polymers only

discrete size $i \in \mathbb{N}$, $c_i(t) \geq 0$, $c = (c_i)$

$$d_t c_i(t) = Q_{coag}(c,c) + Q_{frag}(c)$$
$$= Q_1(c,c) - Q_2(c,c) + Q_3(c) - Q_4(c)$$

Fragmentation of monomers from polymers

$Q_3(c)$: gain of particles of size i

$$\{i+1\} \xrightarrow{b_{i+1}} \{i\} + \{1\}, \qquad 1 \leq i$$

$Q_4(c)$: loss of particles of size i

$$\{i\} \xrightarrow{b_i} \{i-1\} + \{1\}, \qquad 1 < i$$

The Becker-Döring model

Interaction between monomers and polymers

In the Becker-Döring model all coagulation and fragmentation events involve monomers/clusters-of-size-one.

System of a monomer-equation and polymer-equations:

$$\begin{cases} d_t c_1 = -W_1(c) - \sum_{i=1}^{\infty} W_i(c), & \\ d_t c_i = W_{i-1}(c) - W_i(c), & i \geq 2 \end{cases}$$

where $\quad W_i(c) = a_i \, c_1 \, c_i - b_{i+1} \, c_{i+1}$

little knows about C-F models except with detailed balance

$a_1 = a_{1,2}/2, \; b_2 = b_{1,1}/2,$ and $a_i = a_{i,1}, \; b_i + 1 = b_{i,1}, \; i \geq 2$

Detailed balance condition : continuous and discrete

non-negative equilibrium $E(y) \in L^1_1(Y) := L^1(Y, (1+y)dy)$:

$$a(y,y')E(y)E(y') = b(y,y')E(y+y'), \qquad (y,y') \in Y \times Y$$

This equation is also satisfied by all

$$E_z(y) = E(y)\, z^y, \quad y \in Y, \quad \text{for } z \geq 0$$

but E_z not necessarily in $L^1_1(Y)$. Thus,

$$z_s := \sup\{z \geq 0 : E_z \in L^1_1(Y)\} \in [1, \infty]$$

$$\rho_s := M_1(E_{z_s}(y)) \in [0, \infty].$$

ρ_s is called the saturation mass

Entropy and detailed balance

Entropy functional: $H(f|E) = \int_Y f\left(\ln(\frac{f}{E}) - 1\right) dy$

H-Theorem $\quad f' = f(y')$, $\quad f'' = f(y+y')$

$$\frac{d}{dt}H(f|E) = -\frac{1}{2}D(f),$$
$$D(f) = \int_Y\int_Y (aff' - bf'')(\ln(aff') - \ln(bf''))\, dydy'$$

Dissipation $D(f) = 0$ vanishes only for equilibria, conjecture

$$f(t,y) \xrightarrow{t\to\infty} E_z(y), \begin{cases} z : M_1(E_z)) = M_1(f_0) & M_1(f_0) \le z_s \\ z_s & M_1(f_0) > z_s \end{cases}$$

Becker-Döring and generalisations, strong fragmentation, Aizenman-Bak

Large time saturation phenomenon in Becker-Döring

assume initial mass $\rho = M_1(c_0)$ larger than $\rho_s = M_1(E_{z_s}) < \infty$

Expect $\quad c_i(t) \to E_i z_s^i \quad$ as $\quad t \to \infty$.

The remaining mass $\rho - \rho_s$ should go to larger and larger clusters as $t \to \infty$.

How does this work?

O. Penrose *The Becker-Döring equations at large times and their connection with the LSW theory of coarsening* J. Stat. Phys. **87** (1997) pp. 305-320.

B. Niethammer *On the evolution of large clusters in the Becker-Döring model* J. Nonlinear Science **13** (2003) pp. 115-155.

Large time saturation phenomenon in Becker-Döring

assume initial mass $\rho = M_1(c_0)$ larger than $\rho_s = M_1(E_{z_s}) < \infty$

[Niethammer] extended [Penrose] by considering the coefficients

$$a_i = a_1 i^{\alpha}, \quad b_i = a_i(z_s + q i^{-\gamma}), \quad i \geq 2$$

with $\alpha \in (0,1]$, $\gamma \in [0,1)$, $a_1 > 0$, $z_s > 0$, $q > 0$

rescale time $\tau = \varepsilon^{1-\alpha+\gamma} t$

cut-off i_ε where $i_\varepsilon \to \infty$ and $\varepsilon i_\varepsilon \to 0$ as $\varepsilon \to 0$

Goal is to capture saturation mass in $\sum_{i=1}^{i_\varepsilon} i c_i(\tau) \sim \rho_s$

Large time saturation phenomenon in Becker-Döring

assume initial mass $\rho = M_1(c_0)$ larger than $\rho_s = M_1(E_{z_s}) < \infty$

alternative Becker-Döring

$$\begin{cases} \sum_{i=1}^{\infty} i c_i(\tau) = \rho \\ d_\tau c_i = \frac{1}{\varepsilon^{1-\alpha+\gamma}} \left(W_{i-1}(c) - W_i(c) \right), & i \geq 2 \end{cases}$$

where

$$W_i(c) = a_i \left(c_1 - \frac{b_i}{a_i} \right) c_i - \left(b_{i+1}\, c_{i+1} - b_i\, c_i \right)$$
$$= a_1 i^{\alpha} \left(c_1 - z_s - q i^{-\gamma} \right) - \left(b_{i+1}\, c_{i+1} - b_i\, c_i \right)$$

Large time saturation phenomenon in Becker-Döring

assume initial mass $\rho = M_1(c_0)$ larger than $\rho_s = M_1(E_{z_s}) < \infty$

Continuum approximation

Rewrite for $(\tau, x) \in (0, \infty) \times ((i - 1/2)\varepsilon, (i + 1/2)\varepsilon)$

$$f(\tau, x) = \frac{1}{\varepsilon^2} c_i(\tau), \qquad W(\tau, x) = \frac{1}{\varepsilon^2} W_i(f(\tau))$$

Then,

$$\partial_\tau f = -\partial_x W(f), \qquad W(f)(\tau, x) \sim a_1 \left(x^\alpha u(\tau) - q x^{\alpha-\gamma} \right)$$

where $u(\tau) = \varepsilon^{-\gamma}(c_1(\tau) - z_s)$

with $c_1(\tau) \to E_1 \, z_s$ and $\frac{E_i}{E_{i+1}} = \frac{z_s}{E_1}$ for large i

Large time saturation phenomenon in Becker-Döring

assume initial mass $\rho = M_1(c_0)$ larger than $\rho_s = M_1(E_{z_s}) < \infty$

for $i \geq i_\varepsilon \sim -\ln(\varepsilon)$:
continuum approximation $x \sim i\varepsilon$

One can show that for $\varepsilon \to 0$, $\quad i_\varepsilon \to \infty$, $\quad x \sim i_\varepsilon \varepsilon \to 0$

$$\sum_{i=1}^{i_\varepsilon} i c_i(\tau) \sim \rho_s, \qquad \int_0^\infty x f(\tau, x)\, dx = \rho - \rho_s.$$

For general models saturation is an open problem.

