# Processes of fragmentation and coagulation – Smoluchowski's equations and beyond

Jacek Banasiak

University Pretoria & Technical University of Łódź

Joint work with W. Lamb (Strathclyde), S. Shindin (UKZN)

and M. Mokhtar-Kharroubi (Franche-Comté)

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Marian Smoluchowski, 28 May 1872 – 5 September 1917

XXXVI. DREI VORTRÄGE ÜBER DIFFUSION, BROWN-SCHE MOLEKULARBEWEGUNG UND KOAGULATION VON KOLLOIDTEILCHEN.

Physikalische Zeitschrift, XVII. Jahrgang, pp. 557—571 und 587—599. 1916.

**I. Diffusion im unbegrenzten Raum.**

1. Einleitung.

In den nachstehenden drei Vorträgen [1]) soll eine Übersicht über einige neuere theoretische Untersuchungen gegeben werden, in welchen ich versucht habe, den inneren Mechanismus der Diffusion und einiger damit zusammenhängender Molekularphänomene klarzustellen, indem ich einige Gedanken näher ausgeführt habe, welche in einem vor drei Jahren hier in Göttingen gehaltenen Vortrag [2]) kurz angedeutet waren. Einerseits besitzt dieses Thema eine besondere Bedeutung infolge seiner Anwendung auf die Physik der Kolloide, in welcher diese Erscheinungen eine grundlegende Rolle spielen – einen charakteristischen, hierher gehörigen Fall, den Koagulationsprozeß, werden wir später noch eingehender zu betrachten haben — andererseits sollte es meiner Ansicht nach in der theoretischen Physik die Stellung eines Schulbeispiels einnehmen, an welchem man die relative Berechtigung und Tragweite der thermodynamisch-makroskopischen Betrachtungsweise und der mikroskopisch-molekularen Analyse in allen Einzelheiten und in relativ einfacher Weise vergleichen kann, wobei sich überdies fast jeder Schritt durch direkte experimentelle Erfahrung illustrieren und kontrollieren läßt. Es liegt das daran, daß uns ein und dieselbe

[1]) Veranstaltet durch die Wolfskehlstiftung zu Göttingen, 20 - 22. Juni 1916.

[2]) Vgl. Vorträge üb. kinetische Theorie d. Materie u. Elektrizität, Leipzig 1914, p. 89 [p. 361 du présent Volume. *Ed.*].



Erscheinung, je nach dem von uns eingenommenen Standpunkt, in dreifach verschiedener Weise entgegentritt: makroskopisch betrachtet heißt sie „Diffusion", mikroskopisch entweder „Brown'sche Molekularbewegung", falls man nämlich die Lebensgeschichte eines individuellen materiellen Teilchens verfolgt, oder aber „Konzentrationsschwankung", falls man ein bestimmtes Volumelement im Auge behält und die zeitliche Änderung der Anzahl der jeweilig darinnen befindlichen Teilchen notiert. Natürlich muß zwischen diesen verschiedenen Erscheinungsformen ein innerer Zusammenhang bestehen, und die theoretische Untersuchung dieses Zusammenhangs, sowie die nähere Bestimmung der Gültigkeitsgrenzen der üblichen Diffusionstheorie soll unsere erste Aufgabe bilden, während wir später zu einigen darauf beruhenden Anwendungen übergehen wollen, welche einen mehr konkreten, dem experimentellen Gebiet näherstehenden Charakter besitzen.

2. Brown'sche Molekularbewegung.

Auf die Gefahr hin, genügend Bekanntes zu wiederholen, muß ich vorerst einige Worte über Brown'sche Molekularbewegung [1]) vorausschicken. Der eigentliche innere Mechanismus derselben ist zweifellos äußerst kompliziert, viel komplizierter als unsere mathematische Formelsprache es ausdrücken kann, aber einem eigentümlichen und für diese Untersuchungen sehr vorteilhaften Umstand haben wir es zu verdanken, daß diese Komplikationen und überhaupt die Einzelheiten der Teilchenbewegung auf die Gestalt der praktisch wichtigen Endformel ohne irgendwelchen Einfluß sind. Diese Formel, welche die Wahrscheinlichkeit angibt, daß ein von der Abszisse $x_0$ anfänglich ausgehendes Teilchen zur Zeit $t$ in den Abszissenbereich $x \dots x + dx$ gelangt sei:

$$(1) \qquad W(x)\,dx = \frac{1}{2\sqrt{\pi D t}}\, e^{\frac{-(x-x_0)^2}{4Dt}}\, dx$$

[1]) Zusammenfassende Bearbeitungen und Literatur betreffs dieser und verwandter Erscheinungen: G. L. de Haas-Lorentz, Die Brownsche Bewegung, Braunschweig 1913; The Svedberg, Die Existenz d. Moleküle, Leipzig 1912; Jahrb. d. Radioakt. u. Elektr. **10**, 467, 1913; J. Perrins Bericht in den Rapports Solvay (La théorie du rayonnement etc., Paris 1912; Die Theorie d. Strahlung u. d. Quanten, herausgeg. v. A. Eucken, Leipzig, 1914); J. Perrin, Die Atome, Leipzig 1914; Smoluchowski, Phys. Zeitschr. **13**, 1069, 1912 [voir ci-dessus, p. 226. *Ed.*].





## Versuch einer mathematischen Theorie der Koagulationskinetik kolloider Lösungen.

Von

**M. v. Smoluchowski.**

(Mit 3 Figuren im Text.)

(Eingegangen am 8. 9. 16.)

**I. Einleitung.**

So sehr auch bis heute die Literatur über Koagulation kolloider Lösungen angewachsen ist, sind doch unsere Kenntnisse betreffs des quantitativen Verlaufs, sowie betreffs des Mechanismus des Koagulationsprozesses äusserst mangelhaft. Die meisten Forscher begnügen sich mit qualitativen Beobachtungen oder stellen ihre Messungsreihen in Tabellen oder Kurvenform [1]) dar, da die mathematische Wiedergabe derselben auf aussergewöhnliche Schwierigkeiten stösst.

In den interessanten Arbeiten [2]) von S. Miyazawa, N. Ishizaka, H. Freundlich, J. A. Gann wird allerdings eine formelmässige Zusammenfassung des empirischen Versuchsmaterials, sowie eine Aufklärung desselben nach Analogie mit den Gesetzen der chemischen Kinetik angestrebt. Aber klare Gesetzmässigkeiten haben sich bisher auf diese Weise nicht ergeben, und wurden sogar gewisse, anfangs aufgestellte Gesetzformeln (Paine, Freundlich und Ishizaka) bei exakterer Prüfung (Freundlich und Gann) als unhaltbar zurückgenommen [3]).

