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► **To cite this version:**

Lucas Brivadis, Ludovic Sacchelli. New inversion methods for the single/multi-shape CLD-to-PSD problem with spheroid particles. 21st International Symposium on Industrial Crystallization, Aug 2021, Berlin (on line), Germany. hal-03331899

**HAL Id: hal-03331899**

**<https://hal.science/hal-03331899>**

Submitted on 2 Sep 2021

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# New inversion methods for the single/multi-shape CLD-to-PSD problem with spheroid particles

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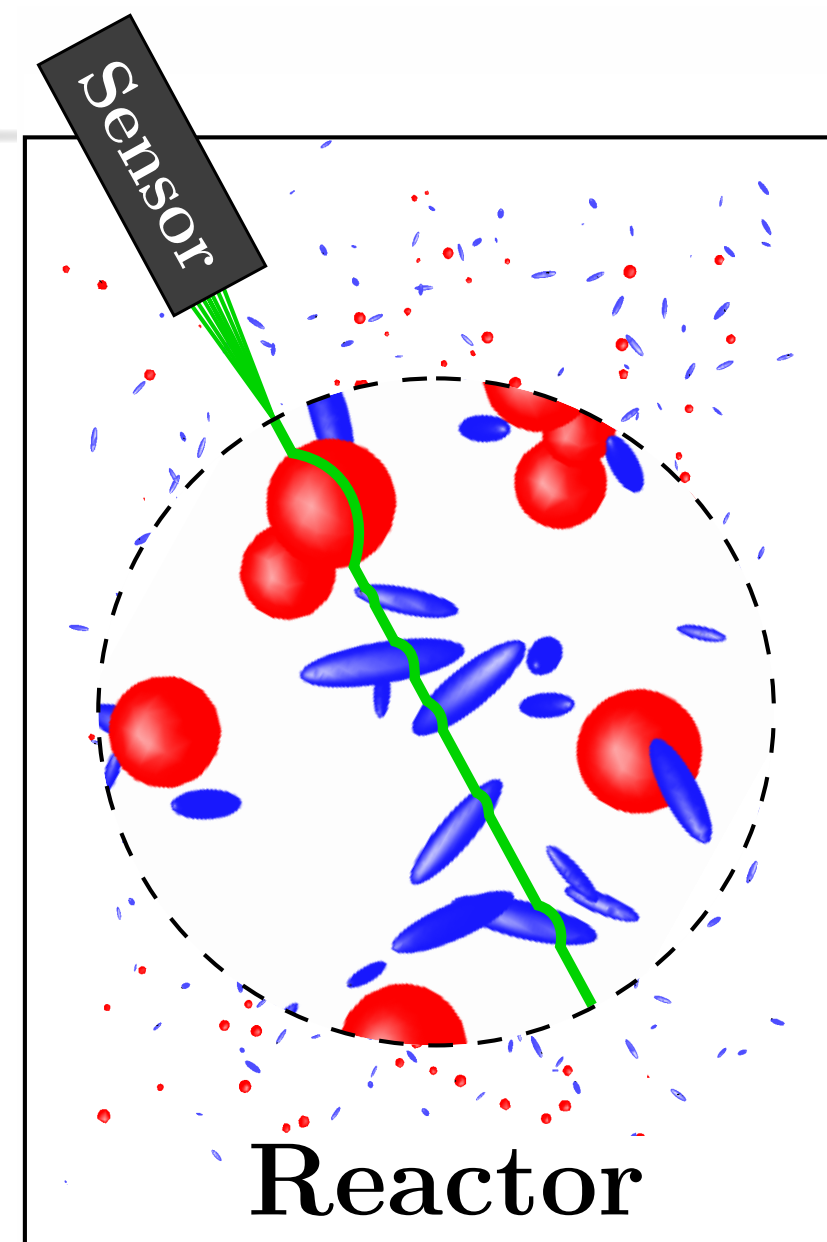
## Introduction

