Unification of Discrete and Continuous Coagulation-Fragmentation Equations

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The Space of Radon Measures: TV Norm and BL norm

There are two norms we associate with $\mathcal{M}(\mathbb{R}^+)$, the space of finite Radon measures on $\mathbb{R}^+ := [0, \infty)$. The first is the total variation norm given by

$$\|\mu\|_{TV} = \sup_{f \in C_c(\mathbb{R}^+),\ \|f\|_\infty \leq 1} \left\{ \int_{\mathbb{R}^+} f d\mu \right\} = |\mu|(\mathbb{R}^+).$$

The second is the Bounded-Lipschitz norm:

$$\|\mu\|_{BL} = \sup_{\phi \in W^{1,\infty}(\mathbb{R}^+),\ \|\phi\|_{W^{1,\infty}} \leq 1} \left\{ \int_{\mathbb{R}^+} \phi d\mu \right\}$$

where $\|\phi\|_{W^{1,\infty}} = \|\phi\|_\infty + \|\phi'\|_\infty$ and $W^{1,\infty}(\mathbb{R}^+)$ is the space of Bounded-Lipschitz functions.

For $\mu \in \mathcal{M}^+(\mathbb{R}^+)$, $\|\mu\|_{TV} = \|\mu\|_{BL}$. However for a general $\mu \in \mathcal{M}(\mathbb{R}^+)$, $\|\mu\|_{BL} \leq \|\mu\|_{TV}$.

Comparison Between TV and BL

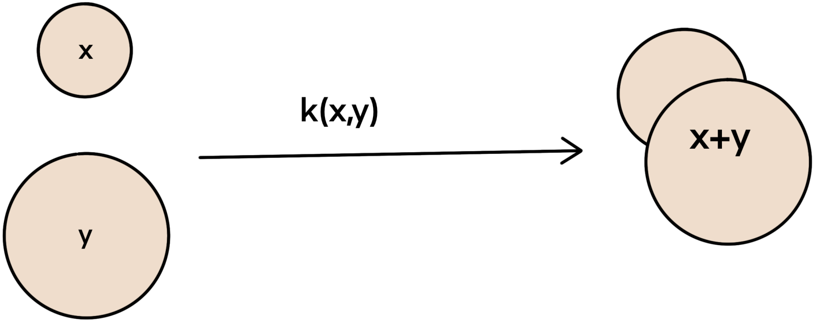
	$\|\cdot\|_{TV}$	$\|\cdot\|_{BL}$
$x_n \longrightarrow x \Rightarrow \delta_{x_n} \longrightarrow \delta_x$	$\times$	$\checkmark$
$\mathcal{M}(\mathbb{R}^+)$ **Banach**	$\checkmark$	$\times$
$\mathcal{M}^+(\mathbb{R}^+)$ **Complete**	$\checkmark$	$\checkmark$
$\mathcal{M}_R(\mathbb{R}^+)$ **Complete**	$\checkmark$	$\checkmark$

Where

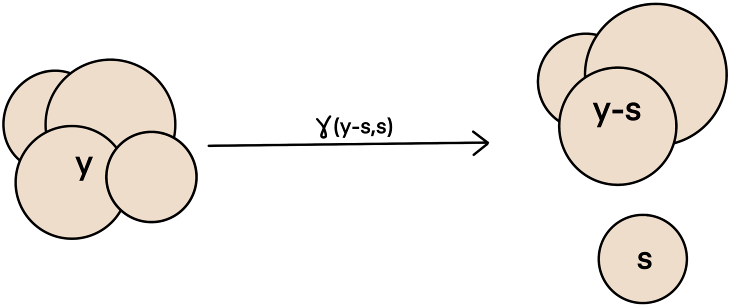
$$\mathcal{M}_R(\mathbb{R}^+) := \{\mu \in \mathcal{M}(\mathbb{R}^+) : \ \|\mu\|_{TV} \le R\}.$$

Description of the Coagulation Process

Coagulation is the process of particles "clumping together". This is described mathematically by particles of size x and y colliding at rate $\kappa(x, y)$ to form a particle of size $x + y$. It is assumed $\kappa(x, y) = \kappa(y, x)$.



Binary fragmentation is the the process of which a cohort of particles of size y splinters off into two separate particles of sizes s and $y - s$ at rate $\gamma(y - s, s)$.



Multiple Fragmentation

Multiple fragmentation allows particles of size y to fracture into a distribution of particles given by $b(y, dx)$ at rate $a(y)$.