Die Erfolglosigkeit der bisherigen Versuche, auf dem empirisch-induktiven Wege zu einem Verständnis der hier geltenden Gesetze zu gelangen, kann man nun als einen Grund auffassen, einmal den um-

[1]) Vgl. z. B.: A. Galecki, Zeitschr. f. anorg. Chemie **74**, 174 (1912); Kolloid-Zeitschr. **10**, 169 (1912); A. Lottermoser, Kolloid-Zeitschr. **15**, 145 (1914); H. H Paine, Kolloidchem. Beihefte **4**, 24 (1912); Kolloid-Zeitschr. **11**, 115 (1912).

[2]) S. Miyazawa, Journ. Chem. Soc. Tokio **33**, 1179, 1210 (1912); N. Ishizaka, Zeitschr. f. physik. Chemie **83**, 97 (1913); H. Freundlich u. N. Ishizaka, ebendort **85**, 398 (1913); Kolloid-Zeitschr. **12**, 230 (1913); J. Gann, Kolloidchem. Beihefte **8**, 64 (1916).

[3]) Siehe Abschnitt VI.

## Fragmentation–coagulation processes

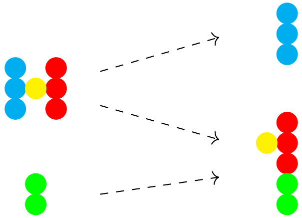


Figure: Pure fragmentation and coagulation

Coagulation and fragmentation belong to the most fundamental processes occurring in animate and inanimate matter. The range of applications includes:

- Chemical engineering: polymerization/depolimerization processes, with possible mass loss through dissolution, chemical reactions, oxidation etc, or mass growth due to the deposition of material on the clusters.
- Biology: Blood cells' coagulation and splitting, animal grouping, phytoplankton at the level of aggregates, flocculation.
- Planetology: merging of planetesimals.
- Aerosol research: coagulation of smoke, smog and dust particles, droplets in clouds.

Thus, together with the Boltzmann equation that describes collision phenomena in rarefied gases, the Navier-Stokes and Euler equations modelling the flow of viscous fuids, the coagulation-fragmentation equation, in its original form going back to Smoluchowski, describing rearrangements of particles, is considered to be one of the most fundamental equations of the classical description of matter.

We shall refer to the fundamental building blocks of the aggregates as monomers and a cluster of $n$ monomers will be called an $n$-mer. The Smoluchowski population balance equations, describing the time-evolution of the number density of $n$-mers of size $n \geq 2$, is given by

$$\begin{aligned} \frac{df_n}{dt}(t) &= -a_n f_n(t) + \sum_{j=n+1}^{\infty} a_j b_{n,j} f_j(t) \\ &+ \frac{1}{2}\sum_{j=1}^{n-1} k_{n-j,j} f_{n-j}(t) f_j(t) - \sum_{j=1}^{\infty} k_{n,j} f_n(t) f_j(t), \qquad (1) \end{aligned}$$

where

- $f_n(t)$ is the *number density* of $n$-mers at time $t \geq 0$;
- $a_n$ is the *net rate of break-up* of an $n$-mer;
- $b_{n,j}$ is the *daughter distribution function* that gives the average number of $n$-mers produced upon the break-up of a $j$-mer;
- $k_{n,j} = k_{j,n}$ represents the *coagulation rate* of an $n$-mer with a $j$-mer.

Since monomers do not fragment and loss of monomers can only arise due to coagulation, for $n = 1$ we have

$$\frac{d}{dt}f_1(t) = \sum_{j=2}^{\infty} a_j b_{1,j} f_j(t) - \sum_{j=1}^{\infty} k_{1,j} f_1(t) f_j(t). \qquad (2)$$

**Continuous fragmentation-coagulation models**

In many applications, such as aerosols or polymers, it makes sense to allow the clusters to be of any size. Then the size of building blocks must be infinitesimal and hence we consider a continuous size variable $x \in \mathbb{R}_+$ as the only variable required to differentiate between the reacting particles.

Then,

$$\begin{aligned} \partial_t f(t,x) &= \mathcal{F}f(t,x) + \mathcal{C}f(t,x)\ , \qquad (t,x) \in (0,\infty)^2\ , & (3)\\ f(0,x) &= \mathring{f}(x)\ , \qquad x \in (0,\infty)\ , & (4) \end{aligned}$$

where

$$\mathcal{F}f(t,x) = -a(x)f(t,x) + \int_x^\infty a(y)b(x,y)f(t,y)\,\mathrm{d}y\,, \qquad (5)$$

and

$$\begin{aligned} \mathcal{C}f(t,x) = \frac{1}{2}\int_0^x k(x-y,y)f(t,x-y)f(t,y)\,\mathrm{d}y \\ - f(t,x)\int_0^\infty k(x,y)f(t,y)\,\mathrm{d}y \qquad (6) \end{aligned}$$

Here $f$ is the density of particles of mass $x$, $a$ is the fragmentation rate and $b$ describes the distribution of particle masses $x$ spawned by the fragmentation of a particle of mass $y$. Further

$$M(t) = \int_0^\infty x f(x,t)dx \tag{7}$$

is the total mass at time $t$. Local conservation principle requires

$$\int_0^y x b(x,y)dx = y, \tag{8}$$

with the expected number of particles produced by a particle of mass $y$ is given by

$$n_0(y) = \int_0^y b(x,y)dx.$$

**Fragmentation–coagulation equation with vital dynamics.**

*Organisms' grouping*

1. active, resulting from conscious actions of individuals (herds, swarms, fish schools),
2. passive, resulting from physical or chemical properties of the organisms and the dynamics of the surrounding medium (bacteria, phytoplankton aggregates).

