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

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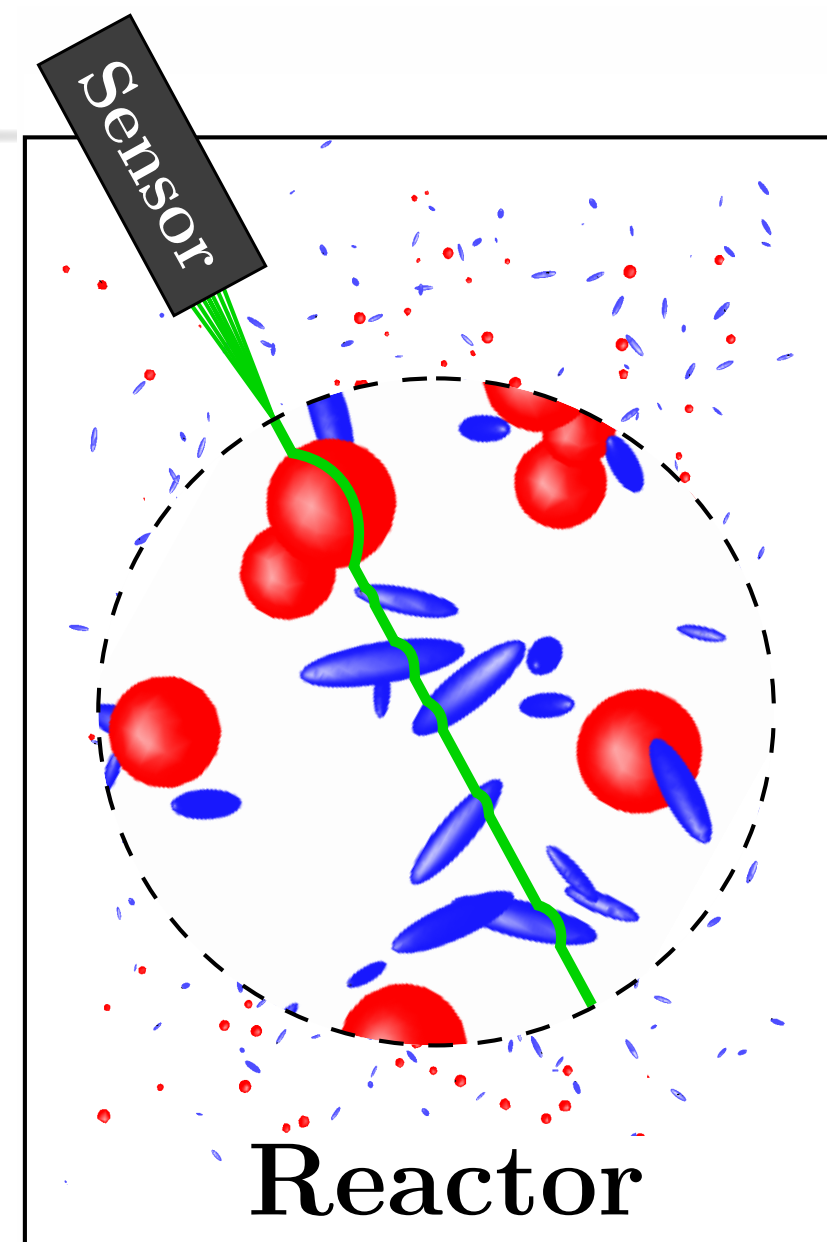
Introduction

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).

