Infinite-dimensional Luenberger observers: application to a crystallization process

SMAI Minisymposium: Control, observation and stabilization

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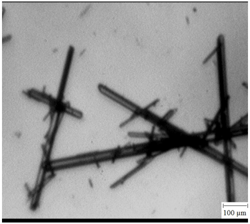
In collaboration with Ludovic Sacchelli

Problem statement

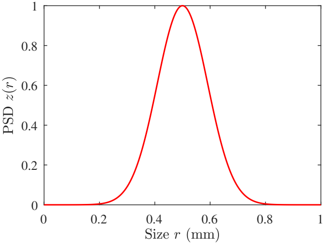
Introduction

Context: During a batch crystallization process, the estimation of the Particle Size Distribution (PSD) is critically important in the industry.



Crystals in the reactor during the process

$\Longrightarrow$



Distribution in characteristic size

Objective: Design an observer to estimate the PSD from an other measurement: the Chord Length Distribution (CLD).

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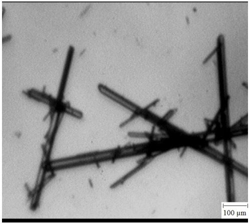

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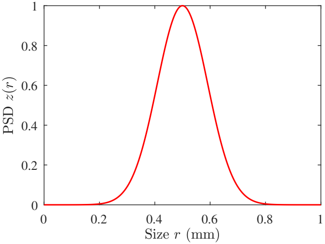

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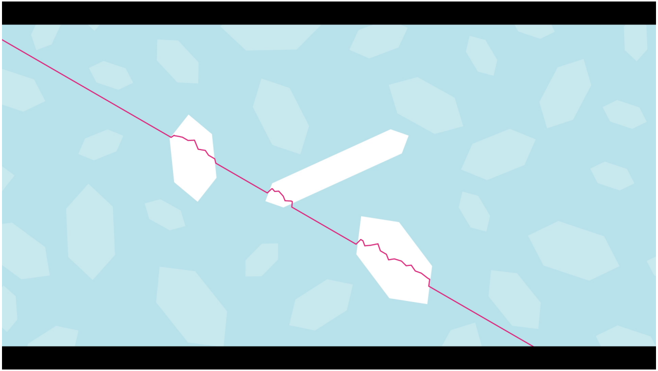
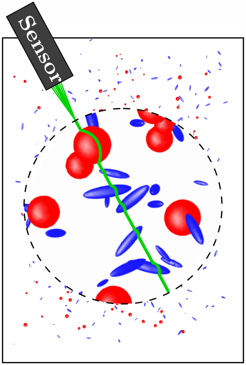
Modeling the CLD



Presentation of the CLD sensor (FBRM)



Reactor

Modeling the CLD

By the **law of total expectation**, the PSD-to-CLD map C is given by:

$$\mathbb{P}(L \leqslant \ell) = \int_{r_{\min}}^{r_{\max}} \mathbb{P}(L \leqslant \ell | R = r) z(r) \mathrm{d}r$$

where

$$k(\ell, r) = \mathbb{P}(L \leqslant \ell | R = r).$$

The kernel $k(\ell, r)$ depends on particle geometry.

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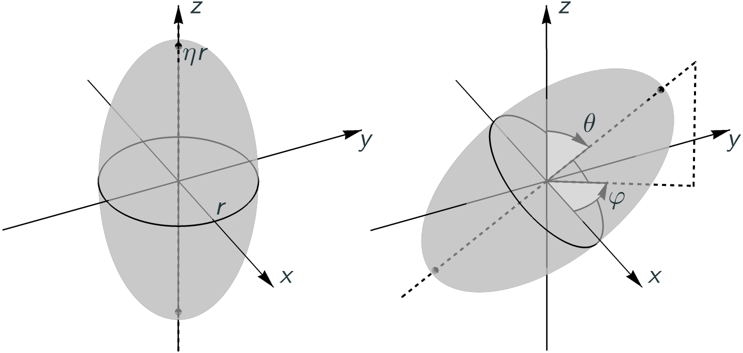
Modeling the CLD

We propose a model for **spheroid** particles.