Coagulation-fragmentation models with diffusion

evolution of a polymer/cluster density $f(t, x, y) \geq 0$

$$\partial_t f - d(y)\triangle_x f = Q_{coag}(f, f) + Q_{frag}(f)$$
$$= Q_1(f, f) - Q_2(f, f) + Q_3(f) - Q_4(f)$$

time $t \geq 0$, size $y \in Y$

position $x \in \Omega$, normalised with $|\Omega| = 1$

homogeneous Neumann $\nabla_x f(t, x, y) \cdot \nu(x) = 0$ on $\partial\Omega$

non-negative initial data $f_0(x, y) \geq 0$

size-dependent diffusion coefficients $d(y)$

Discrete C-F models

discrete in size models $y = i \in \mathbb{N}$, $\quad f(y) = c_i$, $\quad c = (c_i)$

$$Q_{coag}(c,c) = \frac{1}{2}\sum_{j=1}^{i-1} a_{i-j,j}\, c_{i-j}\, c_j - \sum_{j=1}^{\infty} a_{i,j}\, c_i\, c_j$$

$$Q_{frag}(c) = \sum_{j=1}^{\infty} B_{i+j}\, \beta_{i+j,i}\, c_{i+j} - B_i\, c_i$$

coagulation-fragmentation coefficients

$$a_{i,j} = a_{j,i} \geq 0, \qquad \beta_{i,j} \geq 0, \qquad (i,j \in \mathbb{N})$$

$$B_1 = 0, \qquad B_i \geq 0, \qquad (i \in \mathbb{N})$$

(mass conservation) $\quad i = \sum_{j=1}^{i-1} j\, \beta_{i,j}, \qquad (i \in \mathbb{N}, i \geq 2)$

Discrete C-F with diffusion

Weak formulation, conservation of mass

test-sequence φ_i,

$$\sum_{i=1}^{\infty} \varphi_i \, Q_{coal} = \frac{1}{2} \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} a_{i,j} \, c_i \, c_j \, (\varphi_{i+j} - \varphi_i - \varphi_j),$$

$$\sum_{i=1}^{\infty} \varphi_i \, Q_{frag} = - \sum_{i=2}^{\infty} B_i c_i \left(\varphi_i - \sum_{j=1}^{i-1} \beta_{i,j} \varphi_j \right).$$

conservation of total mass or gelation ($\varphi_i = i$)

$$\|\rho(t,\cdot)\|_{L^1} = \int_\Omega \sum_{i=1}^{\infty} i c_i(t,x) \, dx \leq \int_\Omega \sum_{i=1}^{\infty} i c_i^0(x) \, dx = \|\rho^0\|_{L^1}$$

Discrete C-F with diffusion

Existence theory

natural initial data: $0 \leq f^{in}(y) \in L^1_1(Y) = L^1(Y, (1+y)dy)$

two basic approaches:

- fixed-point and compactness methods in spaces of continuous functions

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J.B. McLeod *On the scalar transport equation* Proc. London Math. Soc. (3) **14** (1964) pp. 445-458.

Z.A. Melzak *A scalar transport equation* Trans. Amer. Math. Soc. **85** (1957) pp. 547-560.

P.B. Dubovskii, I. Stewart *Existence, uniqueness and mass conservation for the coagulation-fragmentation equation* Math. Meth. Appl. Sci. **19** (1996) 571-591.

V.A. Galkin, P.B. Dubovskii *Solution of the coagulation equation with unbounded kernels* Differential Equations **22** (1986) pp. 373-378.

Discrete C-F with diffusion

Existence theory

natural initial data: $0 \leq f^{in}(y) \in L^1_1(Y) = L^1(Y, (1+y)dy)$

two basic approaches:

- weak and strong compactness methods in $L^1(Y)$

J.M. Ball, J. Carr, O. Penrose *The Becker-Döring cluster equation : basic properties, uniqueness and asymptotic behaviour of solutions* Comm. Math. Phys. **104** (1986) pp. 657-692.

I.W. Stewart *A global existence theorem for the general coagulation-fragmentation equation with unbounded kernels* Math. Methods Appl. Sci **11** (1989) pp. 627-648

M. Escobedo, Ph. Laurençot, S. Mischler, P. Berthame *Gelation and mass conservation in coagulation-fragmentation models* J. Differential Equations

Ph. Laurençot, S. Mischler *The continuous coagulation-fragmentation equation with diffusion* Arch. Rat. Mech. Anal. **162** (2002) pp. 45-99.

(Global) weak solutions of discrete C-F with diffusion

Let $T \in (0,\infty]$, initial data $0 \le c_i^{in} \in L^1(\Omega)$, $\sum_{i=1}^{\infty} i \|c_i\|_1 < \infty$

A weak solution of C-F on $[0,T)$ is a non-negative function

$$c_i \in C([0,T);L^1(\Omega)), \qquad \sup_{t\in[0,T)} \sum_{i=1}^{\infty} i\|c_i\|_1 < C(c_i^{in})$$

with $Q_2(c) = \sum_{j=1}^{\infty} a_{i,j} c_i c_j \in L^1((0,T)\times\Omega)$,...

Moreover, c_i are mild solutions of

$$c_i(t) = e^{d_i \triangle_x t} c_i^{in} + \int_0^t e^{d_i \triangle_x (t-s)} (Q_{coag} + Q_{frag})(c(s))\, ds$$

and $e^{d_i \triangle_x t}$ is the C_0-semigroup of $d_i \triangle_x$ in $L^1(\Omega)$ with homogeneous Neumann conditions.

Existence of C-F with diffusion

(Global) weak solutions of continuous C-F with diffusion

Let $T \in (0, \infty]$, initial data $0 \leq f^{in} \in L^1(\Omega \times \mathbb{R}_+; (1+y)dxdy)$

A weak solution of C-F on $[0,T)$ is a non-negative function

$$f \in C((0,T); L^1(\Omega \times \mathbb{R}_+)) \cap L^\infty(0,T; L^1(\Omega \times \mathbb{R}_+; ydydx))$$

with $f(0) = f^{in}, \quad f \in L^1((0,T) \times (1/R, R); W^{1,1}(\Omega))$, $\forall R \in \mathbb{R}_+$
and $Q_{1,2,3,4}(f) \in L^1((0,T) \times \Omega \times (0, R))$, which satisfies

$$\int_\Omega \int_0^\infty \left(\psi(t) f(t) - \psi(0) f^{in}\right) dydx + \int_0^t \int_\Omega \int_0^\infty (-f \partial_t \psi$$
$$+ d(y) \nabla f \nabla \psi) \, dydxds = \frac{1}{2} \int_0^t \int_\Omega \int_0^\infty Q(f) \, \psi \, dydxds$$

$\forall t \in (0,T)$ and compactly supported $\psi \in C^1([0,T] \times \Omega \times \mathbb{R}_+)$.

Existence of C-F with diffusion

Stability principle for (global) weak solutions in L^1

For $T \in (0,\infty)$ let (f_n) be weak solutions of C-F with coefficients $a_n \to a$, $b_n \to b$ and $d_n \to d$ and initial datum f^{in}. For all $n \in \mathbb{N}$ let $\mathcal{K}_w \subset L^1(\Omega \times \mathbb{R}_+)$ be a weakly compact with

$$f_n(t) \in \mathcal{K}_w, \qquad \text{for each } t \in [0,T)$$

and suppose moreover for all $R > 0$ and $i \in \{1,2,3,4\}$ that

$$\sup_{t\in[0,T]} \int_\Omega \int_0^\infty f_n(t)(1+y)\,dydx \le C_T,$$

$$Q_{i,n}(f_n) \quad \text{weakly compact in } L^1((0,T) \times \Omega \times (0,R))$$

Ph. Laurençot, S. Mischler *The continuous coagulation-fragmentation equation with diffusion* Arch. Rat. Mech. Anal. **162** (2002) pp. 45-99.

Existence of C-F with diffusion

Stability principle for (global) weak solutions in L^1

Then, there exists a subsequence (f_{n_k}) and f such that

$$f_{n_k} \rightharpoonup f \quad \text{in } C([0,T); w - L^1(\Omega \times \mathbb{R}_+))$$
$$Q_{i,n_k}(f_{n_k}) \rightharpoonup Q_i(f) \quad \text{weakly in } L^1((0,t) \times \Omega \times (0,R))$$

for $R \in \mathbb{R}_+$, $i \in \{1,2,3,4\}$.

Thus, f is a weak solution of C-F on $[0,T)$.

Moreover,

$$\int_0^\infty \psi(y) f_{n_k}\, dy \to \int_0^\infty \psi(y) f\, dy \quad \text{in} \quad L^1((0,T) \times \Omega)$$

for $\psi \in \mathcal{D}(\mathbb{R}_+)$. Thus, $M_1(t) \leq M_1(0)$.