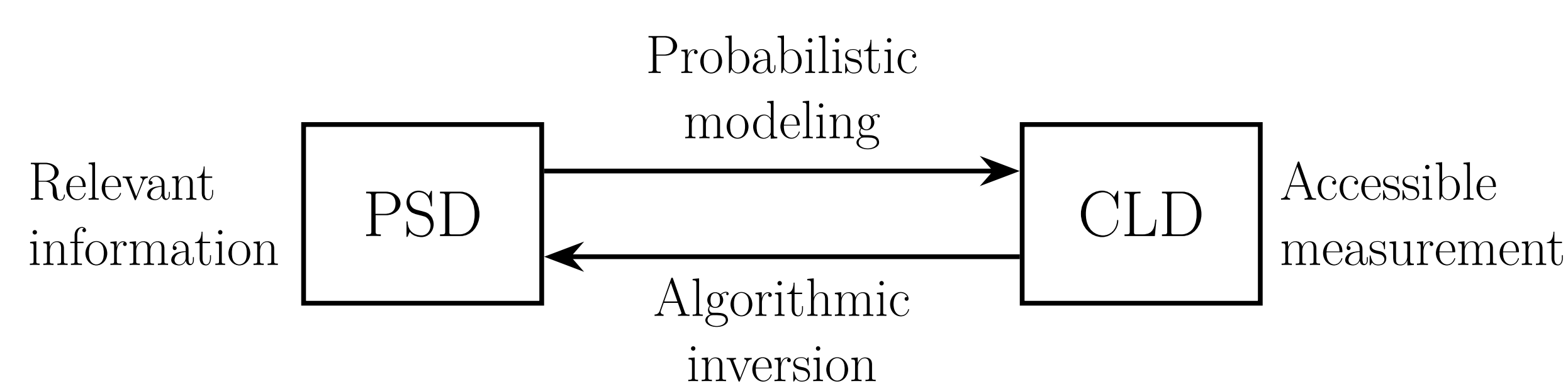
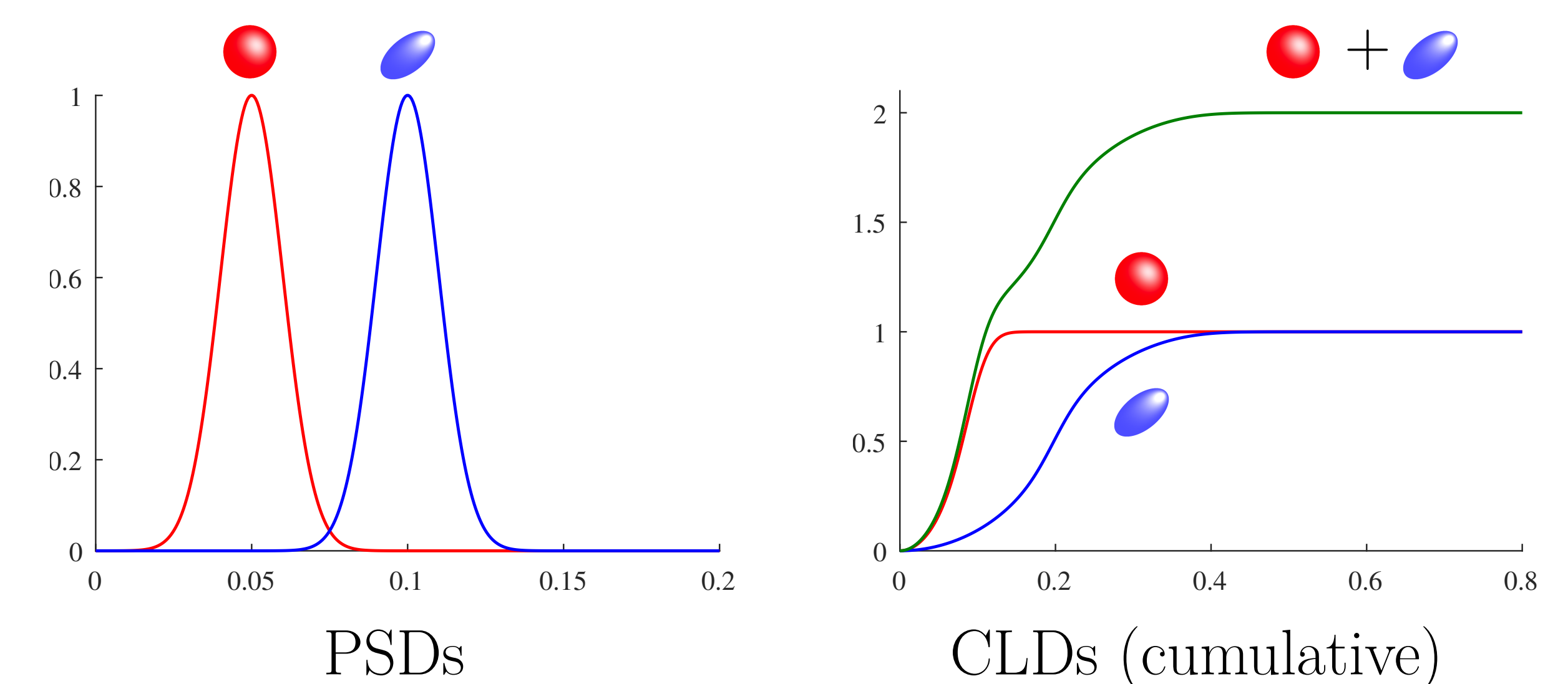
Challenges: The PSD/CLD relation depends on particle geometry; multiple shapes may coexist in the suspension.

