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First Demonstration of AI-assisted automation of single crystal neutron diffraction¹ LEAH ZIMMER, St. Norbert College, ERXI FENG, ZACH MORGAN, HUIBO CAO, Neutron Scattering Division, Oak Ridge National Laboratory — Single-crystal neutron diffraction experiments can provide insight into a material’s atomic structure and the origin of a material’s properties. Current methods of analyzing data from these experiments rely on Bragg peak recognition, signal extraction and multiple codes’ executions. This type of analysis is time-consuming and inefficient. Automated real-time analysis of the images and a common coding language would greatly increase the efficiency of single-crystal neutron diffraction experiments. We present the first demonstration of machine-learning-assisted automated single-crystal neutron diffraction experiments at Oak Ridge National Laboratory. Real-time analysis will optimize the use of neutron beam time and more precisely reduce the data. We plan to integrate our demonstration into real-time analysis methods which will become the new analysis standard at the neutron-scattering user facility at Oak Ridge National Laboratory.

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