**Context:** During a crystallization process, estimating the Particle Size Distribution (PSD) is of major importance.

**Objective:** Estimate the PSD from measurements of the Chord Length Distribution (CLD).

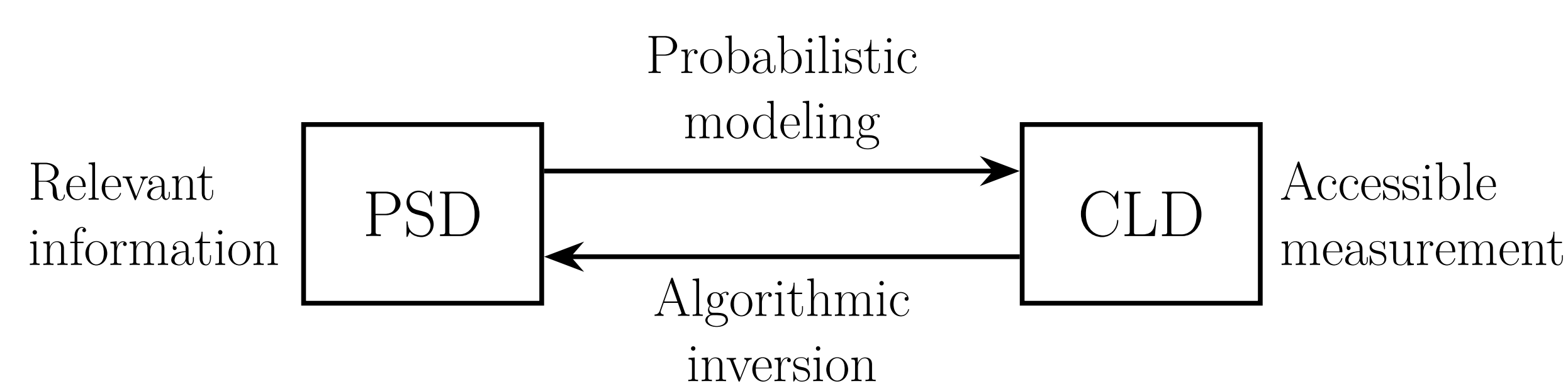
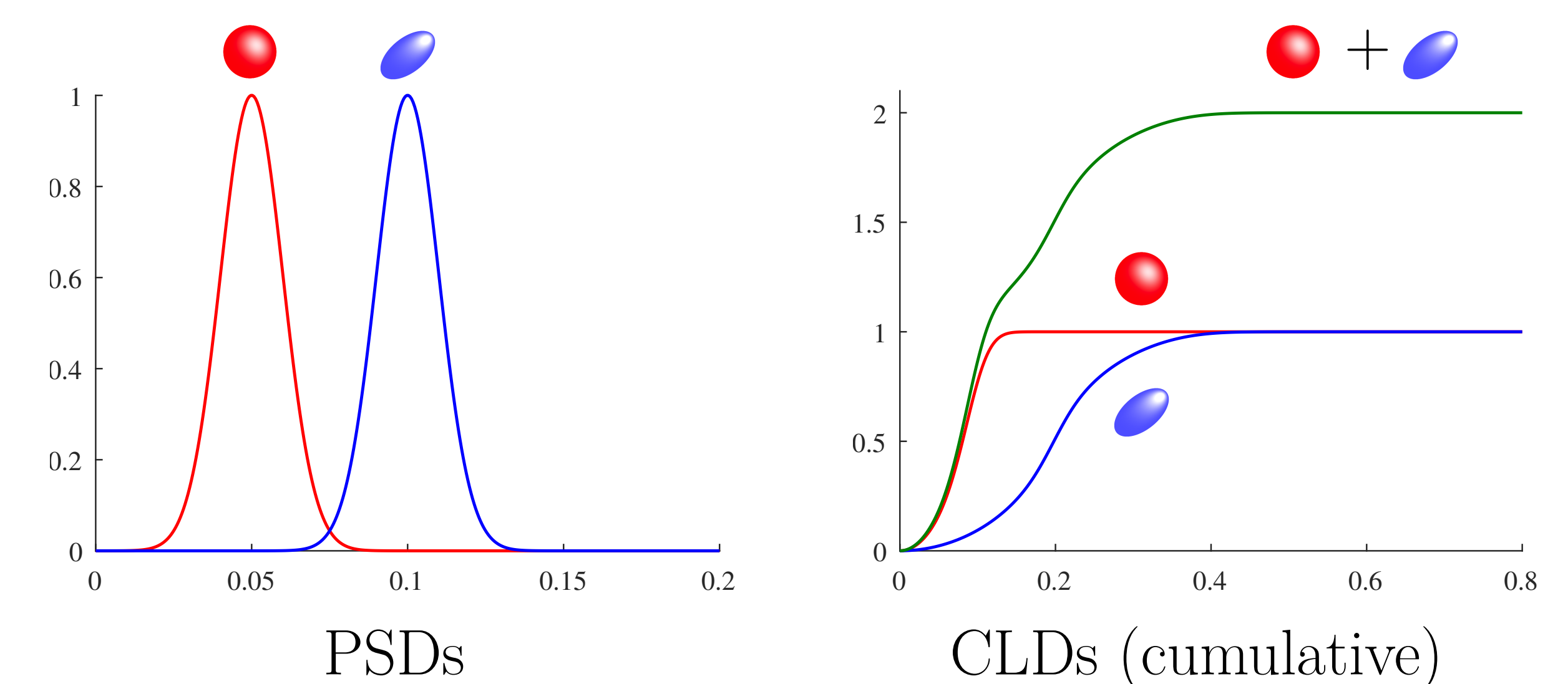
**Challenges:** The PSD/CLD relation depends on particle geometry; multiple shapes may coexist in the suspension.