# Why do animals form groups?

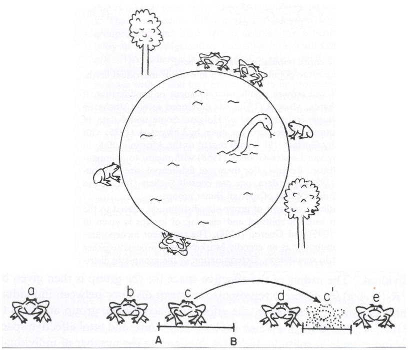



Figure: Frogs' grouping to reduce danger zone, W.D. Hamilton, Geometry of Selfish Herd, JTB, 1971

## Fish schools

Niwa (2003, 2004) observed that fish school-size distribution

$(f_i)_{i\geq 1}$ is well described by

$$f_i \sim \frac{1}{i_{av}}\Phi\left(\frac{i}{i_{av}}\right),$$

where

$$i_{av} = \sum_{i=1}^{\infty} i \frac{if_i}{\sum\limits_{i=1}^{\infty} if_i}$$

is the average size the group an individual belongs to and

$$\Phi(x) = \frac{1}{x}e^{-x+0.5xe^{-x}} \approx \frac{1}{x}e^{-x}.$$

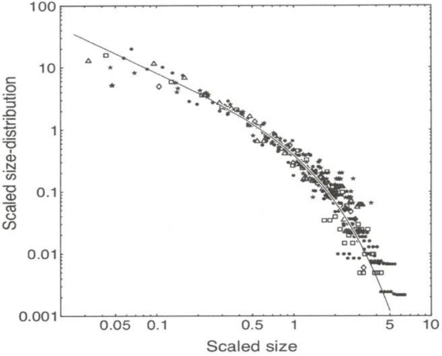



Figure: Empirical school size distribution of six types of pelagic fish (Niwa, 2003)

For a Smoluchowski type model, Degond derives

$$\Phi_\star(x) = 2(6x)^{-2/3} \sum_{n=0}^{\infty} \frac{(-1)^n}{\Gamma\left(\frac{4}{3} - \frac{2}{3}n\right)} (6x)^{n/3}$$

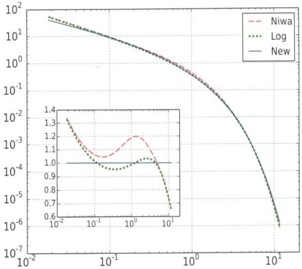
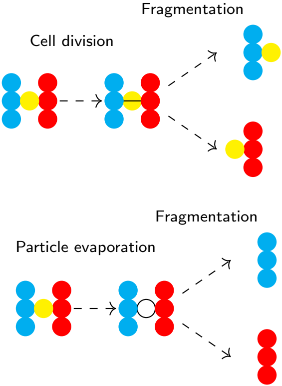



Figure: Plot of $\Phi$ for Niwa's, simplified Niwa's and Degond's distribution profiles. Inset: ratios $\Phi/\Phi_\star$ for all three cases. (Degond et al., 2017)

## Fragmentation-coagulation with growth and decay.

In all discussed models the fragmentation and coagulation processes, which are just rearrangements of monomers, should be accompanied by growth (and death) terms – if a cell divides inside a cluster, it increases in size.



Then, in the continuous case, fragmentation can be supplemented by growth/decay, transport or diffusion processes. For instance,

$$
\begin{aligned}
\partial_t f(x,t) &= \pm\partial_x[r(x)f(x,t)] - a(x)f(x,t) \\
&\quad + \int\limits_x^\infty a(y)b(x,y)f(y,t)dy \\
&\quad + \frac{1}{2}\int_0^x k(x-y,y)f(t,x-y)f(t,y)\,\mathrm{d}y \\
&\quad - f(t,x)\int_0^\infty k(x,y)f(t,y)\,\mathrm{d}y \qquad (9)
\end{aligned}
$$

where $r(x) > 0$ describes either decay of the substance (e.g. by chemical reaction or simply evaporation or dissolving) with "$+$" or growth by birth or multiplication, with "-" (evolution of phytoplankton aggregates.)

**Why do we need functional analysis to deal with such models?**

Fragmentation just rearranges the mass distribution and the total mass should be conserved by (8). However, consider a fragmentation equation describing binary fragmentation: with $b(x,y) = 2/y$ and $a(x) = 1/x$ it takes the form

$$\partial_t f(x,t) = -x^{-1} f(x,t) + 2\int_x^\infty y^{-2} f(y,t)\mathrm{d}y, \qquad (10)$$

For mono-disperse initial condition $f(x,0) = \delta(x-l)$, $l > 0$, it has a solution

$$f_l(x,t) = e^{-t/l}\left(\delta(x-l) + \frac{2t}{l^2} - \frac{t^2}{l^2}\left(\frac{1}{l} - \frac{1}{x}\right)\right), \quad x \le l, \quad (11)$$

and $f_l(x,t) = 0$ for $x > l$. Hence the total mass of the ensemble is given by

$$M(t) = e^{-t/l}\left(l + t + \frac{t^2}{2l}\right), \quad (12)$$

and clearly decreases monotonically in time.

Solutions do not have the properties used for the derivation of the model

**Multiple solutions.**

On the other hand, taking $a(x) = x$, $b(x, y) = 2/y$ yields

$$\partial_t f(x,t) = -xu(x,t) + 2\int\limits_x^\infty f(y,t)dy. \qquad (13)$$

Separating variables we get

$$f_1(x,t) = \frac{e^t}{(1+x)^3}, \qquad (14)$$

with initial condition $f_1(x, 0) = (1 + x)^{-3}$ (of finite mass).

However,

$$f_2(x,t) = e^{-xt}\left(\frac{1}{(1+x)^3} + \int\limits_x^\infty \frac{1}{(1+x)^3}[2t + t^2(y-x)]dy\right),$$

is also a solution to (13) satisfying the same initial condition.

Another example of nonuniqueness for this equation is offered by

$$f(t,x) = t^2 e^{-xt}. \qquad (15)$$

Routine calculations show that this function is a nontrivial solution to (13) emanating from zero so that (13) is not well-posed in the pointwise sense.

This shows that to ensure well-posedness of the problem we must carefully define what we mean by the solution.

## Mathematical setting – state spaces.

**Example 1**

The natural space to analyse the continuous fragmentation - coagulation processes is

$$X_1 = L_1(\mathbb{R}_+, xdx) = \left\{ u;\ \|u\|_1 = \int\limits_0^\infty |u(x)|x\mathrm{d}x < +\infty \right\}$$

as for nonnegative $u$ we have $\|u\|_1 = M(u)$, the mass of the ensemble with density $u$. Best results are obtained in spaces

$$X_{1,\alpha} = L_1(\mathbb{R}_+, (1+x^\alpha)dx) = \left\{ u;\ \|u\|_{0,\alpha} = \int\limits_0^\infty |u|(1+x^\alpha)dx < +\infty \right\},$$

$\alpha > 1$.