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

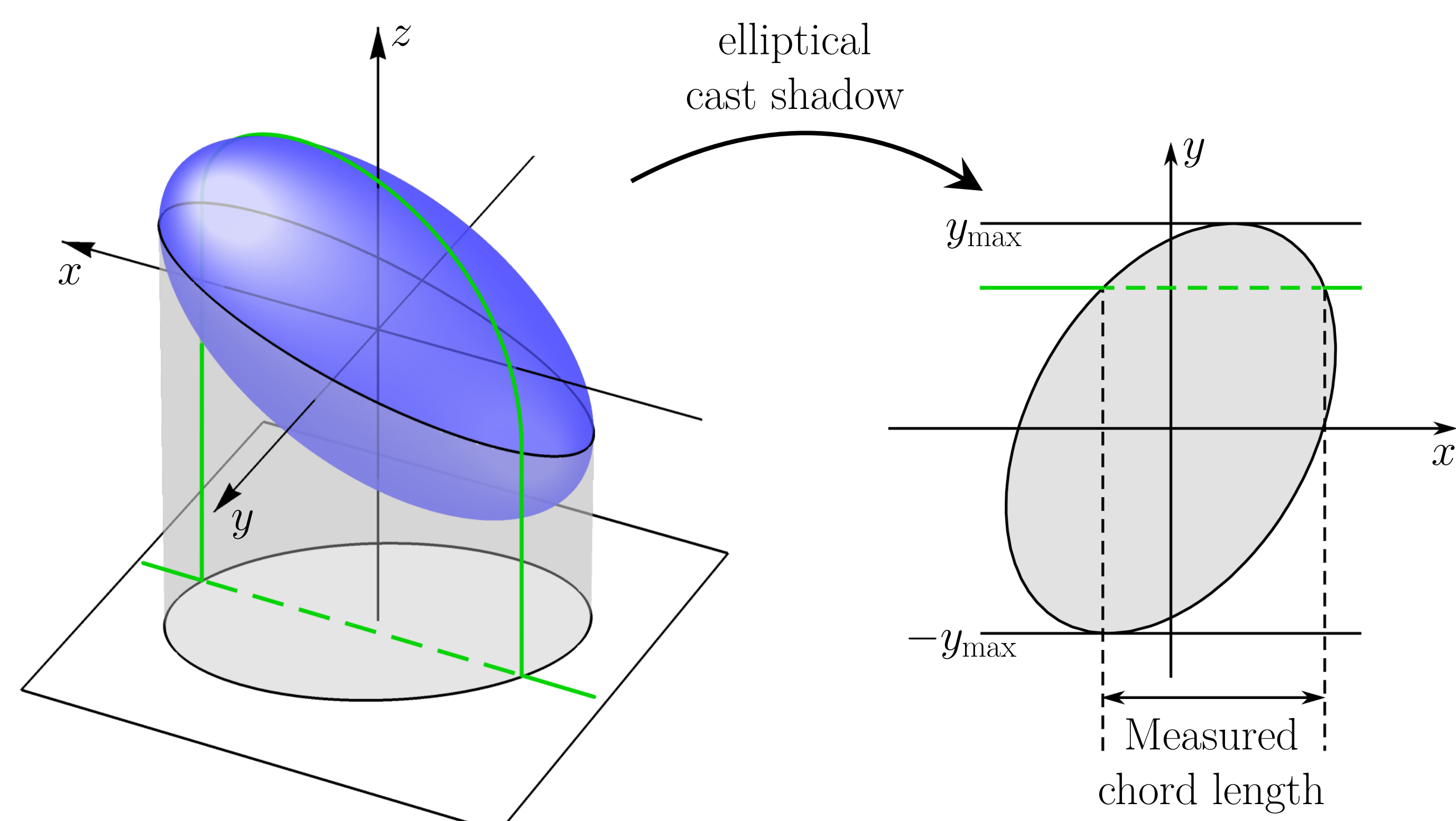


Multi-shape CLD-to-PSD challenge

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:

