

Supporting Information

CrystalCV: A Computer Vision System for Analysis of Crystallization Experiments

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Algorithm S1: Centroid tracking algorithm as implemented in CrystalCV. Adapted from [1]

Require: Set of existing object centroids \mathcal{O}_{t-1} , Set of new detections \mathcal{D}_t , Max disappearance frames τ_{max}

Ensure: Updated set of tracked objects \mathcal{O}_t

- 1: $\mathcal{O}_t \leftarrow \mathcal{O}_{t-1}$
- 2: Let C_{new} be the set of centroids computed from \mathcal{D}_t
- 3: **if** \mathcal{O}_t is empty **then**
- 4: **for** each centroid $c \in C_{new}$ **do**
- 5: Register new object with ID k and centroid c
- 6: **end for**
- 7: **else**
- 8: Let C_{old} be the centroids of objects in \mathcal{O}_t
- 9: Compute distance matrix D where $D_{i,j} = dist(C_{old}[i], C_{new}[j])$
- 10: {Find the optimal assignment of old to new centroids}
- 11: Rows, Cols \leftarrow linear_assignment(D)
- 12: {Update all matched objects immediately}
- 13: **for** each (r, c) in (Rows, Cols) **do**
- 14: Update object r with new centroid $C_{new}[c]$
- 15: Reset disappearance counter for object r
- 16: **end for**
- 17: {Identify unassigned indices based on matrix dimensions}
- 18: $U_{rows} \leftarrow \{i \mid i \notin Rows\}$
- 19: $U_{cols} \leftarrow \{j \mid j \notin Cols\}$
- 20: {Handle lost objects}
- 21: **for** each $r \in U_{rows}$ **do**
- 22: Increment disappearance counter for object r
- 23: **if** counter $> \tau_{max}$ **then**
- 24: Deregister object r from \mathcal{O}_t
- 25: **end if**
- 26: **end for**
- 27: {Register new objects}
- 28: **for** each $c \in U_{cols}$ **do**
- 29: Register new object with next available ID and centroid $C_{new}[c]$
- 30: **end for**
- 31: **end if**
- 32: **return** \mathcal{O}_t

Crystallization methods

MAPbBr₃ and CsPbBr₃ crystallizations shown in case studies 1 and 2 were performed by the FRC method detailed in [2]. MAPbBr₃ solution was prepared by dissolving MAPbBr₃ in DMF. CsPbBr₃ solution was prepared by dissolution in DMSO. Then, solution was poured into a crystallization dish (diameter, 100 mm) after filtration with a 0.22 μm PTFE filter. A hydrophobically treated cover slip was placed in the dish to create a flat bottom. The dish was placed on a hotplate set to 50°C for MAPbBr₃ and 80°C for CsPbBr₃. The growth rate of the main crystal was controlled by the FRC camera system coupled with a syringe pump for additional solvent infusion.

FAPbI₃ crystallization shown in case study 3 was performed by the SC-ITC method described in [3]. Thin single crystals were grown in ambient air via space-confined inverse temperature crystallization (ITC). 1 mL of MAPbI₃ in GBL was sandwiched between two treated substrates preheated to 60 °C. The temperature was gradually ramped to 90 °C.

Figure S1: FRC System schematic. Reproduced from [2]