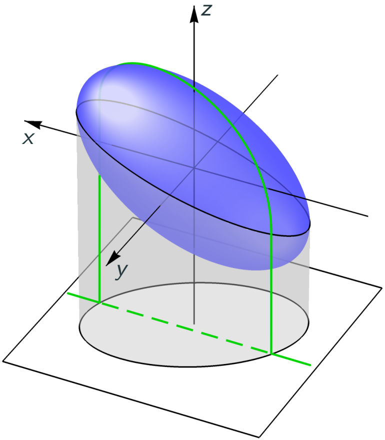
Step 1: Choose an orientation of the spheroid with respect to the probe.

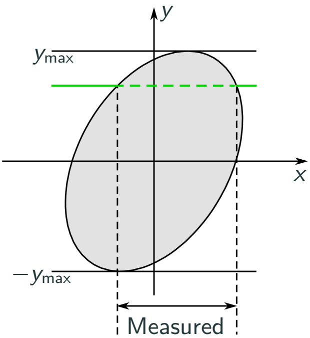


where η is the **shape parameter**.

Modeling the CLD

Step 2: Choose a chord on the projection of the spheroid.





Modeling the CLD

Probabilistic model:

$$k_\eta(\ell, r) = 1 - \int_{\varphi=0}^{2\pi} \int_{\theta=0}^{\pi} \sqrt{1 - \left(\frac{\ell}{2r}\right)^2 \alpha_\eta(\varphi, \theta)} \frac{\sin\theta}{4\pi} \mathrm{d}\theta \mathrm{d}\varphi$$

Proposition (Brivadis, Sacchelli, 2021).
For any shape parameter η, the operator C_η is injective.

⚠ Since C is compact, it has no continuous left-inverse. But one can use a regularization method, such as **Tikhonov regularization**:

$$z = \underset{\hat{z}}{\operatorname{argmin}} \left\| y - C_\eta \hat{z} \right\|_{L^2}^2 + \delta^2 \|\hat{z}\|_{L^2}^2$$

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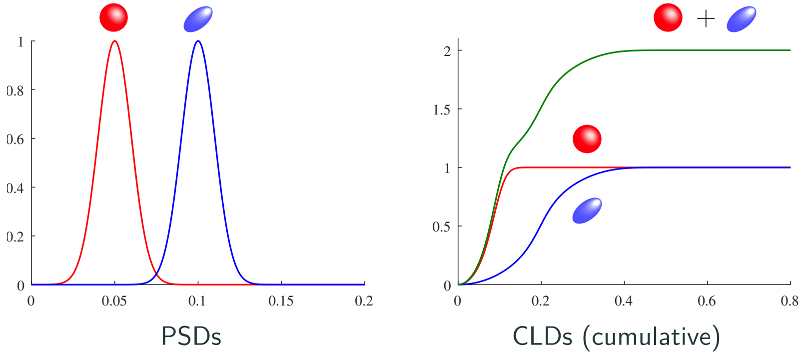
Modeling the CLD

Issue: Due to polymorphism, it frequently occurs that particles in the reactor have different shapes.

Obstacle: There isn't enough information in the CLD to recover PSDs if there are multiple shapes in suspension.



Evolution model

Figure 1: Crystallization process at $t = 50$ min[1]

[1] Experiment LG34, Y. Tahri PhD thesis, 2016

Evolution model

Figure 1: Crystallization process at $t = 70$ min[1]

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Evolution model

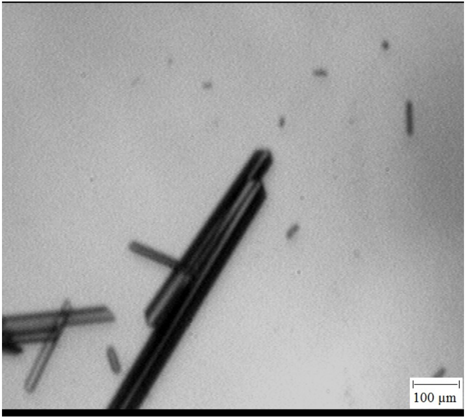


Figure 1: Crystallization process at $t = 80$ min[1]