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

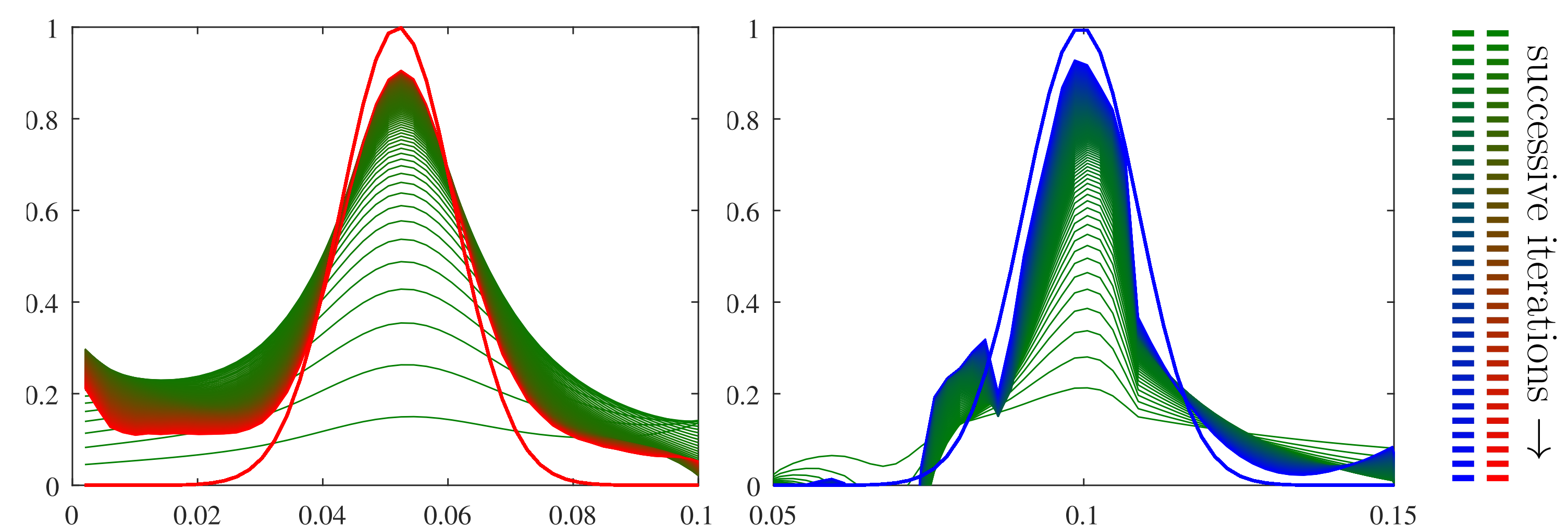
Results with Back and Forth Nudging

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).