## Ways of approaching the fragmentation-coagulation equations.

Difficulties in solving

$$\begin{aligned}
\partial_t f(t,x) &= \mathcal{F}f(t,x) + \mathcal{C}f(t,x)\,, \qquad (t,x) \in (0,\infty)^2\,, \\
f(0,x) &= \mathring{f}(x)\,, \qquad x \in (0,\infty)\,,
\end{aligned} \tag{16}$$

come from the fact that both the fragmentation rate $a$ and the coagulation rate can be unbounded, for instance at $x = \infty$.

1. *Truncation method.* We construct solutions $f_r$ to the problem with the coefficients $a$ and $k$ modified as follows

$$a_r(x) = \begin{cases} a(x) & \text{for} \quad x \leq r \\ 0 & \text{for} \quad x > r, \end{cases} \qquad k_r(x,y) = \begin{cases} k(x,y) & \text{for} \quad x+y \leq r \\ 0 & \text{for} \quad x+y > r. \end{cases}$$

$(f_r)_{r>0}$ is a weakly compact net whose accumulation point is a solution to a suitable weak formulation of (16).

Advantages: possibility to handle very general coagulation coefficients.

Disadvantages: weak solutions, additional work required to prove mass conservation, uniqueness, etc; fragmentation subordinated to coagulation.

2.*Semigroup method.* Considering (16) as a nonlinear perturbation of the linear dynamics generated by

$$\mathcal{F} = \mathcal{A} + \mathcal{B}.$$

Advantages: classical unique mass-conserving solutions.

Disadvantages: The coagulation part subordinated to the fragmentation, typically bounded.

So, first, how to solve

$$\partial_t f = \mathcal{F} f = \mathcal{A} f + \mathcal{B} f \text{ ?}$$

## Between model and its analysis

Equations derived through a modelling process are formulated pointwise: all operations, such as differentiation and integration, are understood in the classical 'calculus' sense and the equation shoud be satisfied for all values of the independent variables:

$$
\begin{aligned}
\frac{\partial}{\partial t} f(t,x) &= [\mathcal{K} f(t,\cdot)](x), \quad x \in \Omega \\
f(t,0) &= \mathring{f},
\end{aligned}
\tag{17}
$$

where $\mathcal{K}$ is a differential, integral, or functional expression. We aim to describe the evolution by a family of operators $(G(t))_{t\geq 0}$ in a state space $X$, parameterised by time, that map an initial state $\mathring{f}$ of the system to all subsequent states in the evolution.

That is, solutions are represented as

$$f(t) = G(t)\mathring{f}. \tag{18}$$

From $G$ we expect some form of continuity in $t$, the semigroup property $G(t+s) = G(t)G(s), t, s \geq 0$, and $G(0) = Id$.

Then we try to write (17) as the Cauchy problem for an ordinary differential equation in $X$: for $t > 0$

$$\partial_t f = Kf, \qquad f(0) = \mathring{f} \in X, \tag{19}$$

where $K$ is certain realization of $\mathcal{K}$ in $X$. Problem (19) is well-posed if $K$ is the generator of $(G(t))_{t\geq 0}$.

## Semigroups – crash course

Let $X$ be a Banach space, $K$ be a linear operator in $X$ with domain $D(K)$.

**Definition 2**

A family $(G(t))_{t\geq 0}$ of bounded linear operators on $X$ with $G(0) = I$, is called a $C_0$-semigroup if

(i) $G(t+s) = G(t)G(s)$ for all $t, s \geq 0$;

(ii) $\lim_{t\to 0^+} G(t)f = f$ for any $f \in X$.

An operator $K$ is called the generator of $(G(t))_{t\geq 0}$ if

$$Kf = \lim_{h\to 0^+} \frac{G(h)f - f}{h}, \tag{20}$$

and $D(K)$ is the set of all $f \in X$ for which this limit exists.

From (20) and (ii), for $\mathring{f} \in D(K)$ we have

$$\partial_t G(t)\mathring{f} = KG(t)\mathring{f}, \quad t > 0,$$
$$G(0)\mathring{f} = \mathring{f}, \tag{21}$$

so the function $f(t, \mathring{f}) = G(t)\mathring{f}$ is a classical solution to the Cauchy problem (19). If $\mathring{f} \in X \setminus D(K)$, the function $f(t, \mathring{f}) = G(t)\mathring{f}$ is continuous but, in general, not differentiable. Thus, if we have a semigroup, we can identify the Cauchy problem of which it is a solution. We are, however, interested in finding the semigroup for a given equation.

Let $\sigma(K)$ denote the spectrum of $K$ and $\rho(K) = \mathbb{C} \setminus \sigma(K)$ be the resolvent set of $K$.

**Theorem 3 (Hille-Yosida)**

*$K \in \mathcal{G}(M, \omega)$ if and only if $K$ is closed and densely defined and there exist $M > 0, \omega \in \mathbb{R}$ such that $(\omega, \infty) \subset \rho(K)$ and for all $n \geq 1, \lambda > \omega$,*

$$\|(R(\lambda, K))^n\| = \|((\lambda I - K)^{-1})^n\| \leq \frac{M}{(\lambda - \omega)^n}. \tag{22}$$

## Analytic semigroups

If a densely defined $K$ is sectorial, that is, if the estimate

$$\|R(\lambda, K)\| \leq \frac{C}{|\lambda|}. \tag{23}$$

holds in some sector

$$S_{\frac{\pi}{2}+\delta} := \{\lambda \in \mathbb{C};\ |\arg \lambda| < \frac{\pi}{2} + \delta\} \cup \{0\}, \quad \delta > 0, \tag{24}$$

then $K$ is the generator of an *analytic* semigroup given by

$$G_K(t) = \frac{1}{2\pi i} \int\limits_{\Gamma} e^{\lambda t} R(\lambda, K) \mathrm{d}\lambda, \tag{25}$$

where $\Gamma$ is an unbounded smooth curve in $S_{\frac{\pi}{2}+\delta}$.

*Benefits of analyticity*

If $K$ is sectorial, then

- $t \to G_K(t)\mathring{f}$ solves the Cauchy problem (21) for arbitrary $\mathring{f} \in X$;
- it is possible to define fractional powers $(-K)^\alpha, 0 < \alpha < 1$, with domains satisfying

$$D(K) \subset D((-K)^\alpha) \subset X;$$

- for every $t > 0$ and $0 \leq \alpha \leq 1$, we have

$$\|t^{-\alpha}(-K)^{-\alpha}G_K(t)\| \leq M_\alpha \tag{26}$$

for some constant $M_\alpha$.

