



**HAL**  
open science

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

Lucas Brivadis, Ludovic Sacchelli

► **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-03331899v1>**

Submitted on 2 Sep 2021

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

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

Lucas Brivadis, Ludovic Sacchelli

LAGEPP, CNRS UMR 5007, Université Claude Bernard Lyon 1, Lyon, France

lucas.brivadis@univ-lyon1.fr, ludovic.sacchelli@univ-lyon1.fr

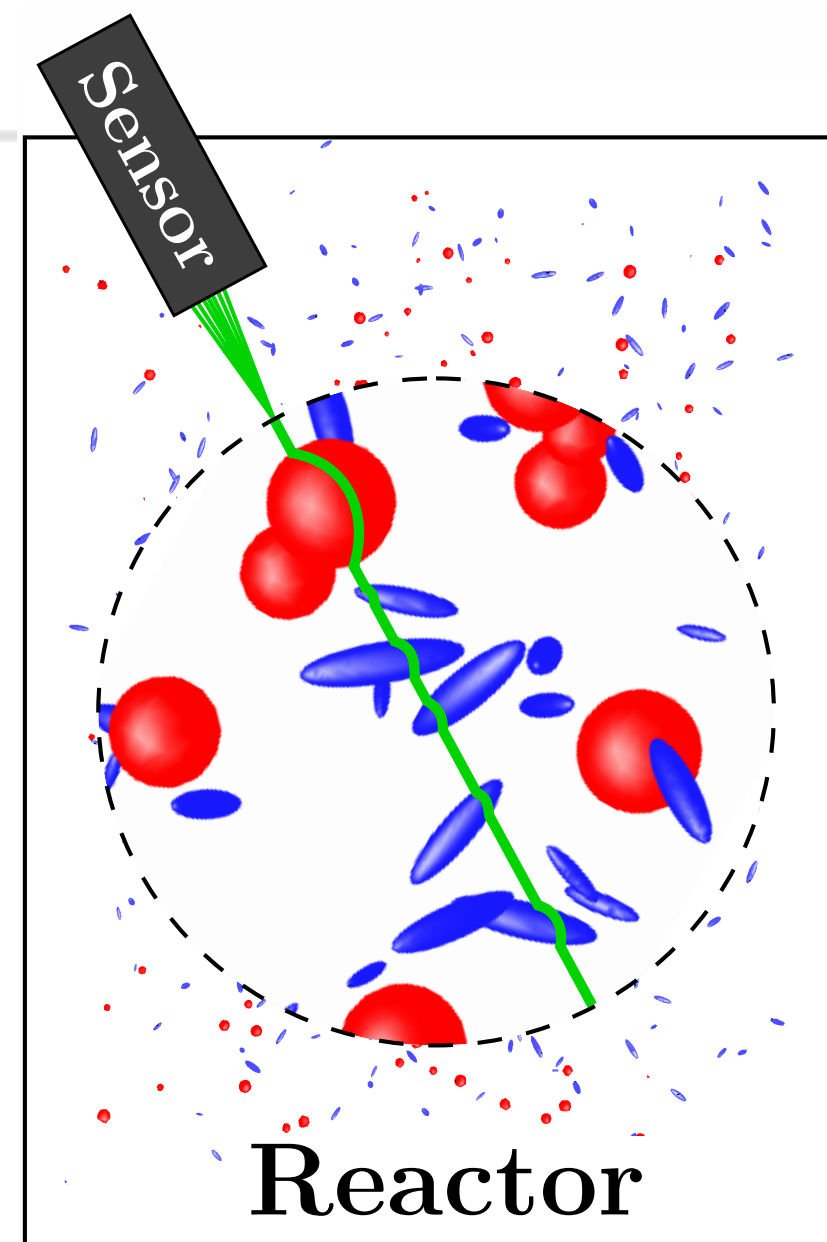
## Introduction

**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).

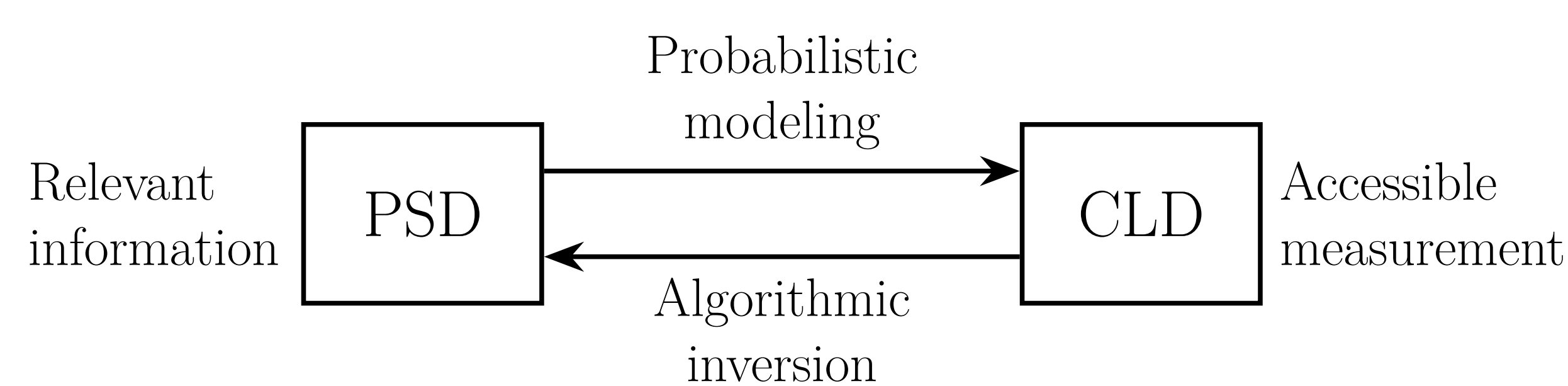
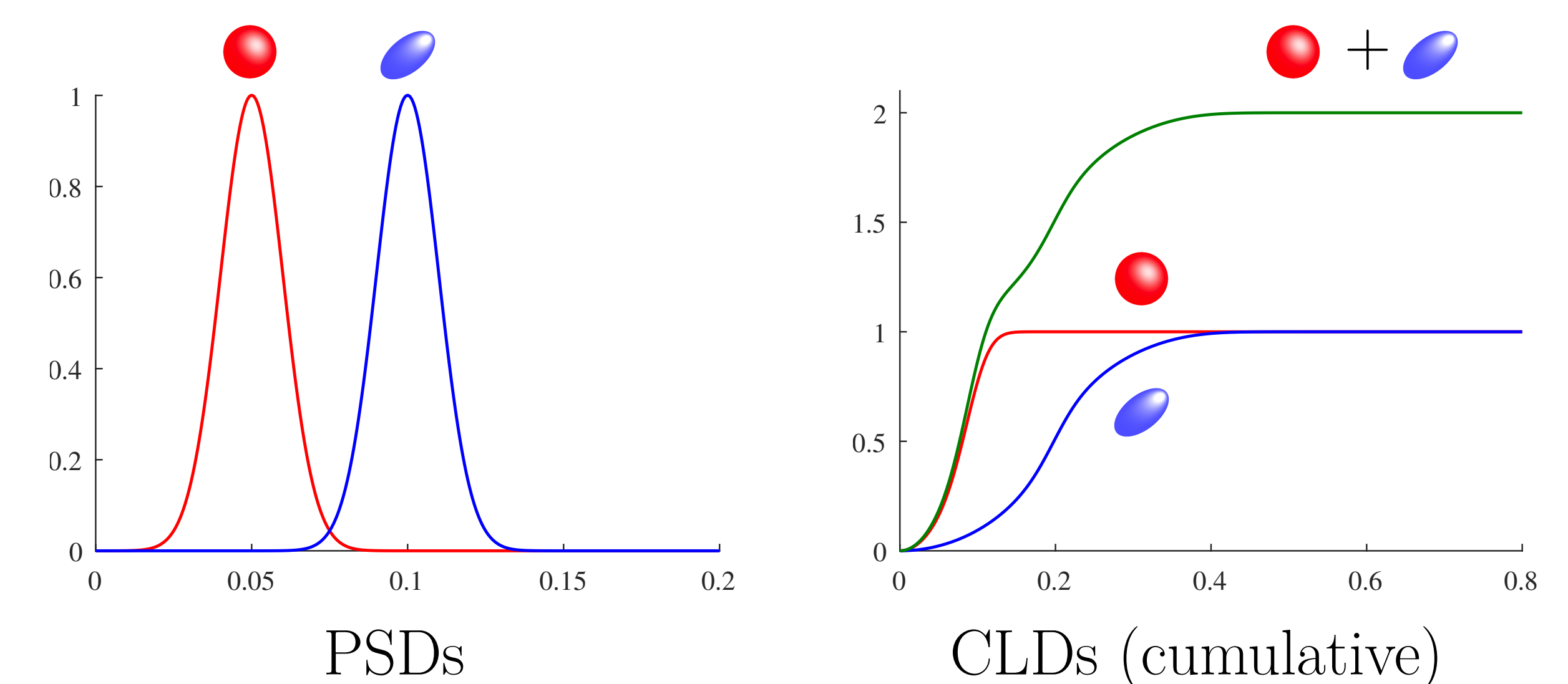
**Challenges:** The PSD/CLD relation depends on particle geometry; multiple shapes may coexist in the suspension.