Existence of C-F with diffusion

A priori estimate with detailed balance

Entropy functional: $H(f|E(y)) = \int_\Omega \int_Y f\left(\ln(\frac{f}{E}) - 1\right) dy$

H-Theorem $\quad f = f(y), \quad f' = f(y'), \quad f'' = f(y+y')$

$$\frac{d}{dt}H(f|E) + \int_\Omega \int_Y d(y)\frac{|\nabla f|^2}{f}\,dydx$$
$$+\frac{1}{2}\int_\Omega \int_Y \int_Y (aff' - bf'')(\ln(aff') - \ln(bf''))\,dydy'dx = 0$$

Total mass $\quad C_0 := \sup_{t\in[0,\infty)} \int_\Omega \int_Y yf(t,x,y)\,dydx < \infty$

Existence of C-F with diffusion

A priori estimate with detailed balance

Initial data $\quad H(f^{in}|E) < C < \infty$

$$\frac{d}{dt}\int_\Omega\int_Y f\Big(\ln\Big(\frac{f}{E}\Big) - 1\Big)dy + \int_\Omega\int_Y d(y)\frac{|\nabla f|^2}{f}\,dydx$$
$$+\frac{1}{2}\int_\Omega\int_Y\int_Y (aff' - bf'')(\ln(aff') - \ln(bf''))\,dydy'dx = 0$$

A priori estimates

- $H(f(t)|E) < C$
- $\int_0^t\int_\Omega\int_Y d(y)\frac{|\nabla f|^2}{f}\,dydxds < C$
- $\int_0^t\int_\Omega\int_Y\int_Y (aff' - bf'')(\ln(aff') - \ln(bf''))\,dydy'dxds < C$

for $C = C(\Omega, E(y), H(f^{in}|E), C_0)$.

A priori estimate and weak compactness

Lemma: Let $\xi \mapsto \{0,1\}$ be measurable on $\mathbb{R}_+ \times \Omega \times \mathbb{R}_+$ and $\alpha \geq e^2$. Then,

$$\int_\Omega \int_Y \xi(t) f(t)\, dy dx \leq 2(\alpha + e^{-1}) \int_\Omega \int_Y \xi(t) E\, dy dx + \frac{2}{\ln(\alpha)} H(f(t)|E)$$

Lemma: For $t \in \mathbb{R}_+$ holds with $f(t)\left|\ln \frac{f(t)}{E(y)}\right| \leq f(t) \ln \frac{f(t)}{E(y)} + \frac{2E}{e}$

$$\int_\Omega \int_Y f(t) \left(1 + \left|\ln\left(\frac{f(t)}{E(y)}\right)\right|\right) dy dx \leq C$$

A priori estimate and weak compactness

Weak compactness lemma:

Let $T \in \mathbb{R}_+$ and $(f_n) \geq 0$ a sequence such that for all $n \geq 1$

$$\sup_{t\in[0,T]} \int_\Omega \int_Y f_n(t) \left(1 + y + \left|\ln\left(\frac{f_n(t)}{E(y)}\right)\right|\right) dydx \leq C_T$$

$$\int_0^t \int_\Omega \int_Y \int_Y (a_n f_n f_n' - b_n f_n'')(\ln(a_n f_n f_n') - \ln(b_n f_n'')) dydy'dxds < C_T$$

Then, (f_n) weakly compact in $L^1((0,T) \times \Omega \times \mathbb{R}_+)$ and $(Q_i(f_n))$ weakly compact in $L^1((0,T) \times \Omega \times (0,R))$ for $i \in 1, 2, 3, 4$ and $R \in \mathbb{R}_+$.

Moreover, exists a weakly compact subset $\mathcal{K}_w \subset L^1(\Omega \times \mathbb{R}_+)$ such that $(f_n(t)) \in \mathcal{K}_w$ for all $t \in [0,T]$ and $n \geq 1$.

Existence of C-F with diffusion

A priori estimate and weak compactness

Proof of weak compactness lemma:

For $S \subset \Omega \times \mathbb{R}_+$ measurable, $|S| < \infty$, $\alpha \geq e^2$ follows from above

$$\int_S f_n(t)\,dydx \leq 4\alpha \int_S E(y)\,dydx + \frac{2C_T}{\ln(\alpha)} \leq C_T(E, |\Omega|, \alpha)$$

$$\int_\Omega \int_\alpha^\infty f_n(t)\,dydx \leq \frac{C_T}{\alpha}$$

Then, $f_n(t) \in \mathcal{K}_w \subset L^1(\Omega \times \mathbb{R}_+)$ for all $n \geq 1$ with $\mathcal{K}_w$ defined that $g \in \mathcal{K}_w$ satisfying the above equations for all measurable $S \subset \Omega \times \mathbb{R}_+$ with $|S| < \infty$ and $\alpha \geq e^2$.

By the Dunford-Pettis theorem is $\mathcal{K}_w$ weakly compact.

Existence of C-F with diffusion

A priori estimate and weak compactness

Dunford-Pettis theorem:

A sequence (f_n) is contained in a weakly compact subset $\mathcal{K}_w \subset L^1(\Omega \times \mathbb{R}_+)$ if (f_n) bounded in $L^1(\Omega \times \mathbb{R}_+)$ and for all $\varepsilon > 0$, there exists a measurable $S \subset \Omega \times \mathbb{R}_+$ with $|S| < \infty$ such that

$$\sup_{n \geq 1} \int_{(\Omega \times \mathbb{R}_+) \setminus S} |f_n| \leq \varepsilon$$

A priori estimate and weak compactness

Proof of weak compactness lemma:

For all $R \in \mathbb{R}_+$

$$Q_{4,n}(f_n) = \frac{f_n(t,x,y)}{2} \int_0^y b_n(y', y-y')\, dy' \leq R \|b_n\|_\infty f_n$$

Therefore, the sequence $(Q_{4,n}(f_n))$ (where $Q_{4,n}$ may be an approximation of Q_4 with coefficients $a_n \longrightarrow a$, $b_n \longrightarrow b$ and $d_n \longrightarrow d$) is weakly compact in $L^1((0,T) \times \Omega \times (0,R))$ since (f_n) is weakly compact and $\|b_n\|_\infty$ is assumed bounded.

Existence of C-F with diffusion

A priori estimate and weak compactness

Proof of weak compactness lemma:

For all $\alpha \geq e^2$, the elementary inequality $\eta \leq \alpha\xi + \frac{(\eta-\xi)\ln(\eta/\xi)}{\ln(\alpha)}$ yields for measurable $S \subset (0,T)\times\Omega\times(0,R)$

$$\int_S a_n(y', y-y') f_n(y') f_n(y-y')\, dy dx dt$$
$$\leq \alpha \sup_{n\geq 1} \int_S Q_4(f_n)\, dy dx dt + \frac{C_T}{\ln(\alpha)}$$

and letting $\alpha \to \infty$ shows that the sequence $(Q_{1,n}(f_n))$ is weakly compact in $L^1((0,T)\times\Omega\times(0,R))$ for all $R \in \mathbb{R}_+$.

A priori estimate and weak compactness

Proof of weak compactness:

For all $\alpha \geq 2R \in \mathbb{R}_+$

$$\int_S Q_{3,n}(f_n)\, dydxdt \leq \int_S \int_0^\alpha b_n(y, y-y') f_n(y')\, dy'dydxdt$$
$$+ \|b_n\|_{L^\infty(a-R,\infty)} \int_S \int_\alpha^\infty f_n(y')\, dy'dydxdt$$
$$\leq C \int_S \int_0^\alpha f_n(y')\, dy'dxdt + \|b_n\|_{L^\infty(a-R,\infty)} C(T,R)$$

and the sequence $(Q_{3_n}(f_n))$ is weakly compact in $L^1((0,T)\times\Omega\times(0,R))$ since (f_n) is weakly compact.

A priori estimate and weak compactness

Proof of weak compactness:

From

$$\int_0^t \int_\Omega \int_Y \int_Y (a_n f_n f_n' - b_n f_n'') \ln\left(\frac{a_n f_n f_n'}{b_n f_n''}\right) dy dy' dx ds \ < \ C_T$$

follows also that $(Q_{2,n}(f_n))$ is weakly compact in $L^1((0,T)\times\Omega\times(0,R))$ from the weak compactness of $(Q_{3,n}(f_n))$ in a similar argument as above showing the weak compactness of $(Q_{1,n}(f_n))$.