**Method:** We model the CLD acquisition with a PSD-to-CLD mapping for spheroid particles.

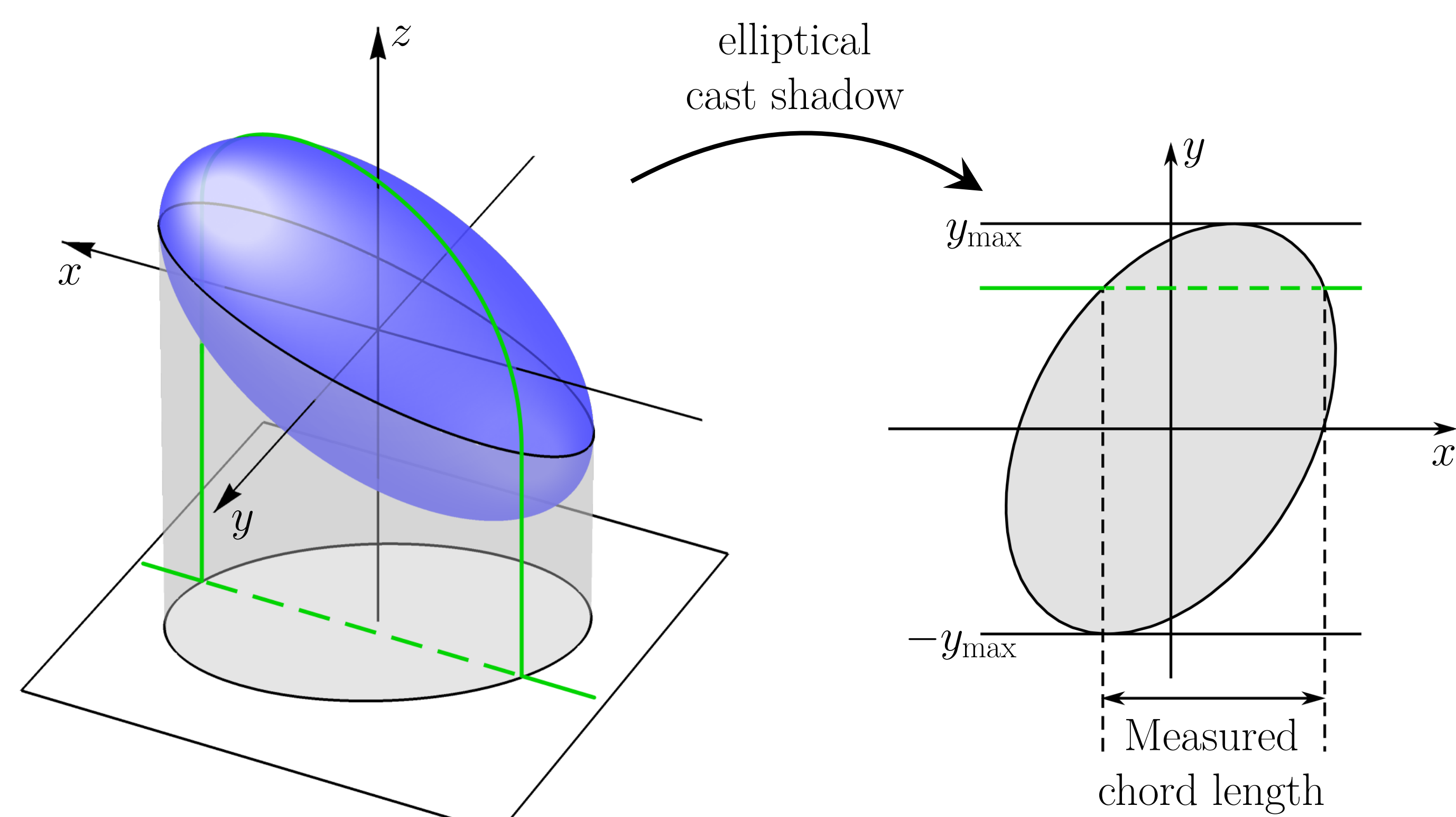


## Multi-shape CLD-to-PSD challenge

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



## PSD-to-CLD with spheroid particles



Law of **total expectation**:  $q(\ell) = \int_{r_{\min}}^{r_{\max}} k(\ell, r) \times \psi(r) dr$

• PSD:  $\psi(r)$ , with radius  $r_{\min} \leq r \leq r_{\max}$  and **fixed shape**.

• CLD:  $q(\ell)$ , with length  $0 \leq \ell \leq \ell_{\max}$ .

•  $k(\ell, r)$  is determined through a **probabilistic analysis**.

It depends on the shape of the spheroids.

## Single-shape CLD-to-PSD challenge

**Theorem:** For all CLD of spheroid particles of fixed shape, there exists a unique corresponding PSD.

**Problem:** Small CLD measurement noise leads to high PSD uncertainty. How to **robustly inverse** the PSD-to-CLD relation?

**Tikhonov regularization method:**

• Goal: Numerically estimate the **distributed** solution of

$$\operatorname{argmin}_{\hat{\psi}} \left\| q(\ell) - \int k(\ell, r) \hat{\psi}(r) dr \right\|_2^2 \quad (\text{least squares})$$

• Idea: Add a regularization term (**measure confidence**):

$$\operatorname{argmin}_{\hat{\psi}} \left\| q(\ell) - \int k(\ell, r) \hat{\psi}(r) dr \right\|_2^2 + \delta^2 \left\| \hat{\psi}(r) \right\|_2^2$$

**Solution:** Equip the crystallization process with a dynamical model.

**Population Balance Equation:**

$$\begin{cases} \partial_t \psi_i(t, r) = -G_i(t) \partial_r \psi_i(t, r) \\ \psi_i(t_0, r) = \psi_{i,0}(r) \\ \psi_i(t, r_{\min}) = u_i(t) \end{cases} \quad \begin{aligned} &\bullet \psi_i(t, r): \text{PSD at time } 0 \leq t \leq t_{\max} \\ &\quad \text{of particles of shape } i. \\ &\bullet G_i(t): \text{growth kinetic} \\ &\bullet u_i(t): \text{nucleation} \end{aligned}$$