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

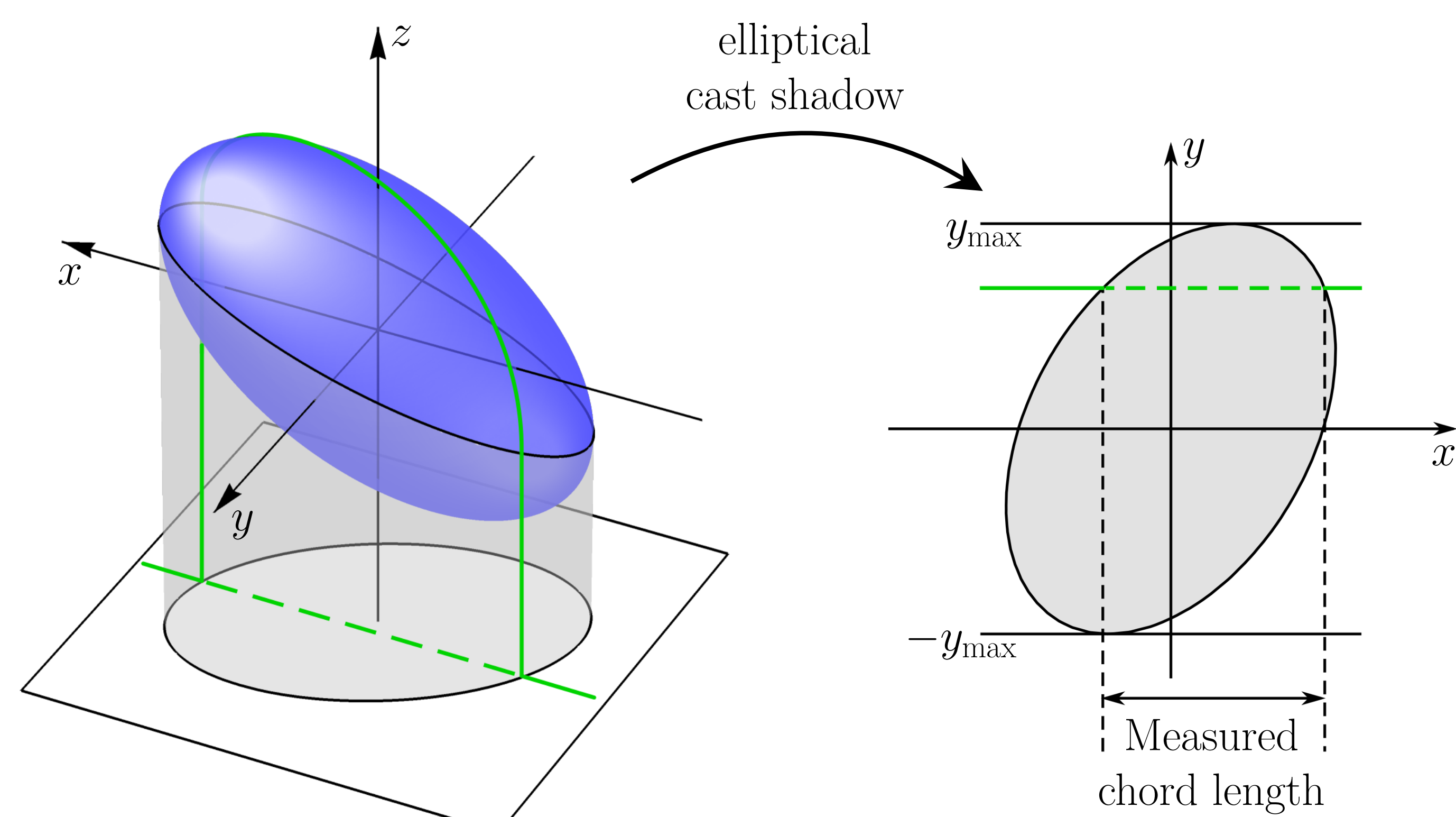


## Multi-shape CLD-to-PSD challenge

**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:**