Discrete C-F with diffusion

Existence of global weak solutions in L^1

Assumptions on coefficients

$$\lim_{j\to\infty} \frac{a_{i,j}}{j} = \lim_{j\to\infty} \frac{B_{i+j}\,\beta_{i+j,i}}{i+j} = 0, \qquad (\text{for fixed } i \geq 1),$$

Then, global weak solutions $c_i \in \mathcal{C}([0,T];L^1(\Omega))$, $i \in \mathbb{N}$, $T > 0$

$$\sum_{j=1}^{\infty} a_{i,j} c_i c_j \in L^1([0,T]\times\Omega),$$

$$\sup_{t\geq 0} \int_\Omega \left[\sum_{i=1}^{\infty} i c_i(t,x)\right] dx \leq \int_\Omega \left[\sum_{i=1}^{\infty} i c_i^0(x)\right] dx,$$

Ph. Laurençot, S. Mischler *Global existence for the discrete diffusive coagulation-fragmentation equation in* L^1 Rev. Mat. Iberoamericana **18** (2002) pp. 731-745

Discrete C-F with diffusion

Lemma: L^2 estimates via duality

Assume coefficients like above and $\rho_0 = \sum_{i=1}^{\infty} i c_i^0 \in L^2(\Omega)$

Then, for all $T > 0$

$$\|\rho\|_{L^2(\Omega_T)} \leq \left(1 + \frac{\sup_i\{d_i\}}{\inf_i\{d_i\}}\right) T \, \|\rho_0\|_{L^2(\Omega)},$$

or for degenerate diffusion

$$\int_0^T \int_\Omega \left[\sum_{i=1}^{\infty} i \, d_i \, c_i(t,x)\right] \left[\sum_{i=1}^{\infty} i \, c_i(t,x)\right] \leq 4 \, T \, \sup_{i \in \mathbb{N}^*}\{d_i\} \|\rho_0\|_{L^2(\Omega)}.$$

J.A. Cañizo, L. Desvillettes, K. F. *Regularity and mass conservation for discrete coagulation-fragmentation equations with diffusion*, Ann. Inst. H. Poincaré (C) Anal. Non Linéaire, **27** no.2 (2010) pp. 639–654

Discrete C-F with diffusion

Proof of duality bounds

Denoting $A(t,x) = \frac{1}{\rho} \sum_{i=1}^{\infty} i\, d_i\, c_i$, then $\|A\|_\infty \leq \sup_{i\in\mathbb{N}^*}\{d_i\}$ and

$$\partial_t \rho - \Delta_x(A\,\rho) = 0.$$

Multiplying with the solution w of the dual problem:

$$-\left(\partial_t w + A\,\Delta_x w\right) = H\,\sqrt{A},$$

$$\nabla_x w \cdot n(x)|_{\partial\Omega} = 0, \qquad w(T,\cdot) = 0$$

for any smooth function $H := H(t,x) \geq 0$ leads to

$$\int_0^T \int_\Omega H(t,x)\,\sqrt{A(t,x)}\,\rho(t,x)\,dxdt = \int_\Omega w(0,x)\,\rho(0,x)\,dx.$$

Discrete C-F with diffusion

Proof of duality bounds

Multiplying the dual problem by $-\Delta_x w$ yields

$$-\int_0^T\int_\Omega \partial_t(|\nabla w|^2/2)\,dxdt + \int_0^T\int_\Omega A\,(\Delta_x w)^2\,dxdt$$
$$\leq \int_0^T\int_\Omega H\,\sqrt{A}(-\Delta_x w)dxdt.$$
$$\leq \frac{C}{\varepsilon}\int_0^T\int_\Omega H^2\,dxdt + \varepsilon\int_0^T\int_\Omega A(\Delta_x w)^2 dxdt$$

and with $\nabla w(T) = 0$

$$\int_0^T\int_\Omega A\,(\Delta_x w)^2\,dxdt \leq \int_0^T\int_\Omega H^2\,dxdt.$$

Proof of duality bounds

Multiplying the dual problem by $-\Delta_x w$ yields

$$\int_0^T \int_\Omega A\,(\Delta_x w)^2\,dxdt \leq \int_0^T \int_\Omega H^2\,dxdt.$$

and

$$\int_0^T \int_\Omega \frac{|\partial_t w|^2}{A}\,dxdt \leq 4\int_0^T \int_\Omega H^2\,dxdt.$$

Hence, $|w(0,x)|^2 \leq \big(\int_0^T \sqrt{A}\,\frac{|\partial_t w|}{\sqrt{A}}\,dt\big)^2$ and

$$\int_\Omega |w(0,x)|^2\,dx \leq 4\,T\,\|A\|_{L^\infty(\Omega)} \int_0^T \int_\Omega H^2\,dxdt.$$

Proof of duality bounds

Recalling above

$$\int_0^T \int_\Omega H \sqrt{A}\, \rho \, dxdt \le \|\rho(0,\cdot)\|_{L^2(\Omega)} \, \|w(0,\cdot)\|_{L^2(\Omega)}$$
$$\le 2\sqrt{T \, \|A\|_{L^\infty(\Omega)}} \, \|H\|_{L^2([0,T]\times\Omega)} \, \|\rho(0,\cdot)\|_{L^2(\Omega)}.$$

for all (nonnegative smooth) functions H, we obtain by duality that

$$\|\sqrt{A}\, \rho\|_{L^2(\Omega)} \le 2\sqrt{T\, \|A\|_{L^\infty(\Omega)}} \, \|\rho(0,\cdot)\|_{L^2(\Omega)}.$$

L. Desvillettes, K. F., M. Pierre, J. Vovelle *About Global Existence for Quadratic Systems of Reaction-Diffusion*, J. Advanced Nonlinear Studies **7** no 3. (2007) pp. 491–511.

Discrete C-F with diffusion

Absence of gelation

Theorem: Assume $a_{i,j} \leq (i+j)\,\theta(j/i)$ for all $j \geq i \in \mathbb{N}$ for a bounded function $\theta(x) \to 0$ as $x \to +\infty$.

Then, a superlinear moment is bounded on bounded time intervals $[0,T]$ for all $T > 0$,
i.e. for a test-sequence $\{\psi_i\}_{i\geq 1}$ with $\lim_{i\to\infty} \psi_i \to \infty$, we have:

$$\int_\Omega \sum_{i=1}^{\infty} i\,\psi_i c_i \leq C(T)$$

As a consequence, the mass is conserved

$$\int_\Omega \rho(t,x)\,dx = \int_\Omega \rho_0(x)\,dx \quad \text{for all } t \geq 0.$$

Proof of absence of gelation in special case

Consider $a_{i,j} = \sqrt{ij}$ and $B_i = 0$, $\int_\Omega \sum_{i=0}^{\infty} i \log i \, c_i(0,x)\, dx < \infty$

Then, (using $\log(1+x) \le C\sqrt{x}$)

$$\frac{d}{dt} \int_\Omega \sum_{i=1}^{\infty} i \, \log i \, c_i \, dx$$

$$= \int_\Omega \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \sqrt{ij}\, c_i \, c_j \left(i \, \log(1 + \frac{j}{i}) + j \, \log(1 + \frac{i}{j}) \right) dx$$

$$\le 2 \int_\Omega \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} i \, j \, c_i \, c_j \, dx \le 2 \int_\Omega \rho(t,x)^2 \, dx.$$

Proof of absence of gelation in special case

Consider $a_{i,j} = \sqrt{ij}$ and $B_i = 0$, $\int_\Omega \sum_{i=0}^{\infty} i \log i \, c_i(0,x)\, dx < \infty$

As a consequence, we have for all $T > 0$

$$\int_\Omega \sum_{i=0}^{\infty} i \ \log i \, c_i(T,x)\, dx \le \int_\Omega \sum_{i=0}^{\infty} i \ \log i \, c_i(0,x)\, dx + 2 \int_0^T \int_\Omega \rho(t,x)^2 \, dx dt,$$

and the propagation of the moment $\int \sum_{i=0}^{\infty} i \ \log i \, c_i(\cdot, x) dx$ ensures the conservation of the mass.