For example, if $K = \Delta$ on the maximal domain in $L_2(\mathbb{R}^n)$, then $D(K) = W_2^2(\mathbb{R}^n)$ and $D((-K)^\alpha) = W_2^{2\alpha}(\mathbb{R}^n)$ and the heat semigroup regularizes initial conditions.

**Perturbation techniques**

Verifying conditions of the Hille–Yosida theorem for a concrete problem is usually an impossible task. Then we consider

> **Problem P.** Let $(A, D(A))$ be a generator of a $C_0$-semigroup on a Banach space $X$ and $(B, D(B))$ be another operator in $X$. Under what conditions does $A + B$, or an extension $K$ of $A + B$, generate a $C_0$-semigroup on $X$?

## Power of positivity and $L_1$ spaces

Recall that natural state spaces for fragmentation and coagulation problems are $X_1 = L_1(\mathbb{R}_+, xdx)$ and $X_{0,\alpha} = L_1(\mathbb{R}_+, (1+x^\alpha)dx)$. They are Banach lattices. In a Banach lattice $X$ we can identify the cone of positive elements $X_+$ and define $Z_+ := Z \cap X_+$ for $Z \subset X$.

**Definition 4**

We say that the semigroup $(G(t))_{t\geq 0}$ on $X$ is positive if for any $f \in X_+$ and $t \geq 0$,

$$G(t)f \geq 0.$$

From now on, $X$ is an $L_1$-space. We say that $(G(t))_{t\geq 0}$ is a *substochastic semigroup* if for any $t \geq 0$ and $f \geq 0$, $G(t)f \geq 0$ and $\|G(t)f\| \leq \|f\|$, and a *stochastic semigroup* if additionally $\|G(t)f\| = \|f\|$ for $f \in X_+$.

With regards to Problem P., the existence of a semigroup $(G_K(t))_{t\geq 0}$ associated with

$$f_t = Af + Bf$$

depends to large extent on whether we can prove

a) $\|BR(\lambda, A)\| < 1$, or only

b) $\|BR(\lambda, A)\| \leq 1$.

In case b), we have Kato type theorem:

**Theorem 5**

*Let $X = L_1(\Omega, \mu)$ and suppose that the operators $A$ and $B$ satisfy*

1. *$(A, D(A))$ generates a substochastic semigroup $(G_A(t))_{t\geq 0}$;*
2. *$D(B) \supset D(A)$ and $Bf \geq 0$ for $f \in D(A)_+$;*
3. *for all $f \in D(A)_+$*

$$\int_{\Omega} (Af + Bf) d\mu \leq 0. \tag{27}$$

*Then there is an extension $(K, D(K))$ of $(A + B, D(A))$ generating a positive $C_0$-semigroup of contractions, say, $(G_K(t))_{t\geq 0}$.*

In case a), we have the Desch–Miyadera type theorem,

**Theorem 6 (W. Desch)**

*Let $(G_A(t))_{t\geq 0}$ be a positive $C_0$-semigroup on some $L^1$ space $X$ with generator $A$ and let $B$ be positive on $D(A)_+$. If $\|BR(\lambda, A)\| < 1$ for large $\lambda > 0$, then*

$$K = A + B : D(A) \to X$$

*is the generator of a positive $C_0$-semigroup on $X$.*

*Moreover, if $(G_A(t))_{t\geq 0}$ is analytic, $(G_K(t))_{t\geq 0}$ is also analytic.*

## Back to the pathologies of the fragmentation problem

Recall

$$
\begin{aligned}
f_t(x,t) &= \mathcal{A}f(x,t) + \mathcal{B}f(x,t) \\
&= -a(x)f(x,t) + \int\limits_x^\infty a(y)b(x,y)f(y,t)\mathrm{d}y. \qquad (28)
\end{aligned}
$$

We denote

$$F_{\min} = A + B, \quad \text{on} \quad D(F_{\min}) = D(A) = \{f, af \in L_1(\mathbb{R}_+, x\mathrm{d}x)\}$$

and

$$F_{\max} = \mathcal{A} + \mathcal{B} \quad \text{on} \quad D(F_{\max}) = \{f, \mathcal{A}f + \mathcal{B}f \in L_1(\mathbb{R}_+, x\mathrm{d}x)\}.$$

Since, using (8), we get

$$\int_0^\infty \left( -a(x)u(x) + \int_0^\infty a(y)b(x,y)u(y)\mathrm{d}y \right) x\mathrm{d}x = 0$$

for $0 \leq f \in D(F_{\min}) = D(A)$, there is a generator, say $F$, of a substochastic fragmentation semigroup associated to (28).

Hence, if the solutions are in $D(F_{min}) = D(A) = D(B)$, then

$$\begin{aligned} \partial_t \|u(t)\|_{X_1} &= \int_0^\infty (Au(t) + Bu(t))x\mathrm{d}x \\ &= \int_0^\infty Au(t)\, x\mathrm{d}x + \int_0^\infty Bu(t)\, x\mathrm{d}x = 0 \end{aligned} \qquad (29)$$

so that $(G_K(t))_{t\geq 0}$ is mass-conserving.

The conservativeness may be extended to the case, when the solutions stay in $D(\overline{F_{\min}})$, where $\overline{F_{\min}}$ is explicitly defined as

$$\overline{F_{\min}}f = \lim_{n\to\infty}(Af_n + Bf_n)$$

where $D(F_{\min}) \ni f_n \to f \in D(\overline{F_{\min}})$, whenever the limits exist. Then it is easy to see that (29) holds for $f(t) \in D(\overline{F_{\min}})$

$$\int\limits_0^\infty \overline{A+B}f(t)x\mathrm{d}x = 0. \qquad (30)$$

But does $f(t) \in D(\overline{F_{\min}})$?

## $F, F_{min}, \overline{F_{min}}, F_{max}$ and pathologies of the model.

The generator $F$ always satisfies $F_{\min} \subset F \subset F_{\max}$. The place of $F$ on this scale determines the well-posedness of the problem (28).

All following situations are possible

1. $F_{\text{min}} = F = F_{\text{max}}$,
2. $F_{\text{min}} \subsetneq F = \overline{F_{\text{min}}} = F_{\text{max}}$,
3. $F_{\text{min}} = F \subsetneq F_{\text{max}}$,
4. $F_{\text{min}} \subsetneq F = \overline{F_{\text{min}}} \subsetneq F_{\text{max}}$,
5. $\overline{F_{\text{min}}} \subsetneq F \subsetneq F_{\text{max}}$.

