Contribution ID: **76** Type: **Poster**

Artificial intelligence methods for synchrotron radiation image and diffraction data analysis

Tuesday, 9 April 2024 18:30 (20 minutes)

High-energy synchrotron radiation (SR) light sources provide precise and deep insights that have been driving cutting-edge scientific research and innovation in a wide range of scientific fields. High Energy Photon Source (HEPS) is one of the fourth-generation SR light sources and the first one in China. With the advantage of high energy and ultra-low emittance, HEPS will provide more sensitive, finer and faster experimental tools to observe the complex samples and collect multidimensional, real-time and in-situ information at the molecular, atomic, electronic, and spin levels. Along with those advanced techniques, HEPS will generate about 1 petabyte of high-dimensional and complex data per day. Therefore, it is an urgent key scientific and technical challenge to develop artificial intelligence (AI) analysis methods to automatically and efficiently deal with SR data. To address this urgent need and challenge, our researches focus on developing AI analysis methods for SR image and diffraction data. First, regarding image data, we implement a novel localization quantitative analysis method based on deep learning to analyze X-ray nano-computed tomography. We achieve localization quantitative three-dimensional imaging analysis of single-cell HfO2 nanoparticles and demonstrate the notable effect of the nanoparticles in tumor treatment. Our approaches show the potential to explore the localization quantitative three-dimensional distribution information of specific molecules at the nanoscale level. Second, regarding diffraction data, we develop two sets of data-driven and physics-knowledge-driven machine learning (ML) methods to analyze the X-ray diffraction and extract three-dimensional orientation information of nanofibers. The data-driven ML model achieves high accuracy and fast analysis of experimental data and is available to be applied in multi light sources and beamlines. The physics-knowledge-driven ML method enables high-precision, self-supervised, interpretable analysis and lays the foundation for systematic knowledge-driven scientific big data analysis. Overall, our work aims to analyze high-energy SR data quickly and accurately in real-time through advanced AI algorithms, which support AI for SR-based Science strongly.

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Session Classification: Posters

Track Classification: MLC