Discrete C-F with diffusion

Degenerate Diffusion: Absence of gelation

Assume decaying diffusion coefficients with $\gamma \in [0, 1]$

$$d_i \geq C\, i^{-\gamma},$$

and coagulation coefficients bounded like

$$a_{i,j} \leq C \left(i^\alpha\, j^\beta + i^\beta\, j^\alpha \right),$$

with $\alpha + \beta + \gamma \leq 1$, $\alpha, \beta \in [0, 1)$.

Then, the mass is conserved $\int_\Omega \rho(t, x)\, dx = \int_\Omega \rho_0(x)\, dx$, $t \geq 0$.

S. Simons, D.R. Simpson *The effect of particle coagulation on the diffusive relaxation of a spatially inhomogeneous aerosol* J. Phys. A **21** (1988) pp. 3523-3536.

Existence theory of discrete C-F with diffusion

By duality we have uniform L^2-bound of approximating systems independent of $a_{i,j}$.

The assumption $\lim_{j\to+\infty} \frac{a_{i,j}}{j} = 0$ is needed for the limit of

$$Q^{-,M}_{coag} = c_i^M \sum_{j=1}^{\infty} a_{i,j}\, c_j^M.$$

as c_i^M converges to c_i weak-$*$ in $L^\infty(\Omega_T)$,
we need $\sum_{j=1}^{\infty} a_{i,j}\, c_j^M \to \sum_{j=1}^{\infty} a_{i,j}\, c_j$ strongly in $L^1(\Omega_T)$

$$\int_0^T \int_\Omega \left| \sum_j a_{i,j}(c_j^M - c_j) \right| dxdt \leq 2 \sup_{j\geq J_0} \left| \frac{a_{i,j}}{j} \right| \|\rho\|_2 + \sup_{j\leq J_0} \|c_j^M - c_j\|_{L^1}$$

Discrete C-F with diffusion

Existence theory generalised quadratic C-F models

$$\partial_t c_i - d_i\, \Delta_x c_i = \frac{1}{2} \sum_{k+l=i} a_{k,l}\, c_k\, c_l - \sum_{k=1}^{\infty} a_{i,k}\, c_i\, c_k$$

$$+ \frac{1}{2} \sum_{k,l=1}^{\infty} \sum_{i<\max\{k,l\}} b_{k,l}\, c_k\, c_l\, \beta_{i,k,l} - \sum_{k=1}^{\infty} b_{i,k}\, c_i\, c_k$$

global L^1-existence in 1D provided

$$\lim_{l\to\infty} \frac{a_{k,l}}{l} = 0, \ \lim_{l\to\infty} \frac{b_{k,l}}{l} = 0, \ \lim_{l\to\infty} \sup_k \left\{ \frac{b_{k,l}}{kl}\, \beta_{i,k,l} \right\} = 0 \quad k, i \in \mathbb{N}$$

J.A. Cañizo, L. Desvillettes, K. F. *Regularity and mass conservation for discrete coagulation-fragmentation equations with diffusion*, Ann. Inst. H. Poincaré (C) Anal. Non Linéaire, **27** no.2 (2010) pp. 639–654

Strong solutions of C-F with diffusion?

Reversible reaction-diffusion of 4 species $\mathcal{A}_1 + \mathcal{A}_2 \leftrightarrow \mathcal{A}_3 + \mathcal{A}_4$
concentrations a_i, individual diffusivities $d_i > 0$

$$\partial_t a_1 - d_1 \triangle_x a_1 = -a_1\, a_2 + a_3\, a_4$$

$$\partial_t a_2 - d_2 \triangle_x a_2 = -a_1\, a_2 + a_3\, a_4$$

$$\partial_t a_3 - d_3 \triangle_x a_3 = +a_1\, a_2 - a_3\, a_4$$

$$\partial_t a_4 - d_4 \triangle_x a_4 = +a_1\, a_2 - a_3\, a_4$$

bounded, smooth domain $\Omega \subset \mathbb{R}^N$, $|\Omega| = 1$
homogeneous Neumann boundary conditions

mass action kinetics (quadratic, no invariant regions)

integrable and bounded initial data $a_{i,0}(x) \geq 0$

Strong solutions of C-F with diffusion?

- 1D: global classical solutions (Amann)
  exponential convergence to equilibrium in all Sobolev norms.
- 2D: global classical (De Giorgi's method)
- 2D: global classical (duality method)
- allD: global weak L^2-solutions via duality
  explicit exponential decay (rates) in L^p, $1 \leq p < 2$

T. Goudon, A. Vasseur *Regularity analysis for systems of reaction-diffusion equations* Annales de l'École Normale Supérieure

J.A. Cañizo, K.F., L. Desvillettes, F. Otto, in preparation

L. Desvillettes, K. F., Revista Mat. Ibero. (2008), Proc. Equadiff 2007

Continuous C-F with diffusion

Inhomogeneous C-F with normalised rates

Continuous in size density $f(t,x,y)$, $t \geq 0$, $x \in \Omega$, $y \in [0,\infty)$
coagulation-fragmentation coefficients $a(y,y') = b(y) = 1$

$$\partial_t f - d(y)\triangle_x f = \int_0^y f(y-y')\, f(y')dy' - 2f(y)\int_0^\infty f(y')\, dy' + 2\int_y^\infty f(y')\, dy' - y\, f(y)$$

homogeneous Neumann, non-negative initial density $f_0(x,y)$
diffusion may degenerate at most linearly for large sizes

$$d(y) \leq d^*(\delta)\,,\ \forall y \in [\delta, \delta^{-1}], \qquad 0 < \frac{d_*}{1+y} \leq d(y)\,,\ \forall y \in [0,\infty)$$

M. Aizenman, T. Bak *Convergence to equilibrium in a system of reacting polymers* Comm. Math. Phys. **65** (1979) pp. 203-230

Inhomogeneous C-F with normalised rates

Macroscopic densities

amount of monomers or mass density N, number density M

$$N = \int_0^\infty y' f(y')\, dy' , \quad M = \int_0^\infty f(y')\, dy'$$

conservation of the total mass

$$\partial_t N - \triangle_x \left(\int_0^\infty d(y')\, y'\, f(y')\, dy' \right) = 0$$

$$\partial_t M - \triangle_x \left(\int_0^\infty d(y')\, f(y')\, dy' \right) = N - M^2$$

Large time behaviour?

Large Time Behaviour

Entropy Method

E entropy functional, nonincreasing

D entropy dissipation

$$\frac{d}{dt}(E - E_\infty) \; = \; -D \leq 0$$

provided conservation laws: $D = 0 \Longleftrightarrow$ steady state

$$D \geq \Phi(E - E_\infty)\,, \quad \Phi(0) = 0,\ \Phi \geq 0$$

$\Rightarrow$ convergence in entropy, exponential if $\Phi'(0) > 0$

convergence in L_1: Cziszár-Kullback-Pinsker type inequalities

Entropy Method

Advantages

- based on functional inequalities $\rightarrow$ "robust"
- avoids linearisation $\rightarrow$ "global" results
- explicit constants

(non)linear diffusion: [O], [CJMTU], [AMTU], . . .

inhomogeneous kinetic equations: [DV]

reaction-diffusion systems: [DF]
(no Bakry-Emery for systems)

Inhomogeneous C-F with normalised rates

Entropy (free energy functional)

Entropy functional

$$H(f)(t,x) = \int_0^\infty (f \ln f - f)\, dy\,,$$

Entropy dissipation: $f = f(y)$, $f' = f(y')$, $f'' = f(y+y')$

$$\frac{d}{dt}\int_\Omega H(f)\,dx = -D_H(f)$$

$$D_H(f) = \int_\Omega \int_0^\infty d(y)\frac{|\nabla_x f|^2}{f}\,dy\,dx$$

$$+ \int_\Omega \int_0^\infty\int_0^\infty (f'' - f\,f')\ln\left(\frac{f''}{f\,f'}\right) dy\,dy' dx \geq 0$$

Inhomogeneous C-F with normalised rates

Inequality by [Aizenman, Bak]'79

$$\int_0^\infty \int_0^\infty (f(y+y') - f(y)f(y')) \ln\left(\frac{f(y+y')}{f(y)f(y')}\right) dy\, dy' \geq M\, H(f|f_{\sqrt{N},N}) + 2(M - \sqrt{N})^2$$

