MLExchange, bringing machine learning to the beamline*

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Abstract

The scientific user facilities (SUF) of the Department of Energy (DOE) are some of the world's largest producers of scientific data from experiments, modeling, and simulation in the world. The data generated span multidisciplinary sciences covering multi-faceted and complex interactions that require domain expertise to decipher intricate relationships within natural phenomena. There is tremendous potential in coordinating complex data analysis. This can aid in building, optimize use of experimental facilities, increase transparency, and widen the pool of available knowledge. As it is now, each experimentalist gathers data and scientific insight into a small part of complex physical phenomena. Restricted to limited pools of scientific data or summarized content of formal publications, intricate relationships are lost. Machine learning and artificial intelligence promises ready-to-use approaches to solve complex problems and accelerate data analysis and knowledge extraction. Driven by industry, machine learning frameworks are being developed at rapid speed. However, the applications in science and in particular the world of scientific user facilities is less evolved. The threshold to develop, train, and test machine learning models is still very steep and requires significant time commitment by beamline scientists. MLExchange is targeting this threshold with the development and deployment of easy-to-use solutions that target science performed at SUF's. We will present our first developments in the field of labeling, segmentation, and XRD.

* Title and Abstract of an Invited Presentation at the Workshop: AI/ML for Particle Accelerator, X-Ray Beamlines and Electron Microscopy at Argonne National Laboratory, November 1-3, 2021.