[1] Experiment LG34, Y. Tahri PhD thesis, 2016

Evolution model

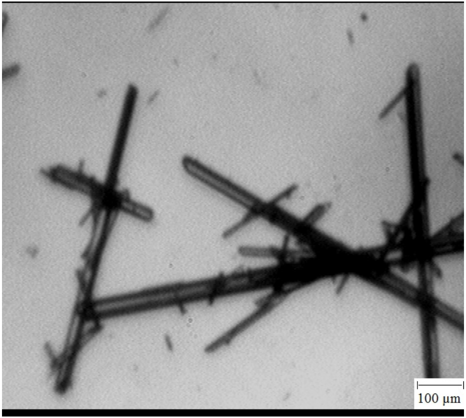


Figure 1: Crystallization process at $t = 110$ min[1]

[1] Experiment LG34, Y. Tahri PhD thesis, 2016

Evolution model

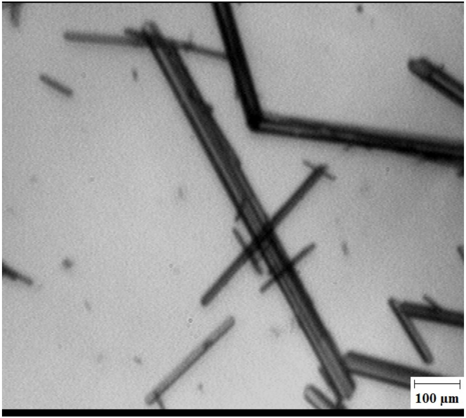


Figure 1: Crystallization process at $t = 130$ min[1]

[1] Experiment LG34, Y. Tahri PhD thesis, 2016

Evolution model

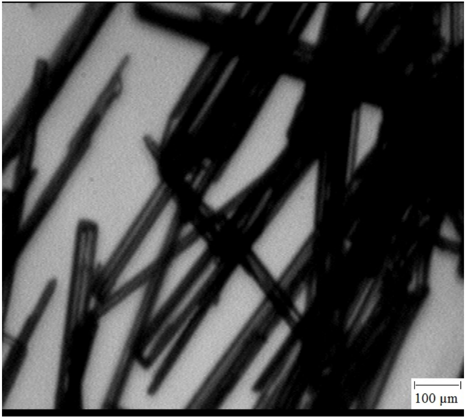


Figure 1: Crystallization process at $t = 345$ min[1]

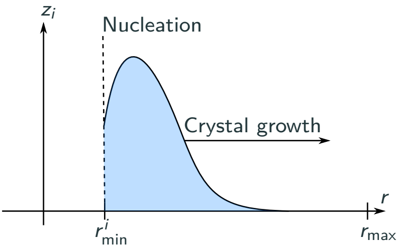
[1] Experiment LG34, Y. Tahri PhD thesis, 2016

Evolution model

Population balance equation:

$$\begin{cases} \partial_t z_i(t,r) = -G_i(t,r)\partial_r z_i(t,r) \\ z_i(0,r) = z_{i,0}(r), \quad \forall r \in [r^i_{\min}, r_{\max}] \\ z_i(t, r^i_{\min}) = u_i(t), \quad \forall t \in [0, t_{\max}] \end{cases}$$

- $z_i(t)$: PSD of particles of shape $1 \leqslant i \leqslant N$ for $t \in [0, t_{\max}]$
- $G_i(t,r)$: grow rate
- u_i: nucleation at $r^i_{\min}$



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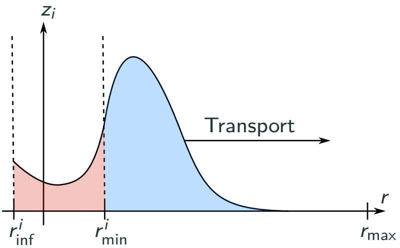