Lower bound of entropy dissipation

$$D_H(f) \geq \int_\Omega \int_0^\infty d(y) \frac{|\nabla_x f|^2}{f} dy\, dx + M\, H(f|f_{\sqrt{N},N}) + 2(M - \sqrt{N})^2$$

Relative entropy $\quad H(f|f_{\sqrt{N},N}) = H(f) - H(f_{\sqrt{N},N})$

Inhomogeneous C-F with normalised rates

Local and global equilibria

Intermediate equilibria with the moments N and $M = \sqrt{N}$

$$f_{\sqrt{N},N} = e^{-\frac{1}{\sqrt{N}}y}$$

Global equilibrium

$$f_\infty = e^{-\frac{y}{\sqrt{N_\infty}}}$$

- constant in x satisfying $M_\infty^2 = N_\infty$
- preserves the initial mass $N_\infty = \int_0^\infty N(x)\,dx$

Inhomogeneous C-F with normalised rates

relative entropy, additivity

Relative entropy

$$H(f|g) = H(f) - H(g)$$

Additivity

$$H(f|f_\infty) = H(f|f_{\sqrt{N},N}) + H(f_{\sqrt{N},N}|f_\infty)$$

$f_{\sqrt{N},N}$ and f_∞ do not need to have the same L^1_y-norm, but nevertheless

$$\int_\Omega H(f_{\sqrt{N},N}|f_\infty)\,dx = 2\left(\sqrt{\int_\Omega N\,dx} - \int_\Omega \sqrt{N}\,dx\right) \geq 0$$

Existence results

Global existence and uniqueness of classical solutions (in 1D with coefficients not quite [Aizenman, Bak])

H. Amann *Coagulation-fragmentation processes*, Arch. Rat. Mech. Anal. **151** (2000), pp.339-366.

H. Amann, C. Walker *Local and global strong solutions to continuous coagulation-fragmentation equations with diffusion*, J. Differential Equations **218** (2005), pp.159-186.

Inhomogeneous C-F with normalised rates

Existence results

Global existence of weak solutions satisfying the entropy dissipation inequality

$$\int_\Omega H(f(t))\,dx + \int_0^t D_H(f(s))\,ds \leq \int_\Omega H(f_0)\,dx$$

Diffusivity $d(y) \in L^\infty([1/R, R])$ for all $R > 0$

Equilibria attract all global weak solutions
(no rate, De la Salle principle)

Ph. Laurençot, S. Mischler, *The continuous coagulation-fragmentation equation with diffusion* Arch. Rat. Mech. Anal. **162** (2002), pp.45-99.

Inhomogeneous C-F with normalised rates

Exponential convergence to equilibrium

Nonnegative initial data $(1+y+\ln f_0)f_0 \in L^1((0,1)\times(0,\infty))$ with positive initial mass $\int_0^1 N_0(x)\,dx = N_\infty > 0$ on $\Omega = (0,1)$. At most linearly degenerating diffusion coefficients.

Then, for $\beta < 2$ and $t > 0$

$$\|f(t,\cdot,\cdot) - f_\infty\|_{L^1_{x,y}} \leq C_\beta\, e^{-(\ln t)^\beta},$$

and for all $t \geq t_* > 0$

$$\int_0^\infty (1+y)^q \, \|f(t,\cdot,y) - f_\infty(y)\|_{L^\infty_x} \, dy \leq C_{\beta,q}\, e^{-(\ln t)^\beta} \,,$$

L. Desvillettes, K. F. *Large time asymptotics for a Continuous Coagulation-Fragmentation Model with Degenerate Size-dependent Diffusion*, SIAM J. Math. Anal. **41** no.6 (2009) pp. 2315–2334.

Entropy Entropy-Dissipation Estimate

needs $\|M\|_{L^\infty_x}$, $\|M\|_{L^\infty_t(L^1_x)}$, $\mathcal{M}_* > 0$

Step 1) Additivity

$$\int_0^1 H(f|f_\infty)\,dx = \int_0^1 H(f|f_{\sqrt{N},N})\,dx + 2\left(\sqrt{\overline{N}} - \overline{\sqrt{N}}\right)$$

Entropy Entropy-Dissipation Estimate

needs $\|M\|_{L^\infty_x}$, $\|M\|_{L^\infty_t(L^1_x)}$, $\mathcal{M}_* > 0$

Step 2) "Reacting" moments $M \leftrightarrow \sqrt{N}$

$$\int_0^1 H(f|f_\infty)\,dx = \int_0^1 H(f|f_{\sqrt{N},N})\,dx + 2\left(\sqrt{\overline{N}} - \overline{\sqrt{N}}\right)$$

$$\sqrt{\overline{N}} - \overline{\sqrt{N}} \le \frac{2}{\sqrt{N_\infty}}\left[\|M - \sqrt{N}\|^2_{L^2_x} + \|M - \overline{M}\|^2_{L^2_x}\right]$$

This inequality quantifies how a reversible reaction of two species $M \leftrightarrow \sqrt{N}$ passes the diffusion effects from M to N.

Entropy Entropy-Dissipation Estimate

needs $\|M\|_{L^\infty_x}$, $\|M\|_{L^\infty_t(L^1_x)}$, $\mathcal{M}_* > 0$

Step 2) "Reacting" moments N **and** $M > \mathcal{M}_* > 0$

$$\int_0^1 H(f|f_\infty)\,dx \le C\left[\int_0^1 M H(f|f_{\sqrt{N},N})\,dx + 2\|M-\sqrt{N}\|^2_{L^2_x}\right] + \frac{4}{\sqrt{N_\infty}}\|M-\overline{M}\|^2_{L^2_x}$$

$$\le C\int_0^1\int_0^\infty\int_0^\infty (f'' - f f')\ln\left(\frac{f''}{f f'}\right) dy\,dy'\,dx + \frac{4}{\sqrt{N_\infty}}\|M-\overline{M}\|^2_{L^2_x}\,,$$

Entropy Entropy-Dissipation Estimate

needs $\|M\|_{L^\infty_x}$**,** $\|M\|_{L^\infty_t(L^1_x)}$**,** $\mathcal{M}_* > 0$

Step 3) Diffusion For a cut-off size $A > 0$, denote

$M_A(t,x) := \int_0^A f(t,x,y)\,dy$ and $M_A^c(t,x) := \int_A^\infty f(t,x,y)\,dy$

$$\begin{aligned}\|M - \overline{M}\|^2_{L^2_x} &= \int_\Omega \left(M_A - \overline{M_A} + M_A^c - \overline{M_A^c}\right)^2 dx \\ &\leq 2\|M_A - \overline{M_A}\|^2_{L^2_x} + \frac{4}{A^{2p}} \int_\Omega \left(\int_0^\infty y^p f(y)\,dy\right)^2 dx \\ &\leq C(P, d_*)\, A\, \|M\|_{L^\infty_x} \int_\Omega \int_0^\infty d(y) \frac{|\nabla_x f|^2}{f}\,dydx \\ &\quad + \frac{4}{A^{2p}} \|M\|_{L^\infty_x} \mathcal{M}_{2p}\end{aligned}$$

for any $p > 1$.

Entropy Entropy-Dissipation Estimate

Let $f := f(x,y) \geq 0$ be measurable with moments
$0 < \mathcal{M}_* \leq M(x) = \int_0^\infty f(x,y)\,dy \leq \|M\|_{L^\infty_x}$,
$0 < N_\infty = \int_\Omega \int_0^\infty y\, f(x,y)\, dydx$, $\int_\Omega \int_0^\infty y^{2p} f(x,y)\, dxdy \leq \mathcal{M}_{2p}$.

Then, for all $A \geq 1$ and $p > 1$

$$D_1(f) \geq \frac{C}{A\,\|M\|_{L^\infty_x}} \int_\Omega H(f|f_\infty)\,dx - C\,\frac{\mathcal{M}_{2p}}{A^{2p+1}}\,,$$

with a constant $C = C(\mathcal{M}_*, N_\infty, d_*, P(\Omega))$ depending only on $\mathcal{M}_*$, N_∞, d_*, and the Poincaré constant $P(\Omega)$.