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

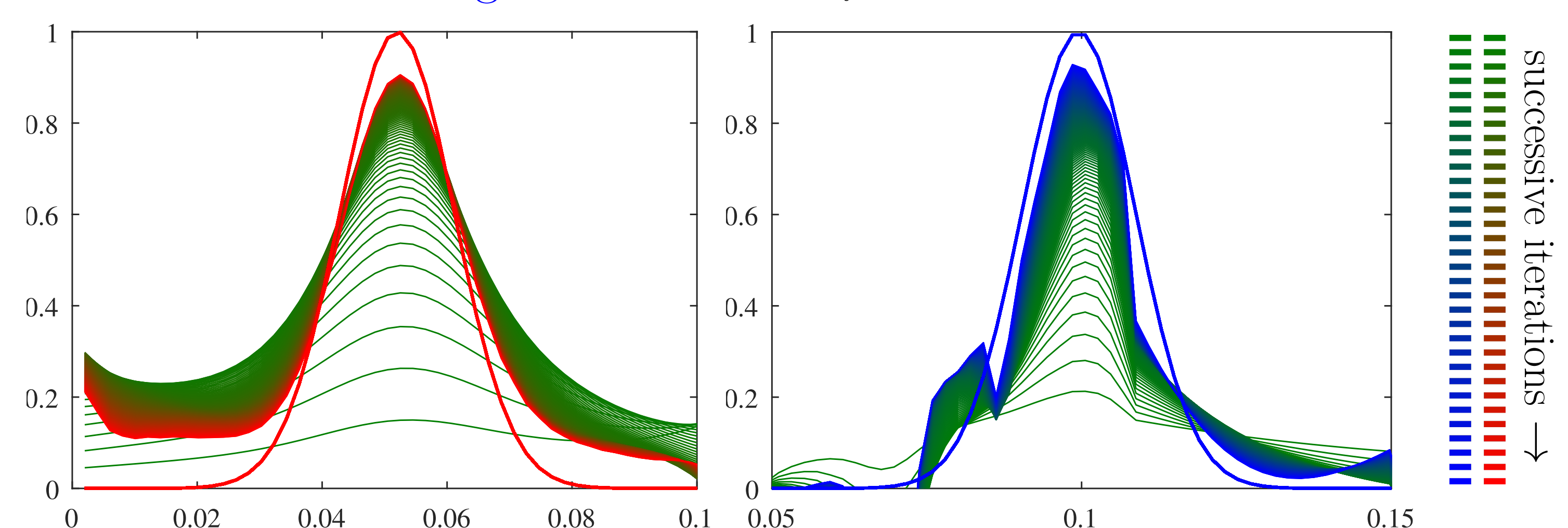
## Results with Back and Forth Nudging

**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).