Each of these cases has its own specific interpretation in the model.

If $F \subsetneqq F_{\max}$, we don't have uniqueness: there are differentiable $X_1$-valued solutions to emanating from zero and therefore they are not described by the semigroup:

*'there is more to life, than meets the semigroup'.*

If $\overline{F_{\min}} \subsetneqq F$, then despite the fact that the equation is formally conservative, the solutions are not: the modelled quantity leaks out from the system and the mechanism of this leakage is not present in the model.

**Typical dynamics in $L_1(\mathbb{R}_+, x\mathrm{d}x)$**

Let $a(x)$ be such that both limits $\lim_{x\to\infty,0} a(x)$ (possibly infinite) exist and let $b(x,y) = (\nu+2)x^\nu/y^{\nu+1}$. Then,

$$F = F_{max} \quad \text{iff} \quad \frac{1}{xa(x)} \notin L_1([N,\infty)), \tag{31}$$

$$F = \overline{F_{min}} \quad \text{iff} \quad \frac{1}{xa(x)} \notin L_1([0,\delta]), \tag{32}$$

for some $N, \delta \in (0,\infty)$.

**Fragmentation in higher moment spaces.**

Assume that

$$a \text{ is bounded at } 0 \ \ \& \ \ \int\limits_0^y b(x,y)\mathrm{d}y = n_0(y) \leq b_0(1+y^l), \quad (33)$$

where $l \in [0,\infty[$ and $b_0 \geq 1$. Recall the notation

$$X_{0,m} = L_1(\mathbb{R}_+, (1+x^m)dx). \quad (34)$$

We note that, due to the continuous injection $X_{0,m} \hookrightarrow X_1,\ m \geq 1$, any solution in $X_{0,m}$ is also a solution in the basic space $X_1$.

Further, define

$$n_m(y) := \int_0^y b(x,y)x^m \mathrm{d}x$$

for any $m \geq 0$ and $y \in \mathbb{R}_+$, and

$$N_0(y) := n_0(y) - 1 \geq 0,$$
$$N_m(y) := y^m - n_m(y) \geq 0, \quad m \geq 1,$$

with $N_1 = 0$.

## Theorem 7

*Let $a, b$ satisfy (33) and for some $m_0 > 1$*

$$\liminf_{y\to\infty} \frac{N_{m_0}(y)}{y^{m_0}} > 0. \tag{35}$$

*Then*

1. *(35) holds for all $m > 1$;*
2. *$F := A + B$ is the generator of a positive analytic semigroup $(G_F(t))_{t\geq 0}$, on $X_{0,m}$ for any $m > \max\{1, l\}$.*

## Example 8

One of the forms of $b(x, y)$ most often used in applications is

$$b(x, y) = \frac{1}{y} h\left(\frac{x}{y}\right) \tag{36}$$

which is referred to as the homogeneous fragmentation kernel. In this case the distribution of the daughter particles does not depend directly on their relative sizes but on their ratio. In this case

$$n_m(y) = \frac{1}{y}\int\limits_0^y h\left(\frac{x}{y}\right) x^m dx = y^m \int\limits_0^1 h(z) z^m dz =: h_m y^m.$$

## Example 9

Since

$$y = n_1(y) = \frac{1}{y}\int_0^y h\left(\frac{x}{y}\right) x dx = y\int_0^1 h(z) z dz = h_1 y$$

we have $h_1 = 1$ so that $h_m < 1$ for any $m > 1$ and

$N_m(y) = y^m(1 - h_m)$. Hence, (35) holds.

On the other hand, fragmentation processes in which daughter particles tend to accumulate close both to 0 and to the parent's size may not satisfy (35).

## Full fragmentation-coagulation problems

Recall that we deal with the equation

$$\partial_t f(x,t) = -a(x)f(x,t) + \int_x^{\infty} a(y)b(x,y)f(y,t)\mathrm{d}y$$

$$- u(x,t)\int_0^{\infty} k(x,y)f(y,t)\mathrm{d}y$$

$$+ \frac{1}{2}\int_0^{x} k(x-y,y)f(x-y,t)u(y,t)dy. \qquad (37)$$

Next, we denote by $C$ the nonlinear part of (37) so that the initial value problem for (37) can be written as

$$\partial_t f = Ff + Cf, \qquad u(0) = \mathring{f}. \qquad (38)$$

## A brief on semilinear problems

Next we consider the semilinear abstract Cauchy problem

$$f_t = Kf + g(f), \tag{39a}$$

$$f(0) = \mathring{f}, \tag{39b}$$

where $K$ is the generator of $(G_K(t))_{t\geq 0}$ and $g$ is a known function in $X$. We approach the problem using the integral formulation

$$f(t) = G_K(t)\mathring{f} + \int\limits_0^t G_K(t-s)g(f(s))ds. \tag{40}$$

For this to work, $g$ must be a Lipschitz function on $X$ - no unbounded $g$ is allowed.

It is possible to relax the restrictions on $g$, when $(G_K(t))_{t\geq 0}$ is an analytic semigroup. If we take $0 \leq \alpha < 1$ and $t \mapsto f(t)$ is $D((-K)^\alpha)$-valued, then for $\mathring{f} \in D((-K)^\alpha)$ we can write

$$(-K)^\alpha f(t) = G_K(t)(-K)^\alpha \mathring{f} + \int_0^t (-K)^\alpha G_K(t-s) g((-K)^{-\alpha}(-K)^\alpha f(s))\mathrm{d}s,$$

where the integral is defined if $h(\cdot) = g((-K)^{-\alpha}\cdot)$ is bounded as a function from $D((-K)^\alpha)$ to $X$. In other words, we repeat the Picard iteration process in $X$ for $v(t) = (-K)^\alpha f(t)$; that is,

$$v(t) = G_K(t)\mathring{v} + \int_0^t (-K)^\alpha G_K(t-s) h(v(s))\mathrm{d}s,$$

where $\mathring{v} = (-K)^{\alpha}\mathring{u}$. For this $h$ should be Lipschitz continuous in $X$; that is, it suffices that $g$ be only Lipschitz continuous from $D((-K)^{\alpha})$ to $X$. Due to the integrable singularity that appears under the sign of the integral due to (26),

$$\|t^{-\alpha}(-K)^{-\alpha}G_K(t)\| \leq M_{\alpha},$$

we obtain a Volterra equation with a weakly singular kernel.

