

COSEDA: An open-source pipeline for continuous serial electron diffraction data analysis

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Continuous Serial Electron Diffraction (SerialED) is a powerful method for determining the atomic structure of nanometer-sized, beam-sensitive crystals by recording thousands of diffraction patterns while scanning the sample under a fixed, parallel nanobeam using only stage motion. This approach eliminates the need for specialized beam scanning setups and relies solely on standard TEM hardware, making it highly accessible across different microscopy platforms. [1]

We present COSEDA, an open-source, Python-based data processing suite specifically designed for continuous SerialED. The software provides a complete pipeline from raw diffraction patterns to an integrated reflection dataset, incorporating Bragg spot detection, beam center finding, indexing, integration, and merging. These routines are adapted from XFEL data analysis but modified to account for the characteristics of continuous SerialED data. COSEDA is optimized for parallel processing, enabling efficient handling of large datasets with tens of thousands of patterns.

To improve usability and lower the barrier to adoption, COSEDA includes a lightweight graphical user interface (GUI) that ties the processing workflow together. This GUI enables users to launch jobs, adjust parameters, and visualize diagnostic outputs in real time, all without requiring scripting experience. Advanced users can still access the full functionality programmatically, allowing seamless integration into custom workflows.

The method has been successfully applied to a broad range of samples—including protein nanocrystals, hybrid perovskites, metal-organic frameworks (MOFs), and covalent organic frameworks (COFs)—demonstrating its versatility. Several datasets were processed independently by new users with minimal guidance, underscoring the method's accessibility and reproducibility.

A beta version of COSEDA is available under an MIT open-source license. [2]

[1] Hofer, G., Wang, L., Pacoste, L., Hager, P., Fonjallaz, A., Williams, L., ... Zou, X. (n.d.). Continuous Serial Electron Diffraction for High Quality Protein Structures. Retrieved from <https://urn.kb.se/resolve?urn=urn:nbn:se:su:diva-241602>

[2] Hager, P. *COSEDA: Continuous Serial Electron Diffraction Analysis Software*, GitLab repository. Available at: <https://gitlab.com/kristallorakel/coseda>

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