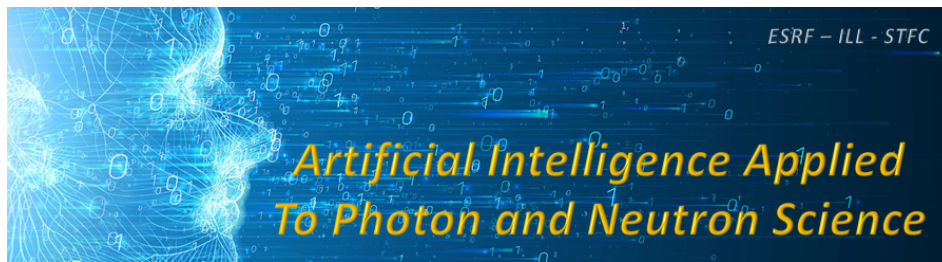


## Artificial Intelligence Applied to Photon and Neutron Science



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# Scientific Machine Learning Benchmarks

*Wednesday, 13 November 2019 15:15 (25 minutes)*

The use of artificial intelligence (AI) technologies, and of deep learning neural networks in particular, is already having a major impact on many aspects of our lives. The challenge for scientists is to explore how these technologies could have a similar impact for scientific discovery. Already Google DeepMind's AlphaFold tool has achieved some impressive results for protein folding predictions.

The Scientific Machine Learning (SciML) Group at the Rutherford Appleton Laboratory in the UK is focused on applying a range of AI technologies, including deep learning, to scientific data generated by the large-scale scientific experimental facilities on the Harwell site. The SciML group is therefore working with researchers at the Diamond Light Source, the cryo-Electron Microscopy facility, the ISIS Neutron and Muon Source, the Central Laser Facility (CLF) and the Centre for Environmental Data Analysis (CEDA).

This talk will share some initial experiences of our 'AI for Science' explorations in collaboration with the UK's Alan Turing Institute. The talk will then focus on the development of a AI-centric benchmark suite specialised for scientific applications. We believe that such a benchmark suite will help scientists map out the suitability of different AI techniques for different scientific problems. Research into the robustness of results from machine learning technologies as well as on uncertainty quantification will be important to gain confidence into the reliability and understandability of these techniques.

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**Session Classification:** Afternoon 1