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A machine learning-empowered automatic loop centering software tool for macromolecular crystallography beamlines

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Synchrotron light source facilities worldwide are evolving into the fourth generation, equipped with diffraction-limited storage rings. These machines generate high quality X-rays with intense brightness, low emittance, ultrafast pulse, and highly coherent beams, offering extreme spatial and temporal resolving power that enables multiscale and ultra-fast characterizations. Consequently, the experimental mode at next-generation beamlines is shifting from static to high-throughput, multimodal, cross-dimensional and dynamic characterizations, greatly facilitating significant scientific outputs. However, regardless of instrumentation advancements, the development of software and algorithms is still lagging behind, becoming the limiting factor to fully unleash the capabilities these facilities have to offer. Cutting-edge light source facilities desire cutting-edge software and algorithms to complement, particularly in key areas such as autonomous beam adjustment and experiment control, intelligent experimental steering and scanning path prediction, data acquisition and orchestration, data analysis and interpretation. Today, we are entering the "fourth paradigm"driven by big data, where artificial intelligence (AI) and machine learning plays a crucial role in advancing scientific discovery (AI for Science). Integrating advanced machine learning techniques into a universal large-scale scientific software system designed for next-generation synchrotron facilities, can ultimately solve the limitations on the software end. This talk first briefly presents our latest effort to develop such large-scale software system (Mamba) designed for China's first fourth-generation light source; then the talk will introduce our recent work on machine learning-empowered automatic loop centering process using SwinTransformer with YOLO object detection models, which is designed for macromolecular crystallography (MX) beamlines. This subject is influential to reduce the man power and labor manually conducted at MX beamlines if one needs to align the X-ray beam with the sample, especially when there exist multiple samples on a single sample plate. The centering process is divided into two stages: automatic loop detection and intelligent crystal recognition. We are integrating the centering process into the software system Mamba with a graphical user interface (GUI) to streamline the centering process at MX beamlines, forming a dedicated software tool to beamline users with detailed operation tutorials provided. Our most recent developmental progress on the centering procedures and the software tool will both be reported. We hope this talk will facilitate inter-institutional cooperation on the development of machine learning-empowered autonomous experiment control system, particularly on those systems relying on automatic and intelligent machine learning object detection and recognition techniques at photon and neutron (PaN) large scale facilities.

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