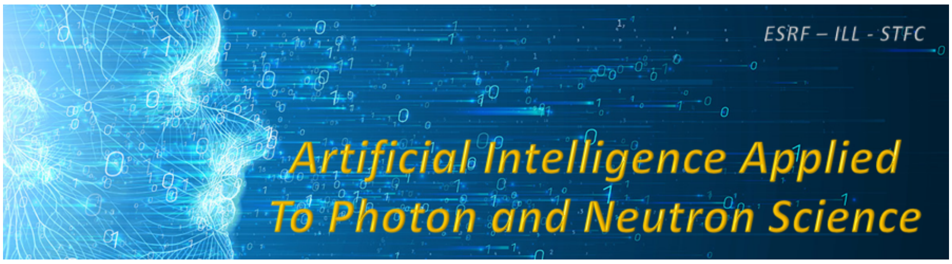

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Machine Learning for accelerating understanding from Neutron Scattering Data

Wednesday, 13 November 2019 16:00 (25 minutes)

In many cases obtaining results from a neutron scattering measurement is solving an inverse problem. Often this problem is solved by time consuming random guessing. However there may be hidden relationships between the model and the data that can be identified by machine learning to accelerate the solution process. A particularly powerful case has been demonstrated for systems with classical magnetic Hamiltonians. Here, using the computational resources of the Oak Ridge Leadership Computing Facility, a network has been trained off simulations of the resulting scattering from Hamiltonians with multiple exchange parameters. Then the network is applied to 3D magnetic diffuse scattering or 4D magnetic spectroscopy data sets acquired from the instruments at ORNL. This network has quickly identified the regions in the vast parameter space requiring greater scrutiny. When additional data is added, (in this case from specific heat measurements) the region of parameter space is further reduced. Similar inverse problem solutions that are less computationally intense, have been demonstrated with SANS and Reflectometery data. More generally systems with itinerant moments can be computationally intensive to model, however using machine learning to search for connections inside the computational model can allow for quicker evaluation of the S(Q,w) and may also open other routes to theoretical understanding of the model systems.

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