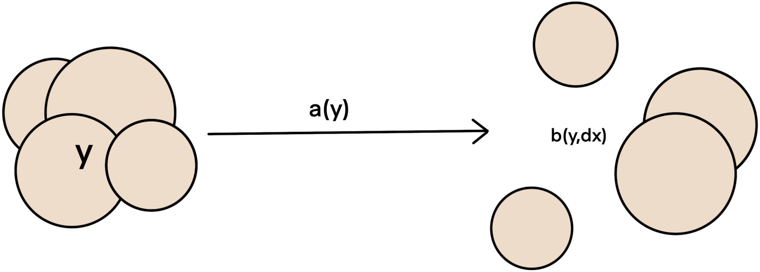


Figure: Marian Smoluchowski, Polish physicist born 28 May, 1872.

In 1916, Smoluchowski introduced the discrete coagulation equation:

$$\frac{\partial}{\partial t}u(t,x_i)=\frac{1}{2}\sum_{j=1}^{i-1}\kappa(x_i-x_j,x_j)u(t,x_i-x_j)u(t,x_j)-\sum_{j=1}^{\infty}\kappa(x_i,x_j)u(t,x_i)u(t,x_j).$$

In 1928, this was extended by Müller to a continuous setting:

$$\frac{\partial}{\partial t}u(t,x)=\frac{1}{2}\int_0^x\kappa(x-y,y)u(t,x-y)u(t,y)dy-\int_0^\infty\kappa(x,y)u(t,x)u(t,y)dy.$$

Important Properties: Diminishing Total Population

Through coagulation, the total number of particles decreases over time. This can be seen by integrating both sides of the coagulation equation and using the substitution $z = x - y$:

$$\begin{aligned}
\frac{d}{dt}\int_0^\infty u(t,x)dx &= \frac{1}{2}\int_0^\infty \int_0^x \kappa(x-y,y)u(t,x-y)u(t,y)dydx \\
&\quad - \int_0^\infty \int_0^\infty \kappa(x,y)u(t,x)u(t,y)dydx \\
&= \frac{1}{2}\int_0^\infty \int_y^\infty \kappa(x-y,y)u(t,x-y)u(t,y)dxdy \\
&\quad - \int_0^\infty \int_0^\infty \kappa(x,y)u(t,x)u(t,y)dydx \\
&= -\frac{1}{2}\int_0^\infty \int_0^\infty \kappa(x,y)u(t,x)u(t,y)dydx
\end{aligned}$$

Important Properties: Conservation of Mass

Coagulation equations also conserve mass ($\int xu(t,x)dx$).

$$\begin{aligned}
\frac{d}{dt}\int_0^\infty xu(t,x)dx &= \frac{1}{2}\int_0^\infty\int_0^x x\kappa(x-y,y)u(t,x-y)u(t,y)dydx \\
&\quad -\int_0^\infty\int_0^\infty x\kappa(x,y)u(t,x)u(t,y)dydx \\
&= \frac{1}{2}\int_0^\infty\int_y^\infty x\kappa(x-y,y)u(t,x-y)u(t,y)dxdy \\
&\quad -\int_0^\infty\int_0^\infty x\kappa(x,y)u(t,x)u(t,y)dydx \\
&= \frac{1}{2}\int_0^\infty\int_0^\infty (z+y)\kappa(z,y)u(t,z)u(t,y)dxdy \\
&\quad -\int_0^\infty\int_0^\infty x\kappa(x,y)u(t,x)u(t,y)dydx = 0
\end{aligned}$$

History: Fragmentation Equations

Later Blatz and Tobolsky (1945) introduced discrete fragmentation terms:

$$\frac{\partial}{\partial t}u(t,x_i) = Coagulation + \sum_{j=i+1}^{\infty} a(x_j)b(x_j,x_i)u(t,x_j) - a(x_i)u(t,x_i).$$

Which were extended to a continuous setting by Melzak (1957):

$$\frac{\partial}{\partial t}u(t,x) = Coagulation + \int_x^{\infty} a(y)b(y,x)u(t,y)dy - a(x)u(t,x).$$

Binary fragmentation:

$$a(y) = \frac{1}{2}\int_0^y \gamma(y-s,s)\,ds, \qquad b(y,x) = \frac{\gamma(x,y-x)}{a(y)}$$

Some Applications

Coagulation-fragmentation models have many applications including:

- particle collision;
- coalescence of aerosols;
- polymerization;
- flocculation;
- hadronization;
- onset and progression of Alzheimer's disease.

