Contribution ID: **46** Type: **Talk**

Adaptive X-Ray Reflectivity Measurements using Deep Reinforcement Learning

Monday 8 April 2024 09:50 (20 minutes)

This presentation focuses on the application of machine learning techniques, specifically deep reinforcement learning, to improve the process of X-ray reflectivity (XRR) measurements. Our study demonstrates how machine learning can be utilized to dynamically adjust measurement angles and integration times, adapting these parameters after acquisition of each new datapoint to optimize the information gathered about the sample.

In our approach, a diffractometer is simulated within a virtual environment including the simulation of the scattering process but also including motor movement times. Here, a machine learning agent is trained to select data points in a smart and adaptive manner, using information from previous simulated measurements to inform its decisions. The agent is designed to prioritize the speed of measurements and accuracy, receiving rewards for achieving quicker measurements and reducing the error in predicting the layer parameters from the measured curve. Once trained, this agent then is used to steer a real laboratory diffractometer via the BLISS (ESRF) control software. The key outcome of this research is a significant increase in measurement efficiency. Our findings indicate that using this machine learning approach one can easily speed up the measurement process by at least a factor of two, and also reduce measurement errors. The "self-driving diffractometer"using a reinforcement learning agent presents an advancement not only for XRR measurements, but the results also apply to many X-ray and neutron scattering experiments using angular scans.

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Session Classification: Session 1

Track Classification: MLC