



Contribution ID: 164

Type: **Talk**

Towards Reflectivity profile inversion through Artificial Neural Networks

Thursday, 10 December 2020 16:30 (15 minutes)

The goal of Specular Neutron and X-ray Reflectometry is to infer materials Scattering Length Density (SLD) profiles from experimental reflectivity curves. This talk will focus on describing an original approach to the ill-posed non-invertible problem which involves the use of Artificial Neural Networks (ANN). In particular, the numerical experiments to be described deal with large data sets of simulated reflectivity curves and SLD profiles, whose aim is to assess the applicability of Data Science and Machine Learning technology to the analysis of data generated at large scale facilities. In fact, under certain circumstances, properly trained Deep Neural Networks are capable of correctly recovering plausible SLD profiles when presented with never-seen-before simulated reflectivity curves. A proper inclusion of such an approach within current data workflows would be able to offer two main advantages over traditional fitting methods when dealing with real experiments, namely, 1. no prior assumptions about the sample physical model are required and 2. the times-to-solution could be shrank by orders of magnitude, enabling faster batch analyses for large datasets.

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Session Classification: DN2020: Digitalization and Machine Learning

Track Classification: DN: Digitalization and Machine Learning