A Particular Example

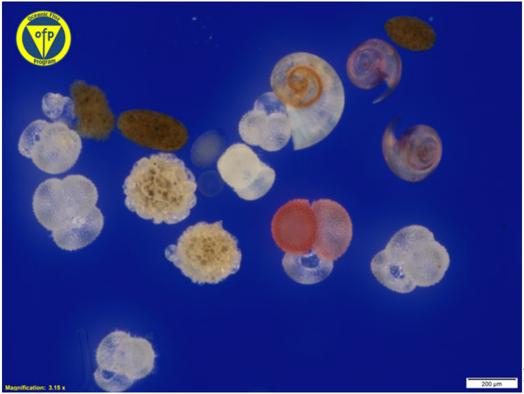
In Baird and Süli (2019), authors consider a mixed fragmentation model

$$\partial_t u = -a_i u + \sum_{j=i+1}^{N} a_j b_{j,i}\, u(x_j, t) + \int_N^{\infty} a(y) b(y,x) u(y,t) dy$$

to account for the phenomenon of "shattering" (i.e. the excessive creation of zero size dust particles).

Application to Oceanic Phytoplankton

These equations have been extensively used in mathematical biology. Jackson (1990), Ackleh et al. (1994) applied such models to phytoplankton aggregations while Gueron and Levin (1994) applied such equations to animal group formation.



[1]

[1] Photo from the Marine Biological Lab at the University of Chicago.

Structured Population Model

We consider the structured population model with boundary

$$\begin{cases} \partial_t \mu + \partial_x (g(t,\mu)\mu) + d(t,\mu)\mu = 0, \quad (t,x) \in (0,T) \times (0,\infty) \\ g(t,\mu)(0) D_{dx}\mu(0) = \displaystyle\int_0^\infty \beta(t,\mu)(y) d\mu(y), \quad t \in [0,T] \\ \mu(0) \in \mathcal{M}^+(\mathbb{R}^+) \end{cases},$$

where

$$\mu : [0,T] \longrightarrow \mathcal{M}^+(\mathbb{R}^+),$$
$$g, d, \beta : [0,T] \times \mathcal{M}^+(\mathbb{R}^+) \longrightarrow W^{1,\infty}(\mathbb{R}^+).$$

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- $\mu(t)(A) = \mu_t(A)$ represents the number of individuals with structure $x \in A$ at time t,
- $D_{dx}\mu(0)$ denotes the Radon-Nikodym derivative of $\mu(t)$ with respect to the Lebesgue measure, dx, at the point $x = 0$.

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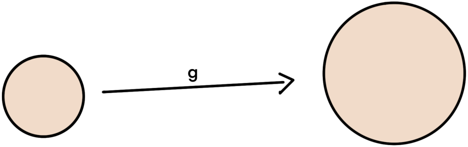
$g(t,\mu)(x)$ represents the growth rate of individuals of structure x.



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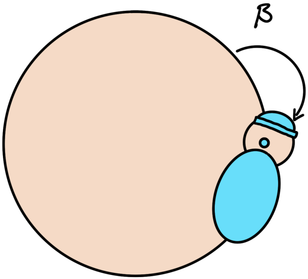
$$\begin{cases} \partial_t \mu + \partial_x(g(t,\mu)\mu) + d(t,\mu)\mu = 0, & (t,x) \in (0,T) \times (0,\infty) \\ g(t,\mu)(0) D_{dx}\mu(0) = \int_0^\infty \beta(t,\mu)(y) d\mu(y), & t \in [0,T] \\ \mu(0) \in \mathcal{M}^+(\mathbb{R}^+) \end{cases},$$

$\beta(t,\mu)(x)$ represents the birth rate of individuals of structure x.



Structured Population Model

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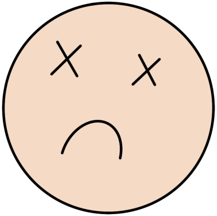
$$\begin{cases} \partial_t \mu + \partial_x (g(t,\mu)\mu) + d(t,\mu)\mu = 0, & (t,x) \in (0,T) \times (0,\infty) \\ g(t,\mu)(0) D_{dx}\mu(0) = \int_0^\infty \beta(t,\mu)(y) d\mu(y), & t \in [0,T] \\ \mu(0) \in \mathcal{M}^+(\mathbb{R}^+) \end{cases},$$

$d(t,\mu)(x)$ represents the death rate of individuals of structure x.