Luenberger observer and BFN

Observer design

Infinite-dimensional linear time-varying system:

$$\begin{cases} \dot{z} = A(t)z, & z_0 \in X \\ y = Cz \end{cases}$$

Luenberger observer:

$$\begin{cases} \dot{\hat{z}} = A(t)\hat{z} - \alpha C^* C\varepsilon, & \hat{z}_0 \in X \\ \dot{\varepsilon} = (A(t) - \alpha C^* C)\varepsilon, & \varepsilon_0 = \hat{z}_0 - z_0 \end{cases}$$

- X and Y are Hilbert spaces, $C \in \mathscr{L}(X, Y)$
- $A(t) : \mathcal{D}(A) \to X$ generates an evolution system $(\mathbb{T}(t,s))_{t \geqslant s \geqslant 0}$
- $z, \hat{z}, \varepsilon \in C^0(\mathbb{R}_+; X)$

Example: $X = L^2(r_{\inf}, r_{\max})^N$, $Y = L^2(\ell_{\min}, \ell_{\max})$,
$A(t) = \mathrm{diag}(-G_i(t,r)\partial_r)$, and $C = \langle k(\ell, \cdot), \cdot \rangle_{L^2(r_{\min}, r_{\max})}$

Observer design

Definition (Exact observability).

The system is **exactly** observable on $[t_0, t_0+\tau]$ if for some $k > 0$,

$$\int_{t_0}^{t_0+\tau} \|C\mathbb{T}(t,t_0)z_0\|_Y^2 \mathrm{d}t \geqslant k\|z_0\|_X^2, \quad \forall z_0 \in X$$

Proposition. (Brivadis, Andrieu, Serres, Gauthier, 2021)

Since k is bounded, the crystallization process is **not** exactly observable.

Definition (Approximate observability).

$$\mathcal{O} = \left\{ z_0 \in X \mid \int_{t_0}^{t_0+\tau} \|C\mathbb{T}(t,t_0)z_0\|_Y^2 \mathrm{d}t = 0 \right\}^{\perp}$$

The system is **approximately** observable on $[t_0, t_0+\tau]$ if $\mathcal{O} = X$.

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Back and Forth Nudging

Inverse problem: How to **estimate** $z(t)$ from the knowledge of $y(t)$ over a **bounded** time interval $[0, \tau]$?

Observer approach: Forward and backward Luenberger observers

Assume that $A(t)$ is the generator of a **bidirectional** evolution system.

$$\forall n \in \mathbb{N}, \forall t \in [0, \tau], \quad \begin{array}{ll} \text{If } n \text{ is even,} & \begin{cases} \dot{\hat{z}}^n = A(t)\hat{z}^n - \alpha C^*(C\hat{z}^n - y(t)) \\ \hat{z}^n(0) = \begin{cases} \hat{z}^{n-1}(0) & \text{if } n \geqslant 1, \\ \hat{z}_0 & \text{otherwise.} \end{cases} \end{cases} \\ \text{If } n \text{ is odd,} & \begin{cases} \dot{\hat{z}}^n = A(t)\hat{z}^n + \alpha C^*(C\hat{z}^n - y(t)) \\ \hat{z}^n(\tau) = \hat{z}^{n-1}(\tau) \end{cases} \end{array}$$

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If $\langle A(t)z,\ z\rangle_X \leqslant p\,\|Cz\|_Y^2$ for some $p > 0$ (**weak detectability**), then

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\,\|\varepsilon(t)\|_X^2 \leqslant -(\alpha - p)\,\|C\varepsilon(t)\|_Y^2$$

Theorem (Brivadis, Andrieu, Serres and Gauthier, 2021).
Assumption:

- Both $((A(t))_{t\geqslant 0}, C)$ and $((-A(t))_{t\geqslant 0}, C)$ are weakly detectable

Let $\mathcal{O}$ be the observable subspace of $(\mathbb{T}, C)$ over $[0,\tau]$. Then

$$\langle \varepsilon^n(t),\ \psi\rangle_X \underset{n\to+\infty}{\longrightarrow} 0, \qquad \forall \varepsilon_0 \in X,\ \forall \psi \in \mathcal{O},\ \forall t \in [0,\tau].$$

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Application to the crystallization process

Theorem (Brivadis, Sacchelli, 2021).