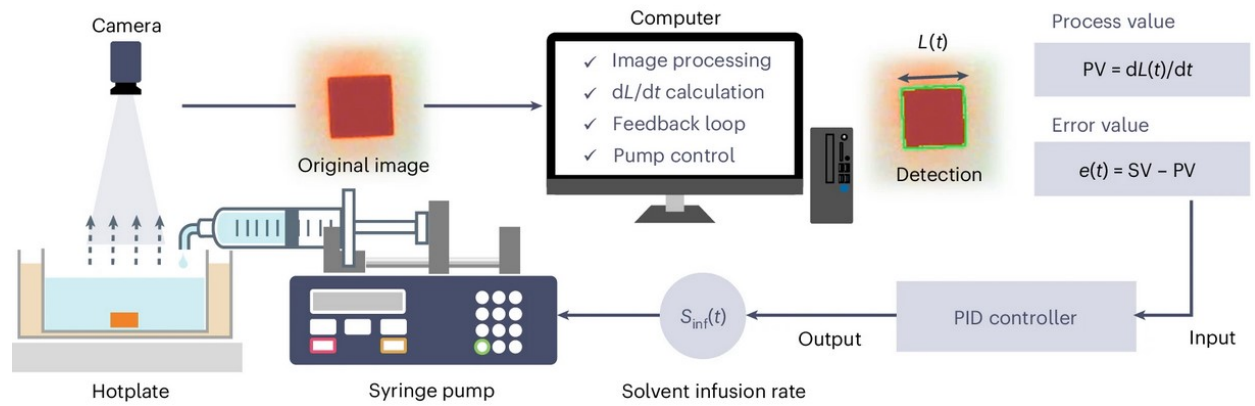


Figure S2: Case Study 1 Postprocessed Growth Rate Tracking Results

Showing only cases where >1 crystal was present.