$$
\begin{cases}
\partial_t \mu + \partial_x (g(t,\mu)\mu) + d(t,\mu)\mu = K[\mu] + F[\mu], \\
g(t,\mu)(0) D_{dx}\mu(0) = \displaystyle\int_{\mathbb{R}^+} \beta(t,\mu)(y)\mu(dy), \\
\mu(0) \in \mathcal{M}^+(\mathbb{R}^+),
\end{cases}
\tag{1}
$$

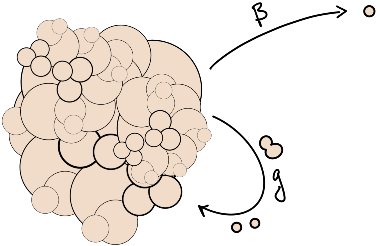
where

$$
\begin{aligned}
\mu : [0,T] &\longrightarrow \mathcal{M}^+(\mathbb{R}^+), \\
g, d, \beta : [0,T] \times \mathcal{M}^+(\mathbb{R}^+) &\longrightarrow W^{1,\infty}(\mathbb{R}^+), \\
K := K^+ - K^- : \mathcal{M}^+(\mathbb{R}^+) &\longrightarrow \mathcal{M}(\mathbb{R}^+), \\
F := F^+ - F^- : \mathcal{M}^+(\mathbb{R}^+) &\longrightarrow \mathcal{M}(\mathbb{R}^+)
\end{aligned}
$$

Our Model

$$\begin{cases} \partial_t \mu + \partial_x (g(t,\mu)\mu) + d(t,\mu)\mu = K[\mu] + F[\mu], \\ g(t,\mu)(0) D_{dx}\mu(0) = \int_{\mathbb{R}^+} \beta(t,\mu)(y)\mu(dy), \\ \mu(0) \in \mathcal{M}^+(\mathbb{R}^+), \end{cases} \tag{1}$$

Through single-cell division, aggregates can grow in size or shed off single cells. This is captured by the transport term and the boundary condition.



Reformulation into a Measure Setting: Coagulation

We reformulate these terms as measures by writing them as distributions. Taking

$$K^+(u)(x) = \frac{1}{2}\int_0^x \kappa(y, x-y)u(x-y)u(y)dy,$$

we can multiply by a test function ϕ and integrate over $\mathbb{R}^+$ to see

$$\begin{aligned}(K^+[u], \phi) &= \frac{1}{2}\int_0^\infty \int_0^x \kappa(y, x-y)u(x-y)u(y)dy\phi(x)\, dx \\ &= \frac{1}{2}\int_0^\infty \int_0^\infty \kappa(y, x)\phi(x+y)u(x)dx\, u(y)dy.\end{aligned}$$

Letting $\mu = u(x)dx$ we have

$$(K^+[\mu], \phi) = \frac{1}{2}\int_0^\infty \int_0^\infty \kappa(y, x)\phi(x+y)\mu(dx)\mu(dy)$$

Reformulation into a Measure Setting

Similarly,

$$(K^-[\mu], \phi) = \int_0^\infty \int_0^\infty \kappa(y, x)\phi(x)\, \mu(dy)\, \mu(dx).$$

Using kernel symmetry, we arrive at the following formulations:

$$(K[\mu], \phi) = \frac{1}{2}\int_0^\infty \int_0^\infty \kappa(y, x)[\phi(x+y) - \phi(x) - \phi(y)]\, \mu(dx)\, \mu(dy)$$

Using similar ideas we obtain this formulation for F.

$$(F[\mu], \phi) = \int_{\mathbb{R}^+} (b(y, \cdot), \phi)a(y)\, \mu(dy) - \int_{\mathbb{R}^+} a(y)\phi(y)\mu(dy),$$

where $(b(y, \cdot), \phi) = \int_0^y \phi(x)b(y, dx)$.

We apply the following assumptions to our model functions. Let $f = g, d, \beta$:

(A1) For any $R > 0$, there exists $L_R > 0$ such that for all $\|\mu_i\|_{TV} \leq R$ and $t_i \in [0, \infty)$ $(i = 1, 2)$ the following hold

$$\|f(t_1, \mu_1) - f(t_2, \mu_2)\|_\infty \leq L_R(|t_1 - t_2| + \|\mu_1 - \mu_2\|_{BL}),$$

(A2) There exists $\zeta > 0$ such that for all $T > 0$

$$\sup_{t\in[0,T]} \sup_{\mu\in\mathcal{M}^+(\mathbb{R}^+)} \|f(t, \mu)\|_{W^{1,\infty}} < \zeta,$$

(A3) For all $(t, \mu) \in [0, \infty) \times \mathcal{M}^+(\mathbb{R}^+)$,

$$g(t, \mu)(0) > 0.$$

Our Model: Assumptions on Coagulation and Fragmentation

We assume the coagulation kernel κ satisfies the following assumption:

(K) κ is symmetric, nonnegative, bounded by a constant C_κ, and globally Lipschitz with Lipschitz constant L_κ.