Assumptions:

- Only two clusters of crystals: $i \in \{1, 2\}$, $N = 2$
- $G_i(t, r) = g_i f(t) h(r)$, $g_i \neq 0$, f in C^2 has a finite number of zeros and $h(r) = 1/r^m$, $m \geqslant 0$.

Then $H^2(r_{\inf}, r_{\max})$ lies in the observable subspace of the system over any positive time interval if:

- $g_i > 0$, $h(r) = 1$, $r^1_{\min} = r^2_{\min}$, $\eta_1 = 1$ and $\eta_2 > 1$

or

- $(r^1_{\min})^2 A(\eta_2) \neq (r^2_{\min})^2 A(\eta_1)$ with $\begin{cases} A(\eta) = 1 & \text{if } \eta \geqslant 1 \\ A(\eta) = 1/\eta^2 & \text{if } \eta < 1 \end{cases}$
  and ($g_i > 0$ and m is even) or ($g_i < 0$ and m is odd)

Thus, the back and forth observer converges in the weak topology for initial conditions in $H^2(r_{\inf}, r_{\max})$.

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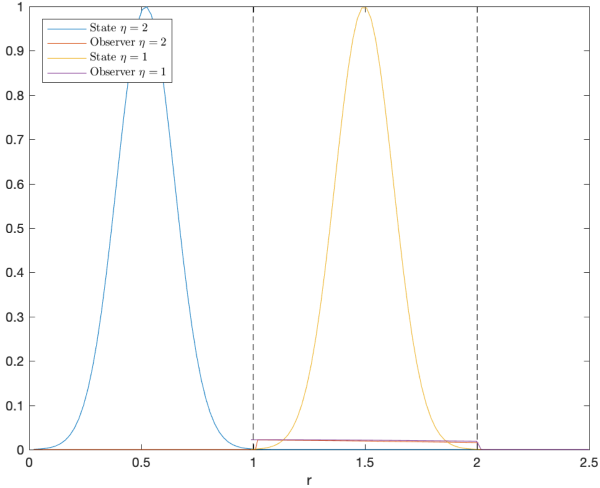

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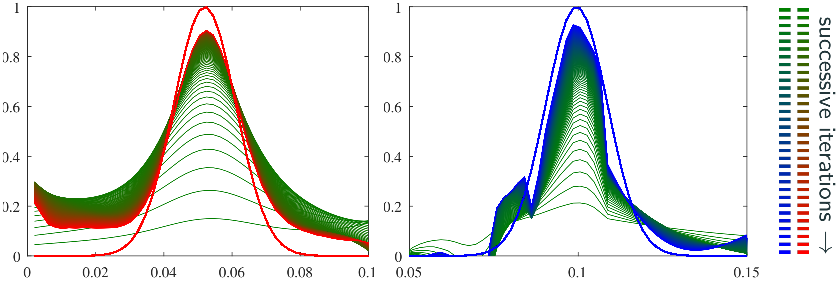

200 successive estimates of the PSDs as returned by the BFN algorithm.

Conclusion and perspectives

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- We propose a **model** of the PSD-CLD mapping for **spheroids**.
- The **Back and Forth Nudging** algorithm can employed to recover the PSD from the CLD in the multi-shape case.
- **Weak convergence** has been proved for various pairs of shapes.

Conclusion and perspectives

Some open questions about the theoretical results:

- Speed of convergence
- Unbounded operator C
- Online back and forth observer

Some open questions about the application:

- Crystals with other shapes
- Test different probability models
- Observability analysis with spheroids

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