## Back to the fragmentation–coagulation equation

We assume that $b$ satisfies (33), $F = A + B$ generates an analytic semigroup, and the coagulation kernel $k(x, y)$ satisfies

$$0 \leq k(x, y) \leq L((1 + a(x))^{\alpha}(1 + a(y))^{\alpha}, \qquad (41)$$

for some $L > 0$ and $0 \leq \alpha < 1$. This will suffice to show local in time solvability of (37), whereas to show that the solutions are global in time we need to strengthen (57) to

$$0 \leq k(x, y) \leq L((1 + a(x))^{\alpha} + (1 + a(y))^{\alpha}). \qquad (42)$$

To formulate the main theorem we have to introduce a new class of spaces which, as we shall see later, is related to intermediate spaces which play the role of the domains of fractional powers of $-F$,

$$X_m^{(\alpha)} := \left\{ f \in X_{0,m};\ \ \int_0^\infty |f(x)|(\omega + a(x))^\alpha (1 + x^m)\, dx < \infty \right\},$$

where $\omega$ is a sufficiently large constant. We assume that all assumptions that ensure analyticity of $(G_F(t))_{t\geq 0}$ are satisfied. Then

### Theorem 10

*1. If k satisfies (57), then, for each* $\mathring{f} \in X_{m,+}^{(\alpha)}$*, there is* $t_{max}(\mathring{f}) > 0$ *such that the initial-value problem (38) has a unique nonnegative classical solution f in* $X_m^{(\alpha)}$*, that is,*

$$f \in C\left([0, t_{max}(\mathring{f})), X_m^{(\alpha)}\right) \cap C^1\left((0, t_{max}(\mathring{f})), X_m^{(\alpha)}\right).$$

*2. If k satisfies (42), then, for each* $\mathring{f} \in X_{m,+}^{(\alpha)}$*, the corresponding local nonnegative classical solution is global in time.*

## Example 11

Suppose we have $a(x) = x^j, j > 0$, and $k(x,y) = x^\beta + y^\beta$. Then we can write

$$k(x,y) = a(x)^{\beta/j} + a(y)^{\beta/j}$$

so that $\alpha = \beta/j$. The assumption for local solvability require $\alpha < 1$; that is, $\beta < j$. The same condition is required for global solvability. On the other hand, if $k(x,y) = x^\beta y^\beta$, then the conditions of the local solvability remain the same, while from

$$2x^\beta y^\beta \leq x^{2\beta} + y^{2\beta},$$

it follows that we require $\beta < j/2$.

## Relation to weak solutions

Weak solutions to (37) are constructed as weak limits of solutions $u_r$ to the problem with the coefficients $a$ and $k$ modified as follows

$$a_r(x) = \begin{cases} a(x) & \text{for} \quad x \le r \\ 0 & \text{for} \quad x > r, \end{cases} \qquad k_r(x,y) = \begin{cases} k(x,y) & \text{for} \quad x+y \le r \\ 0 & \text{for} \quad x+y > r. \end{cases}$$

**Theorem 12**

*Assume that the assumptions of Theorem 10 are satisfied and $u$ is the solution to (38). If $(u_r)_{r>0}$ are approximate solutions defined above, then*

$$\lim_{r\to\infty} u_r = u \tag{43}$$

*in $C([0,T], X_m^{(\alpha)})$ for any $T < t_{max}(\mathring{f})$.*

## Back to the fragmentation–coagulation equation with growth

Let us recall that we are dealing with the problem

$$\partial_t f(x,t) = -\partial_x[r(x)f(x,t)] + Ff(x,t) + Cf(x,t),$$
$$f(x,0) = \mathring{f}(x), \qquad (44)$$

where we assume

$$0 \le a \in L_{\infty,loc}([0,\infty)); \qquad (45)$$
$$1/r \in L_{1,loc}(\mathbb{R}_+) \text{ and } 0 < r(x) \le r_0 + r_1 x \le \tilde{r}(1+x), \qquad (46)$$

for some nonnegative constants $r_0, r_1$ and $\tilde{r}$.

We distinguish two cases of behaviour of $r(x)$ close to $x = 0$:

$$\int_{0^+} \frac{\mathrm{d}x}{r(x)} = +\infty \text{ or } \int_{0^+} \frac{\mathrm{d}x}{r(x)} < +\infty. \tag{47}$$

In the latter, we need a boundary condition at $x = 0$ and hence we define $T_0 f := -(rf)_x - af$, in the first case on

$$D(T_0) := \{f \in X_{0,m} : (rf)_x, qf \in X_{0,m}\}, \tag{48}$$

and in the second case we use

$$D(T_0) := \{f \in X_{0,m} : (rf)_x, qf \in X_{0,m}, r(x)f(x) \to 0 \text{ as } x \to 0\}. \tag{49}$$

We consider the full linear part in the abstract form

$$f_t = T_0 f + Bf,\ t > 0;\quad f(0) = \mathring{f}, \tag{50}$$

where $B$ is the restriction to $D(T_0)$ of

$$f \mapsto \int_x^\infty a(y)b(x,y)f(y)\mathrm{d}y.$$

Then, under the same assumptions on $b$ that ensured analyticity of the fragmentation semigroup, we have

**Theorem 13**

*Then $(K, D(T_0)) = (T_0 + B, D(T_0))$ generates a positive $C_0$-semigroup, $(G_K(t))_{t\geq 0}$, on $X_{0,m}$.*

The proof is carried out by the Desch theorem, applicable since we deal with positive operators in $L_1$ spaces.

## An application to spectral gap and AEG.

**Theorem 14**

*Let the assumptions of the previous theorem be satisfied, and let* $r$ *be continuous, satisfy* (46) *and* $1/r$ *be integrable close to* $0^+$*. Further, let the sublevel sets of* $a$ *be thin at infinity in the sense that for any* $c > 0$

$$\int_1^{+\infty} 1_{\{x>0:\, a(x)<c\}} \frac{1}{r(y)} dy < +\infty \tag{51}$$

*(e.g., let* $\lim_{x\to+\infty} a(x) = +\infty$ *). Then* $(G_K(t))_{t\geq 0}$ *has AEG, that is,*

## Theorem 14

*there is* $\varepsilon > 0$ *such that*

$$\left\| e^{-\lambda t} G_K(t)\mathring{f} - (\boldsymbol{e}^* \cdot \mathring{f})\boldsymbol{e} \right\| = O(e^{-\varepsilon t}), \qquad (52)$$

*where* $\lambda$ *is the isolated algebraically simple dominant eigenvalue of* $K$, *and* $\mathbf{e}$ *and* $\mathbf{e}^*$ *are strictly positive eigenvectors of, respectively, the generator and its dual.*

## Application to problems with coagulation

For pure fragmentation and coagulation problems (with $r \equiv 0$), the linear part generates an analytic semigroup $(G_F(t))_{t\geq 0}$ which allows to deal with the integral equation

$$f(t) = G_F(t)\mathring{f} + \int_0^t G_F(t-s)Cf(s)\,\mathrm{d}s,\ \ t \in \mathbb{R}_+. \qquad (53)$$

even when the kernel $k$ of $C$ is unbounded (but with growth controlled by $a$).

