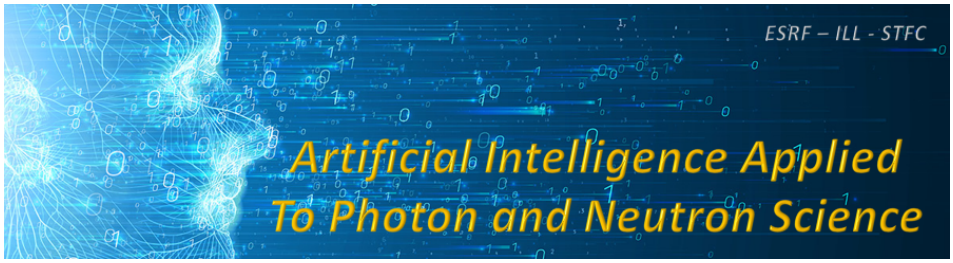

Contribution ID: **124** Type: **not specified**

Towards automated analysis for neutron reflectivity

Wednesday, 13 November 2019 17:40 (25 minutes)

The current workflow of neutron (and x-ray) reflectivity requires human intervention at almost every stage, from data capture, through data reduction, and into data analysis. While some of these steps necessitate expert knowledge and judgement, being able to remove the ones which do not remains a goal, enabling on experiment feedback for the system being measured, and lowering the barrier to fully analysed data for expert and beginner alike.
We have been investigating the application of machine learning methods to model selection in neutron reflectivity, starting from simple metrics like cosine similarity and working up to complex deep or convolutional neural networks. We present here our journey, and lessons learned, with everything from data representation, to optimising network architectures and the difficulties associated with them all.
Our work enables a generalised reflectivity input (R vs. Q) to be fed into the network, which predicts a scattering length density profile for the sample, then outputs that information into fitting software. Both input priors and output uncertainty are dealt with through a variety of methods. We discuss the implementation of both of these features.

Presenter: Dr MIRONOV, Daniil (STFC)

Session Classification: Afternoon 2