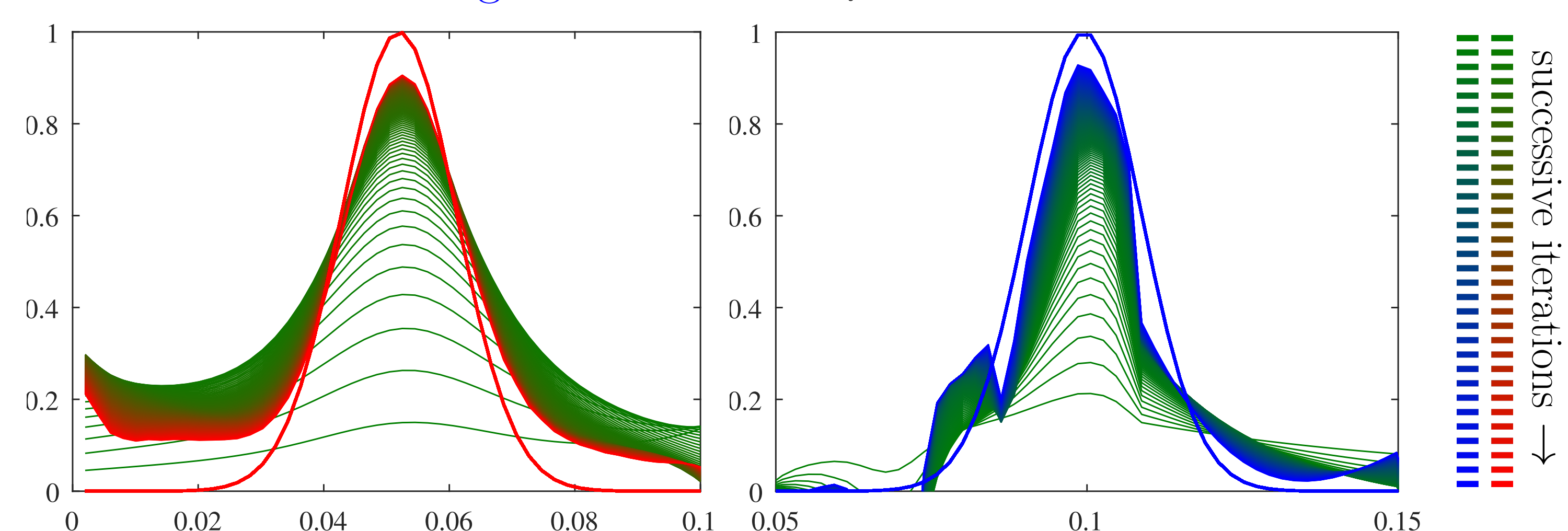
## Results with Back and Forth Nudging

**Observer-based strategy:** Luenberger asymptotic observer design with gain  $\mathcal{L}$ :

$$\partial_t \hat{\psi}_i(t, r) = -G_i(t) \partial_r \hat{\psi}_i(t, r) - \mathcal{L}(\hat{q} - q)$$

**Back and Forth Nudging** algorithm: on the finite experiment time interval, we refine the estimate by iteration of the asymptotic observer.

**No prior knowledge on the nucleation**  $u_i$  is required. However, we need an **estimation of the growth kinetic**  $G_i$ .



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

• At first, the algorithm assigns PSDs indiscriminately in order to match the shared CLD.

• Using the dynamics, the observer then refines its estimation.

We proved that **estimate accuracy increases** at each iteration and ultimately **converges** for most pairs of spheroids.

## Conclusion

We propose a **new algorithm** to estimate the PSD from the knowledge of the CLD during a batch crystallization process.

We rely on an evolution model of the process and an estimation of the growth kinetic. We use a **Back and Forth Nudging** strategy based on a Luenberger observer.

The method has been **theoretically** validated and **numerically** tested. In the future, we wish to apply this method to **experimental** data.

References:

- [1] L. Brivadis and L. Sacchelli, New inversion methods for the single/multi-shape CLD-to-PSD problem with spheroid particles, Submitted to Journal of Process Control.
- [2] L. Brivadis, L. Sacchelli, Approximate observability and back and forth observer of a PDE model of crystallization process, Submitted to IEEE CDC, Austin (2021).