With $r \neq 0$, however, $(G_K(t))_{t\geq 0}$ is not analytic.

**Moment regularization.** We have the following result.

Theorem 15 (E. Bernard & P. Gabriel, 2020)

*In addition to the conditions required for Theorem 13 to hold, assume that positive constants $a_0, \gamma_0$ and $x_0$ exist such that*

$$a(x) \geq a_0 x^{\gamma_0}, \qquad \textit{for all } x \geq x_0. \tag{54}$$

*Then, for any $n$, $p$ and $m$ satisfying $\max\{1, l\} < n < p < m$, there are constants $C > 0$ and $\theta > 0$ such that*

$$\|G_K(t)\mathring{f}\|_{0,m} \leq Ce^{\theta t} t^{\frac{n-m}{\gamma_0}} \|f\|_{0,p}, \quad \textit{for all } f \in X_{0,p}. \tag{55}$$

**Full problem** (44)

Here, the coagulation kernel is required to satisfy

$$k(x,y) \leq k_0(1+x^\alpha)(1+y^\alpha), \tag{56}$$

for some $0 < \alpha < \gamma_0$.

Assume that the generation assumptions of this section hold, $k$ satisfy (56) and, in addition, $m > \alpha + \max\{1, l\}$.

## Theorem 16

*Then, for each* $\mathring{f} \in X_{0,m,+}$, *the problem* (44) *has a unique nonnegative mild solution* $f \in C([0, t_{\max}), X_{0,m})$ *defined on its maximal interval of existence* $[0, t_{\max}(\mathring{f}))$. *If* $t_{\max}(\mathring{f}) < \infty$, *then* $\|f(t)\|_{0,m}$ *is unbounded as* $t \to t_{\max}(\mathring{f})^-$.

In the next theorem we address the issue of differentiability of the mild solution and it being a classical solution. The result is similar to that for analytic semigroups in that the mild solution in a smaller space (here $X_{0,m}$) is a classical solution in a bigger space (here $X_{0,p}$). Denote by $D_p(K)$ the domain of $K$ in $X_{0,p}$.

**Theorem 17**

*Assume that $\mathring{f} \in X_{0,m} \cap D_p(K)$, where $p = m - \alpha$. Then the mild solution $f$ constructed in Theorem 16, defined on its maximal interval of existence $[0, t_{\max})$, satisfies*

$$f \in C([0, t_{\max}), X_{0,m}) \cap C^1((0, t_{\max}), X_{0,m}) \cap C((0, t_{\max}), D_p(K))$$

*and is a classical solution to (44) in $X_{0,p}$.*

**Global solvability.** For this, we assume

$$k(x, y) \leq k_0(1 + x^\alpha + y^\alpha), \tag{57}$$

$0 < \alpha < \gamma_0$.

**Theorem 18**

*If for $x \geq 0$ either*

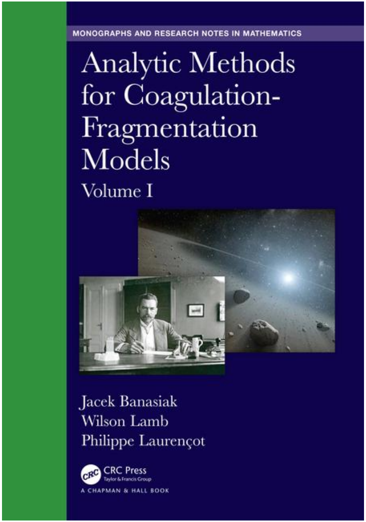
*a) there are constants $m_0$ and $m_1$ such that*

$$(n_0(x) - 1)a(x) \leq m_0 + m_1 x,$$

*or*

*b) $r(x) \leq \tilde{r}x$,*

*then the solutions of Theorem 16 are global in time.*



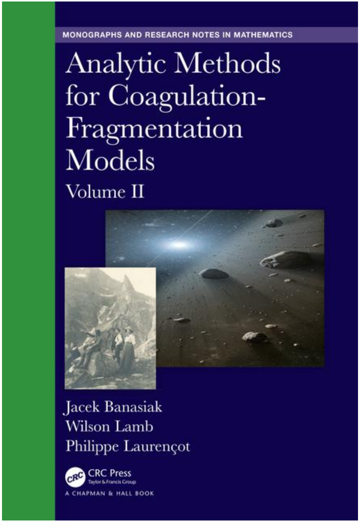
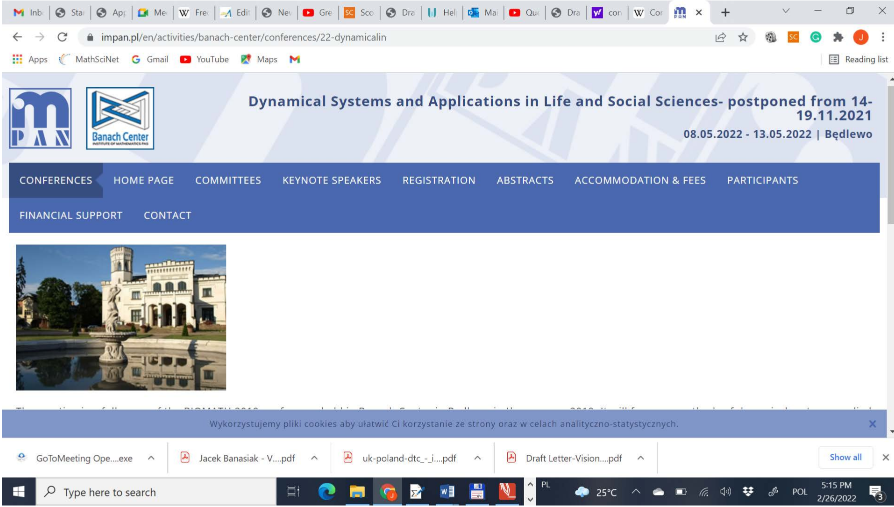




Figure: Shameless self-promotion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