Proof of Theorem

Algebraic rate for all $p > 1$

We have for any $A > 1$

$$\frac{d}{dt}\int_0^1 H(f|f_\infty)\,dx \le -\frac{C}{\|M\|_{L^\infty_x}}\frac{1}{A}\int_0^1 H(f|f_\infty)\,dx + \frac{C_p\,2^{8p^2}}{A^{2p+1}}\,,$$

where $\|M\|_{L^\infty_x}(t) \le m_\infty + m_2(t)$.

Balancing the r.h.s. (e.g. positive term = 1/2 negative term) by choosing $A = A(t) > 2$ yields

$$\frac{1}{A} \le C^{-1/2}\left(\frac{C\int_0^1 H(f|f_\infty)\,dx}{\|M\|_{L^\infty_x}\,2^{8p^2}}\right)^{\frac{1}{2p}}\,,$$

Thus, Gronwall yields algebraic rate $2p$ for all $p > 1$.

Proof of Theorem

Algebraic rate for all $p > 1$

Faster than polynominal rate

Then, by summing w.r.t. $p \in \mathbb{N}$

$$\int_0^1 H(f(t)|f_\infty)\,dx \leq L(t - C),$$

where (for all $1 < \alpha < 2$)

$$L^{-1}(t) = \sum_{q \geq 1,\ \text{even}} \frac{t^q}{(C\,q)^q\,2^{2q^2}} = \sum_{q \geq 1,\ \text{even}} t^q\,e^{-2q^2\ln 2 - q\ln(q\,C)}$$

$$\geq C(\alpha)\,e^{\ln^{2(\alpha-1)}(t)}$$

for all t large enough and any $1 < \alpha < 2$.

A-priori Estimates

$(L^1 \cap L^2) + L^\infty$ bounds in 1D

Lemma:

$$\|M(t,\cdot)\|_{L^\infty_x} \leq m_\infty + m_2(t)$$

Proof: $f(t,x,y) - f(t,\tilde{x},y) = 2\int_{\tilde{x}}^{x} \sqrt{f}(t,\xi,y)\,\partial_x\sqrt{f}(t,\xi,y)\,d\xi$

$$\int_0^\infty \left| f(t,x,y) - \int_0^1 f(t,\tilde{x},y)\,d\tilde{x} \right| dy$$

$$\leq 2\left[\int_0^\infty\!\!\int_0^1 \frac{f(t,x,y)}{d(y)} dxdy\right]^{\frac{1}{2}} \left[\int_0^\infty\!\!\int_0^1 d(y)|\partial_x\sqrt{f}(t,x,y)|^2 dxdy\right]^{\frac{1}{2}}$$

$$M(t,x) \leq \int_0^1 M(t,\tilde{x})\,d\tilde{x} + d_*^{-1/2}\,(\mathcal{M}_0^* + N_\infty)^{1/2}\,D(f(t))^{1/2}.$$

A-priori Estimates

Lemma: $\int_\Omega M(t,x)\,dx \geq \mathcal{M}_{0*}$

$$\frac{d}{dt}\int_0^1 M(t,x)\,dx = \int_0^1 (N - M^2)\,dx$$
$$\geq \int_0^1 N_{in}(x)\,dx - (m_\infty + m_1(t)) \int_0^1 M(t,x)\,dx$$

$$\int_0^1 M(t,x)\,dx \geq \int_0^1 M_{in}(x)\,dx\, e^{-\int_0^t (m_\infty + m_1(\sigma))\,d\sigma}$$
$$+ \int_0^1 N_{in}(x)\,dx \int_0^t e^{-\int_s^t (m_\infty + m_1(\sigma))\,d\sigma}\,ds$$
$$\geq e^{-\mu_1}\left[e^{-m_\infty t}\|M_{in}\|_{L^1_x} + \frac{1 - e^{-m_\infty t}}{m_\infty}\|N_{in}\|_{L^1_x}\right]$$

A-priori Estimates

Moments $M_p(f)(t) := \int_0^1 \int_0^\infty y^p \, f \, dy \, dx$

Lemma: For $p > 1$ and for a.a. $t \geq t_* > 0$

$$M_p(f)(t) \leq (2^{2p} \, C)^p =: \mathcal{M}_p^*$$

for $C = C(t_*, f_{in})$ depending only on the initial datum and t_*.

Idea: fragmentation produces moments

$$\frac{d}{dt} M_p(f)(t) \leq (2^p - 2) \, M_p(f)(t) \, [m_\infty + m_2(t)] - \frac{p-1}{p+1} M_{p+1}(f)(t).$$

interpolation $-\frac{p-1}{p+1} M_{p+1}(f) \leq \frac{\epsilon^{-p}}{p+1} N_\infty - \frac{p}{p+1} \epsilon^{-1} \, M_p(f)$

use Duhamel's formula, $\int_{t_*}^t m_2 \, ds \leq \mu_2 \sqrt{t - t_*}$

A-priori Estimates

Moments $M_p(f)(t) := \int_0^1 \int_0^\infty y^p \, f \, dy \, dx$

How start with $(1+y) f_{in} \in L^1$??

Vallée-Poussin lemma:

for any $f \in L^1$ exists $\varphi \nearrow \infty$ such that $\varphi f \in L^1$.

Idea: $F = \int_x^\infty f(t) \, dt$ and $\varphi = F^{-\alpha}$ for $\alpha < 1$

$$\int_0^\infty \varphi f \, dy = \int_0^\infty \frac{-F'}{F^\alpha} \, dy = \frac{1}{1-\alpha} F(0)^{-\alpha+1}$$

Then, for a regularised version of $\varphi(y)$, calculate

"$y \, \varphi(y)$-moment" and $y \, \varphi(y) \, Q_{frag} \leq -C_1 y^{1+\delta}$

A-priori Estimates

Lower bound $M(t,x) \geq \mathcal{M}_* > 0$

Lemma: Let $t_* > 0$ be given. Then, there is a strictly positive constant $\mathcal{M}_*$ (depending on t_*, d_* and $d^*(\delta)$)

$$M(t,x) \geq \mathcal{M}_*.$$

Idea: linear lower bound for lost terms

$$\partial_t f - d(y)\,\partial_{xx} f = g_1 - y\,f - \|M(t,\cdot)\|_{L^\infty_x} f$$

where g_1 is nonnegative, then

$$(\partial_t + d(y)\,\partial_{xx})\left(f\, e^{ty + \int_0^t \|M(s,\cdot)\|_{L^\infty_x}\, ds}\right) = g_2$$

where g_2 is nonnegative.

A-priori Estimates

Lower bounds $M(t,x) \geq \mathcal{M}_*$ **and** $N(t,x) \geq \mathcal{N}_*$

Fourier series and Poisson's formula for $\partial_t h - d\,\partial_{xx} h = G \in L^1$ with homogeneous Neumann boundaries on $(0,1)$

$$h(t,x) = \frac{1}{2\sqrt{\pi}} \int_{-1}^{1} \tilde{h}(0,z) \sum_{k=-\infty}^{\infty} \frac{1}{\sqrt{d\,t}}\, e^{-\frac{(2k+x-z)^2}{4d\,t}}\, dz$$

$$+ \frac{1}{2\sqrt{\pi}} \int_{0}^{t} \int_{-1}^{1} \tilde{G}(s,z) \sum_{k=-\infty}^{\infty} \frac{1}{\sqrt{d\,(t-s)}}\, e^{-\frac{(2k+x-z)^2}{4d\,(t-s)}}\, dz ds$$

$\tilde{h}$ and $\tilde{G}$ "mirrored" around 0

A-priori Estimates

Lower bounds $M(t,x) \geq \mathcal{M}_*$ **and** $N(t,x) \geq \mathcal{N}_*$

$$f(t_1+t,x,y) \geq C \int_0^1 f(t_1,z,y)\, e^{-(2t_* + \frac{1}{d_*\, t_*})\, y}\, dz,$$

Moment bound $\int_0^1 \int_0^\infty y^2\, f(t,x,y)\, dy\, dx \leq \mathcal{M}_2^*$

$$M(t_1+t,x) \geq C\, e^{-(2t_* + \frac{1}{d_*\, t_*})\frac{1}{\delta}} \int_0^1 \int_\delta^{1/\delta} f(t_1,z,y)\, dydz$$

$$\geq C\, e^{-(2t_* + \frac{1}{d_*\, t_*})\frac{1}{\delta}} \left(\mathcal{M}_{0*} - \delta\, N_\infty - K\,\delta - \frac{\int_0^1 H(f)\, dx}{\ln K} \right)$$

Choosing δ and K, we get that $M(t_1+t,x) \geq \mathcal{M}_*$.