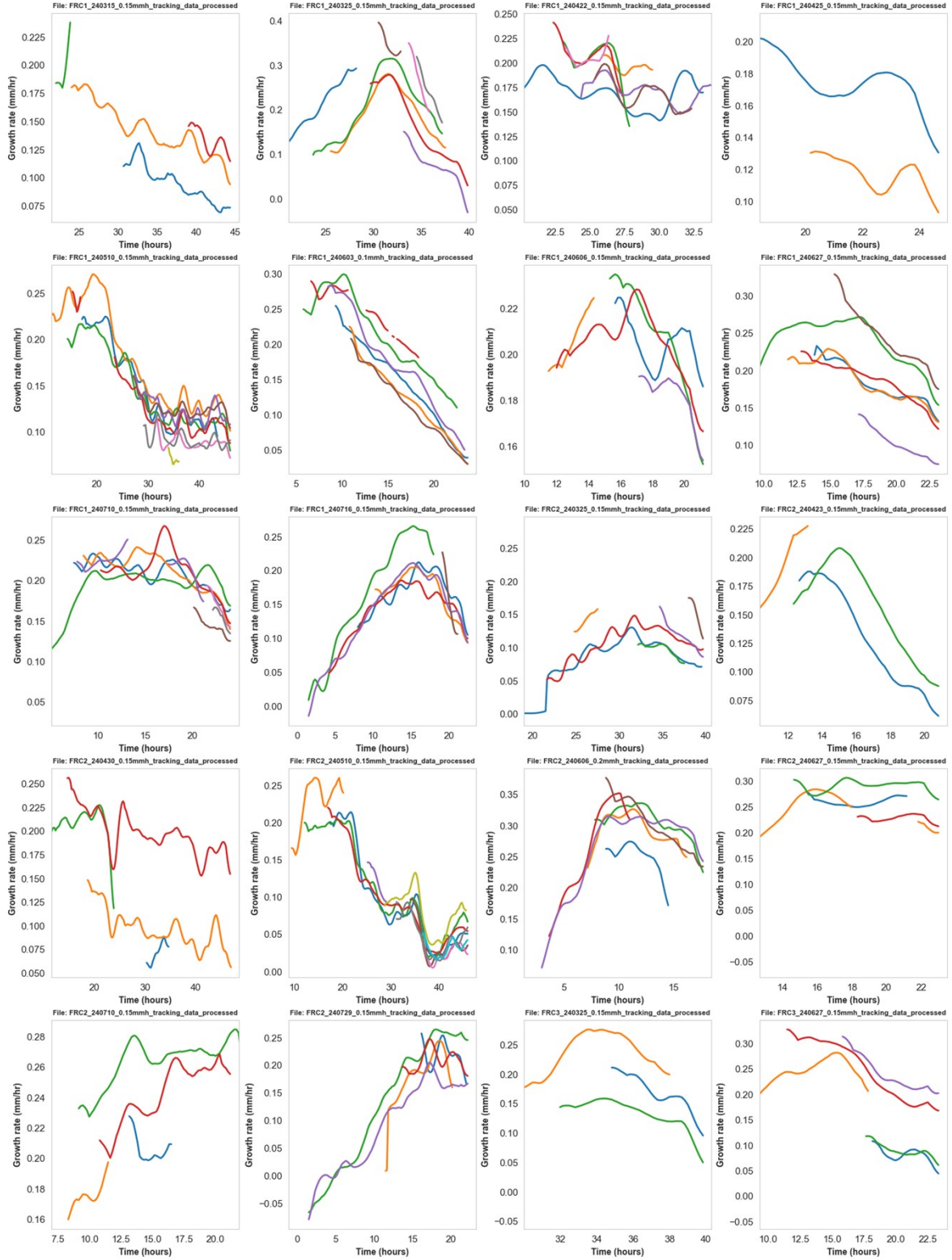
MAPbBr₃







CsPbBr₃



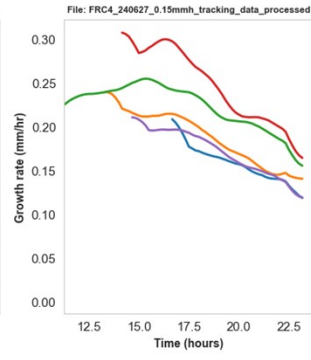
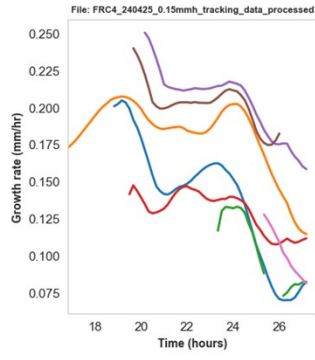
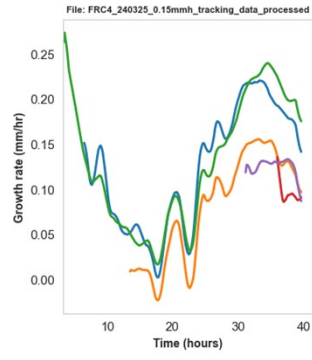