We assume the fragmentation kernel satisfies the following assumptions:

(F1) $a \in W^{1,\infty}(\mathbb{R}^+)$ is non-negative,

(F2) for any $y \geq 0$, $b(y, dx)$ is a measure such that

   (i) $b(y, dx)$ is non-negative and supported in $[0, y]$ so that for all $y > 0$ there exist a $C_b > 0$ such that $b(y, \mathbb{R}^+) < C_b$,

   (ii) there exists L_b such that

$$\|b(y, \cdot) - b(\bar{y}, \cdot)\|_{BL} \leq L_b |y - \bar{y}|$$

   (iii) $(b(y, \cdot), x) = y$

Given $T \geq 0$, we say a function $\mu \in C([0,T], \mathcal{M}^+(\mathbb{R}^+))$ is a weak solution to (1) if for all $\phi \in (C^1 \cap W^{1,\infty})([0,T] \times \mathbb{R}^+)$, and for all $t \in [0,T]$ the following holds:

$$
\begin{aligned}
&\int_{\mathbb{R}^+} \phi(t,x)\mu_t(dx) - \int_{\mathbb{R}^+} \phi(0,x)\mu_0(dx) = \\
&\int_0^t \int_{\mathbb{R}^+} \left[\partial_t \phi(s,x) + g(s,\mu_s)(x)\partial_x \phi(s,x) - d(s,\mu_s)(x)\phi(s,x)\right] \mu_s(dx)ds \\
&\quad + \int_0^t (K[\mu_s] + F[\mu_s], \phi(s,\cdot))ds + \int_0^t \int_{\mathbb{R}^+} \phi(s,0)\beta(s,\mu_s)(x)\mu_s(dx)ds.
\end{aligned}
$$

Our Model

We can extend this model to all of $\mathbb{R}$ by 0 by writing model (1) in the following way

$$\begin{cases} \partial_t \mu + \partial_x (g(t,\mu)\mu) + d(t,\mu)\mu = K[\mu] + F[\mu] + S[\mu_t]\delta_{x=0}, \\ \mu(0) \in \mathcal{M}^+(\mathbb{R}), \end{cases} . \tag{2}$$

where $S[\mu] = \int_{\mathbb{R}^+} \beta(t,\mu)(x)\mu(dx)$. This allows us to use recent well-posedness results for such equations over $\mathbb{R}$.

Existence-Uniqueness of Solutions

Theorem

Assume that assumptions (A1),(A2),(A3),(K),(F1),(F2) hold. Given an initial condition $\mu_0 \in \mathcal{M}^+(\mathbb{R}^+)$*, there exists a unique global solution* $\mu \in C([0,\infty),\mathcal{M}^+(\mathbb{R}^+))$ *of equation* (1)*. Moreover, if* μ_0 *has finite total mass in the sense that* $\int_{\mathbb{R}^+} x\,\mu_0(dx) < \infty$*, then for any* $T \geq 0$ *there exists* $C_T > 0$ *such that*

$$\int_{\mathbb{R}^+} x\,\mu_t(dx) \leq C_T \qquad t \in [0,T].$$

In particular, if $g = d = \beta = 0$ *then mass is conserved in the sense that* $\int_{\mathbb{R}^+} x\,\mu_t(dx) = \int_{\mathbb{R}^+} x\,\mu_0(dx)$ *for any* $t \geq 0$*.*

For the nonlinear problem

$$\partial_t \mu_t + \mathrm{div}(v(t,\mu_t)\mu_t) = N(t,\mu_t)$$

we show for small enough $T > 0$ (depending only on $\|\mu_0\|_{TV}$) the map defined by

$$\Gamma(\mu)_t = T_t^v \sharp \mu_0 + \int_0^t T_{s,t}^v \sharp N(s,\mu_s)\, ds,$$

has a fixed point, which is a solution to the nonlinear problem, in the space

$$X = \{\mu \in C([0,T], \mathcal{M}(\mathbb{R}^d)) : \mu_{|t=0} = \mu_0,\ \|\mu_t\|_{TV} \leq 2\|\mu_0\|_{TV},\ \ t \in [0,T]\}.$$

Here, X is endowed with the sup-norm $\|\mu\|_X = \sup_{t\in[0,T]} \|\mu_t\|_{BL}$.