Regularity, Interpolation

$\int_0^\infty (1+y)^q \, \|f(t,\cdot,y) - f_\infty(y)\|_{L^\infty_x} \, dy \le C \, e^{-\alpha \, t}$

Moment control implies $\int_0^T \int_0^1 \int_0^\infty (1+y)^q \, Q^+(f,f) \, dy \, dx \, dt \le C_T$

Regularising effect of 1D heat equation: $\partial_t f - d(y) \partial_{xx} f = g$

for all $q \in [1,3)$: $\frac{1}{r} + 1 = \frac{1}{p} + \frac{1}{q}$

$$\|f\|_{L^r([0,T]\times\Omega)} \le C_T \, d(y)^{\frac{1-q}{2q}} \, \|f_{in}\|_{L^p_x} + C_T \, d(y)^{\frac{1-q}{2q}} \, \|g\|_{L^p_{t,x}}$$

and while $d(y)^{\frac{1-q}{2q}} \le (1+y)^{1/3}$ for y large. Thus,

$$\|f(\cdot,\cdot,y)\|_{L^{3-\varepsilon}([t_*,T]\times\Omega)} \le C_T \left(\|f(0,\cdot,y)\|_{L^1_x} + \|Q^+(f,f)(\cdot,\cdot,y)\|_{L^1([0,T]\times\Omega)} \right)$$

Regularity, Interpolation

$\int_0^\infty (1+y)^q \, \| f(t,\cdot,y) - f_\infty(y) \|_{L^\infty_x} \, dy \le C \, e^{-\alpha \, t}$

A bootstrap yields after three iteration steps

$$\int_0^\infty (1+y)^q \, \| f(T,\cdot,y) \|_{H^1_x} \, dy \le C_T$$

Interpolation

$$\int_0^\infty (1+y)^q \, \| f(T,\cdot,y) - f_\infty(y) \|_{L^\infty_x} \, dy$$
$$\le \int_0^\infty \Big((1+y)^q \, \| f(T,\cdot,y) - f_\infty(y) \|_{H^1_x}^{3/4} \Big) \, \| f(T,\cdot,y) - f_\infty(y) \|_{L^1_x}^{1/4} \, dy$$
$$\le C_T^{3/4} \, e^{-\alpha \, T}$$

Inhomogeneous Aizenman-Bak

Fast-reaction limit

$$\partial_t f^\varepsilon - d(y)\triangle_x f^\varepsilon = \frac{1}{\varepsilon}\left(Q_{coag}(f^\varepsilon, f^\varepsilon) + Q_{frag}(f^\varepsilon)\right)$$

formal limit: $f^\varepsilon \longrightarrow e^{-\frac{y}{\sqrt{N^0(t,x)}}}$

satisfying the nonlinear, nondegenerate diffusion equation

$$\partial_t N^0(t,x) - \triangle_x n(N^0(t,x)) = 0$$

where

$$n(N) := \int_0^\infty d(y)\, y\, e^{-\frac{y}{\sqrt{N}}}\, dy$$

with $\quad 0 < \inf_{[0,\infty)}\{d(y)\}N \le n(N) \le \sup_{[0,\infty)}\{d(y)\}N$.

Fast-reaction limit

Theorems:

- convergence without rate using compactness
- assuming lower bound: convergence with rate in ε

J.A. Carrillo, L. Desvillettes, K. F., *Rigorous Derivation of a Nonlinear Diffusion Equation as Fast-Reaction Limit of a continuous Coagulation–Fragmentation Model with Diffusion*, Comm. Partial Differential Equations **34** no.10-12 (2009) pp. 1338–1351.

J.A. Carrillo, L. Desvillettes, K. F., *Fast-Reaction Limit for the Inhomogeneous Aizenman-Bak Model.* Kinetic and Related Models **1** no. 1 (2008) pp. 127–137.

Fast-Reaction limit

Dissipation of entropy

$$-\varepsilon \frac{d}{dt} \int_\Omega H(f^\varepsilon)\,dx \geq \int_\Omega M^\varepsilon\, H(f^\varepsilon | f_{\sqrt{N^\varepsilon}, N^\varepsilon})\,dx$$
$$+ 2 \int_\Omega ((M^\varepsilon) - \sqrt{N^\varepsilon})^2\,dx$$

Thus

$$\int_0^\infty \int_\Omega M^\varepsilon H(f^\varepsilon | f_{\sqrt{N^\varepsilon}, N^\varepsilon})\,dx\,dt \leq \varepsilon\, C$$

Assuming $M^\varepsilon \geq \mathcal{M}_*$ it follows from Cziszár-Kullback-Pinsker

$$\| f^\varepsilon - e^{-\frac{y}{\sqrt{N^\varepsilon}}} \|^2_{L^2_t(L^1_{x,y})} \leq \varepsilon\, C(\mathcal{M}_*)$$

Expansion

However, want $f_1^\varepsilon \in L^2_{t,x}(L^1_y((1+y)\,dy))$

An interpolation shows that for a $0<\theta<1$, there exists

$$f^\varepsilon = e^{-\frac{y}{\sqrt{N^\varepsilon}}} + \varepsilon^\theta f_1^\varepsilon, \quad \text{with} \quad \nabla_x f_1^\varepsilon \cdot \nu(x) = 0 \ \text{ on } \ \partial\Omega$$

Then

$$\partial_t N^\varepsilon - \triangle_x n(N^\varepsilon) = \varepsilon^\theta \triangle_x \int_0^\infty d(y) y f_1^\varepsilon \, dy \ := \varepsilon^\theta \triangle_x g^\varepsilon$$

where $g^\varepsilon \in L^2_{t,x}$ with $\nabla_x g^\varepsilon \cdot \nu(x) = 0$ on $\partial\Omega$.

Fast-Reaction limit

Compactness

Let $g^\varepsilon \in L^2_{t,x}$ with $\nabla_x g^\varepsilon \cdot \nu(x) = 0$. Take initial data $N_{in} \in L^2_x$.

Then, the solutions of the nonlinear diffusion equation

$$\partial_t N^\varepsilon - \triangle_x n(N^\varepsilon) = \varepsilon^\theta \triangle_x g^\varepsilon$$

$$\nabla_x N^\varepsilon \cdot \nu(x)|_{\partial\Omega} = 0$$

converge in $L^2_{t,x}$ as $\varepsilon \to 0$ to the solution N of

$$\partial_t N - \triangle_x n(N) = 0$$

$$\nabla_x N \cdot \nu(x)|_{\partial\Omega} = 0$$

Fast-Reaction limit

Compactness : proof

Duality argument: $w \geq 0$, $w(T)=0$, $\nabla_x w \cdot \nu(x)|_{\partial\Omega} = 0$

$$-\partial_t w - \frac{n(N^\varepsilon) - n(N)}{N^\varepsilon - N} \triangle_x w = H$$

Holds that $\|\triangle_x w\|_{L^2([0,T]\times\Omega)} \leq C \|H\|_{L^2([0,T]\times\Omega)}$

Then

$$\left| \int_0^T \int_\Omega (N^\varepsilon - N)\, H dx dt \right| \leq \varepsilon^\theta \|g^\varepsilon\|_{L^2_{t,x}} \, \|\triangle_x w\|_{L^2([0,T]\times\Omega)}$$

Since $H \geq 0 \in C_0^\infty([0,T]\times\Omega)$ is arbitrary

$$\|N^\varepsilon - N\|_{L^2_{t,x}} \leq C\, \varepsilon^\theta \, \|g^\varepsilon\|_{L^2_{t,x}} \leq C\, \varepsilon^\theta$$

THANK YOU!

THANKS TO THE ORGANISERS!

(now and in the future)