Figure S3: Manual Accuracy Verification for Case Study 2

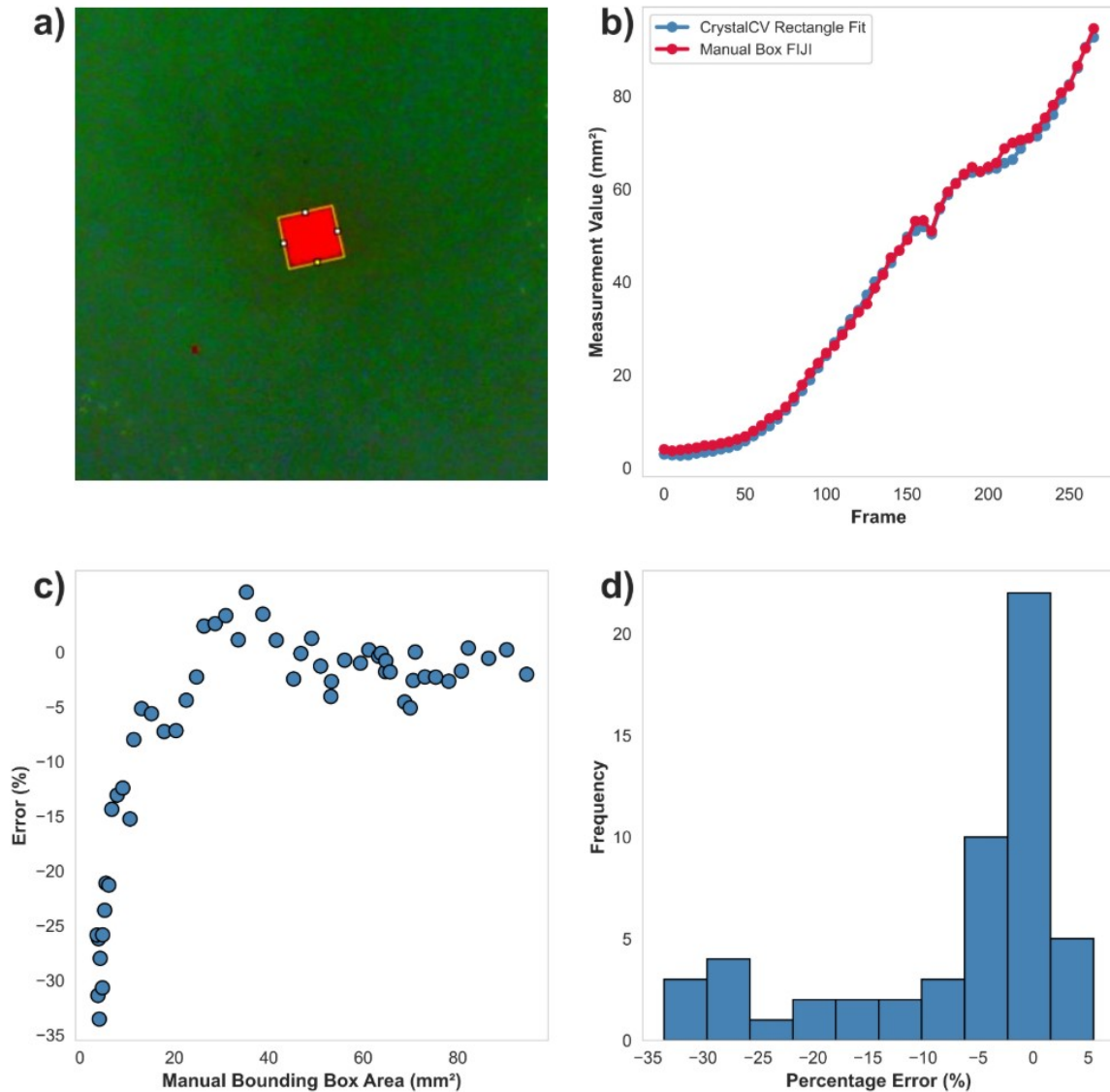


Figure S3: a) Manual bounding box tracing of Crystal ID 1 in thermal cycling experiment performed using FIJI [4]. b) Manual (red) vs CrystalCV area measurements for every 5th frame in thermal cycling experiment video. c) Percentage error vs manually verified error. d) Histogram of percentage errors for full video sequence.

Due to the highly tunable nature of the segmentation method used in *CrystalCV*, establishing a single baseline for accuracy is challenging as it relies on the quality of the lighting and camera setup, as well as the specific choices in image enhancement and segmentation. Here an example of the achievable accuracy is presented for case study 2.

Every 5th frame of the thermal cycling crystallization video sequence was manually analyzed using FIJI [4], with the area of a manually determined bounding box around the crystal with index '1' measured as shown in figure S3(a). The resulting area vs frame plot for the manual and *Crysta/CV* method is shown in figure S3(b). Measuring the percent error between *Crysta/CV* and the manual method and plotting it against the true size of the bounding box as shown in figure S3(c), we see that errors in this specific case study rapidly increase for crystal areas below 10 mm². This is likely due to the fact that segmentation becomes challenging around the edges of the crystals, and for smaller crystals these edge regions represent a larger fraction of the total area. Figure S3(d) shows a histogram of the percentage error values for the entire experiment, which can be seen to be broadly clustered below 10% with a tail due to the aforementioned difficulty in segmenting small crystals.

The error values shown in manuscript figure 4 were calculated as follows: Considering all crystal areas shown in figure 4(c) and 4(d) are >10 mm², the mean absolute percentage error for all crystals above that size, calculated as 2.86%, is used for the error intervals. For the elimination threshold shown in figure 4(e), the relevant claim is about small crystals, so the worst-case error of 33.54% for very small crystals is used.

Table S1: Comparison with other techniques:

Reference	Target environment	Tracking Scope	Persistent tracking of multiple crystals?	Methodology
[5]	Turbulent Crystallizer	Bulk population statistics (Size)	No (Snapshot distributions)	Deep Learning
[6]	Turbulent Crystallizer	Bulk population statistics (Size, Polymorph)	No (Snapshot distributions)	Deep Learning
[7]	Single-crystal growth cell	Single crystal (facet growth rates)	No (1 crystal only)	Classical
[8]	Single-crystal growth cell	Single crystal (facet growth rates)	No (1 crystal only)	Deep Learning
CrystalCV	Lab-scale crystallization experiments	Single crystals (growth rates) and bulk statistics (size, aspect ratio)	Yes (n-crystals, persistent)	Classical

References

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