Idea of Proof: Existence

It then follows as before that this equation has an unique solution defined on a maximal time interval $[0, T*)$. Moreover,

$$T* < \infty \text{ if and only if } \lim_{t \longrightarrow T^*} \|\mu_t\|_{TV} = \infty.$$

Thus to show the solution is global, it is enough to show there is a $C > 0$ such that

$$\|\mu_t\|_{TV} \leq \|\mu_0\|_{TV} \exp(Ct) \qquad \text{for any } t \in [0, T^*).$$

Idea of Proof: Mass Conservation

Let us assume now that $\int_0^\infty x\,\mu_0(dx) < \infty$. After a slight regularization, we can take $\phi_R(x) = \min\{x, R\}$, $R > 0$, in the weak formulation to arrive at

$$\begin{aligned}(\mu_t, \phi_R) \quad &\leq \quad (\mu_0, \phi_R) + \int_0^t \int_{\mathbb{R}^+} g(s, \mu_s)(y)\phi_R'(y)\,\mu_s(dy)ds \\ &\quad + \int_0^t \int_{\mathbb{R}^+} (b(y, \cdot), \phi_R)a(y)\,\mu_s(dy)ds.\end{aligned}$$

Using that $\phi_R(x) \leq x$, $(b(y, dx), x) = y$, and (A2), we have

$$\begin{aligned}(\mu_t, \phi_R) \quad &\leq \quad (\mu_0, x) + C_{T,\zeta} + \int_0^t \int_{\mathbb{R}^+} ya(y)\,\mu_s(dy)ds \\ &\leq \quad (\mu_0, x) + C_{T,\zeta} + \|a\|_\infty \int_0^t (\mu_s, x)\,ds.\end{aligned}$$

Idea of Proof: Mass Conservation

Passing to the limit $R \to \infty$ using the Monotone Convergence Theorem, we deduce

$$(\mu_t, x) \leq (\mu_0, x) + C_{T,\zeta} + \|a\|_\infty \int_0^t (\mu_s, x)\, ds.$$

The Gronwall inequality then gives

$$(\mu_t, x) \leq ((\mu_0, x) + C_{T,\zeta})e^{\|a\|_\infty t}.$$

As a consequence we can use any smooth test-function ϕ with linear growth, i.e. $|\phi(x)| \leq C(1 + |x|)$. In particular, we can take $\phi(x) = x$ to have

$$\begin{aligned}(\mu_t, x) &= (\mu_0, x) + \int_0^t \int_{\mathbb{R}^+} g(s, \mu_s)(y)\, \mu_s(dy) ds \\ &\quad - \int_0^t \int_{\mathbb{R}^+} xd(s, \mu_s)(x)\, \mu_s(dy) ds.\end{aligned}$$

Theorem

Assume additionally for each y, $b(y,\cdot) = b(y,x)dx$, the family $\{b(y,\cdot) : y \geq 0\}$ is uniformly equi-integrable, and , $g(t,\mu_t) \in C^1(\mathbb{R}^+)$ takes strictly positive values, and let μ_t be the solution to (1) for some some initial condition μ_0.
Denote $l_0(t)$ the solution to

$$\begin{cases} \frac{d}{dt} l_0(t) = g(t,\mu(t))(l_0(t)), \\ l_0(0) = 0. \end{cases}$$

Then for any $t > 0$, μ_t is absolutely continuous on $[0, l_0(t))$ with respect to the Lebesgue measure (i.e. $\mu_t \ll dx$).

Unification of Discrete and Continuous Models

It is clear that continuous coagulation-fragmentation models are a special case of our model by undoing the derivations of the model. In order to arrive at the discrete coagulation-fragmentation models, we take for some fixed $h > 0$

(C1) $\mu_0 = \sum_{i \in \mathbb{N}_0} m_i^0 \delta_{ih}$ where for each i, $m_i^0 \in \mathbb{R}^+$,

(C2) $b(y, \cdot) = \sum_{i \in \mathbb{N}} b_i(y) \delta_{ih}$,

and also that

(C3) $g(t, \mu) \equiv 0$.

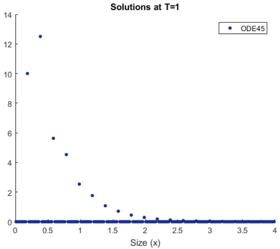
Under all of these assumptions, we have

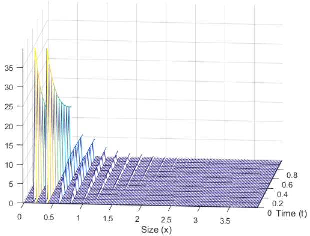
Lemma

For any $t \in [0, \infty)$, the solution μ_t of (1) is supported on $h\mathbb{N}_0$:

$$\mu_t = \sum_{l \in \mathbb{N}_0} m_l(t)\delta_{lh},$$

where the $m_l(t)$, $l \in \mathbb{N}_0$, satisfy the discrete coagulation-fragmentation differential equation system.





Numerical Methods on Measures

The idea behind numerical methods on this space is to approximate the solution by a sum of Dirac measures:

$$\mu^k_{\Delta x} = \sum_{j=1}^{J} m^k_j \delta_{x_j}.$$

The hope is that your numerical method gives a decent approximation of the measure on the interval $(x_{j-1}, x_j]$:

$$\mu_{k\Delta t}((x_{j-1}, x_j]) \approx m^k_j.$$

$$\begin{cases} \dfrac{m_j^{k+1} - m_j^k}{\Delta t} + \dfrac{g_j^k m_j^k - g_{j-1}^k m_{j-1}^k}{\Delta x} + d_j^k m_j^k = \dfrac{1}{2} \displaystyle\sum_{i=1}^{j-1} \kappa_{i,j-i} m_i^k m_{j-i}^k - \sum_{i=1}^{J} \kappa_{i,j} m_i^k m_j^k \\ \qquad + \displaystyle\sum_{i=j}^{J} b_{i,j} a_i m_i^k - a_j m_j^k \qquad j = 1, .., J, \\ g_0^k m_0^k = \Delta x \displaystyle\sum_{j=1}^{J} \beta_j^k m_j^k \end{cases} \tag{3}$$

With CFL condition

$$\Delta t \Big(C_\kappa \|\mu_0\|_{TV} \exp((\zeta + C_b C_a) T) + C_a \max\{1, C_b\} + (1 + \frac{1}{\Delta x})\zeta \Big) \leq 1.$$

Finite Difference Schemes: Semi-implicit

$$
\begin{cases}
\dfrac{m_j^{k+1} - m_j^k}{\Delta t} + \dfrac{g_j^k m_j^k - g_{j-1}^k m_{j-1}^k}{\Delta x} + d_j^k m_j^k = \dfrac{1}{2} \displaystyle\sum_{i=1}^{j-1} \kappa_{i,j-i} m_i^{k+1} m_{j-i}^k - \sum_{i=1}^{J} \kappa_{i,j} m_i^k m_j^{k+1} \\
\qquad\qquad\qquad\qquad + \displaystyle\sum_{i=j}^{J} b_{i,j} a_i m_i^k - a_j m_j^k, \\
g_0^k m_0^k = \Delta x \displaystyle\sum_{j=1}^{J} \beta_j^k m_j^k
\end{cases}
\tag{4}
$$

With CFL Condition:

$$
\bar{\zeta}(2\Delta t + \frac{\Delta t}{\Delta x}) \leq 1 \quad \text{where} \quad \bar{\zeta} = \max\{\zeta, \|a\|_{W^{1,\infty}}\}.
$$

Rewriting the Equation as a Conservation Law

We rewrite the scheme in the following form:

$$\begin{cases} \partial_t(x\mu) + x\partial_x(g(t,\mu)\mu) + xd(t,\mu)\mu = \partial_x \mathcal{Q}_F[\mu] - \partial_x \mathcal{Q}_K[\mu] \\ g(t,\mu)(0)D_{dx}\mu(0) = \int_0^\infty \beta(t,\mu)(x)\mu(dx) \\ \mu_0 \in \mathcal{M}^+(\mathbb{R}^+) \end{cases},$$

where

$$(\mathcal{Q}_K[\mu],\phi) = \int_0^\infty \int_0^\infty \left[\int_z^{z+y} \phi(x)dx\right] z\,\kappa(z,y)\,\mu(dz)\,\mu(dy)$$

and

$$(\mathcal{Q}_F[\mu],\phi) = \int_0^\infty \left(b(y,dx), x\int_x^y \phi(z)dz\right) a(y)\mu(dy).$$

Notice $\partial_x \mathcal{Q}_K[\mu] = -xK[\mu]$ and $\partial_x \mathcal{Q}_F[\mu] = xF[\mu]$ in the sense of distributions.

Explicit Scheme on CL

$$\begin{cases} x_j \dfrac{m_j^{k+1} - m_j^k}{\Delta t} + x_j \dfrac{g_j^k m_j^k - g_{j-1}^k m_{j-1}^k}{\Delta x} + x_j d_j^k m_j^k = \dfrac{\mathcal{Q}_{F,j}^k - \mathcal{Q}_{F,j-1}^k - \mathcal{Q}_{K,j}^k + \mathcal{Q}_{K,j-1}^k}{\Delta x} \\ g_0^k \dfrac{m_0^k}{\Delta x} = \sum_{j=1}^{J} \beta_j^k m_j^k \end{cases}, \tag{5}$$

where

$$\mathcal{Q}_{K,j}^k := \sum_{i=1}^{j} \sum_{l=j-i}^{J} \Delta x \, x_i \kappa_{i,l} m_l^k m_i^k$$

and

$$\mathcal{Q}_{F,j}^k := \sum_{i=j+1}^{J} \sum_{l=1}^{j} x_l \Delta x \, b_{i,l} a_i m_i^k.$$

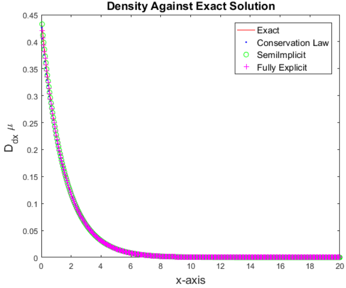
CFL condition:

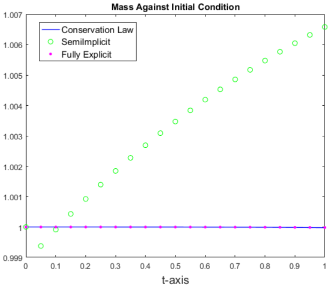
$$\Delta t (C_\kappa \|\mu_0\|_{TV} \exp(\zeta + C_b C_a) + C_b C_a + (1 + \frac{1}{\Delta x})\zeta) \leq 1.$$

Comparison: Coagulation Only

Nx	Nt	Explicit			Semi-Implicit		
		BL Error	Order	Time (secs)	BL Error	Order	Time (secs)
50	100	0.046406			0.059118		
100	200	0.024121	0.94401	1.2972	0.029972	0.97997	1.9879
200	400	0.012296	0.97209	27.511	0.015119	0.98727	41.505
400	800	0.0062079	0.98605	455.73	0.0075973	0.99281	645.54
800	1600	0.0031190	0.99301	5942.6	0.0038088	0.99616	10370

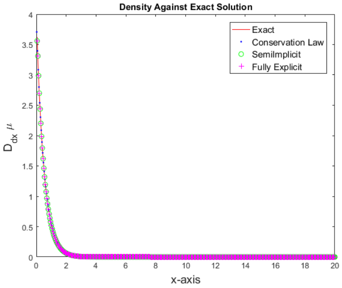
Nx	Nt	Conservation Law		
		BL Error	Order	Time (secs)
50	100	0.076986		
100	200	0.040102	0.94091	19.83
200	400	0.020535	0.96561	338.35
400	800	0.010408	0.98042	6223.8
800	1600	0.0052438	0.98897	88950

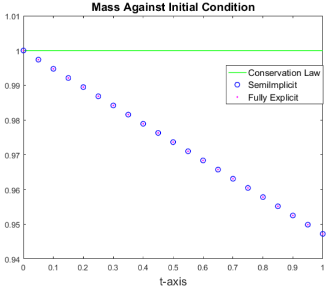




Comparison: Fragmentation Only

Nx	Nt	Explicit/SemiImplicit			Conservation Law		
		BLError	Order	Time (secs)	BLError	Order	Time (secs)
200	10	0.27759			0.51684		
400	20	0.15055	0.88275	2.4223	0.28095	0.87941	23.5
800	40	0.078274	0.94362	49.012	0.14664	0.93804	376.07
1600	80	0.03989	0.97251	765.21	0.074949	0.96829	6957.5
3200	160	0.020133	0.98644	11721	0.037898	0.98379	107980





On Going/Future Work

- Upgrade the finite difference schemes to higher order.
- Asymptotic behavior.
- Stability of these equations.

Our Papers

1. A. S. Ackleh, R. Lyons, and N. Saintier, Structured Coagulation-Fragmentation Equation in the Space of Radon Measures: Unifying Discrete and Continuous Models, *ESAIM: Mathematical Modelling and Numerical Analysis*, (2021).
2. A. S. Ackleh, R. Lyons, and N. Saintier, Finite Difference Schemes for Structured Coagulation-Fragmentation Equation in the Space of Radon Measures, *submitted*.

Thank you for your attention!