Contribution ID: **18** Type: **not specified**

Using Generative Adversarial Networks to match experimental and simulated inelastic neutron scattering data

During the past decades, research in materials science has been accelerated by the rapid development of synchrotron and neutron sources.1 Conventional data analysis approaches using minimization techniques, such as least-squares fitting algorithms, cannot keep up with the amount of increasing size of measured datasets. Consequently, data analysis is becoming a bottleneck for research in materials science.2, 3 Therefore, it is of great importance to improve the current state-of-art for data analysis for materials science, particularly utilizing recent developments in artificial intelligence and machine learning (ML).2-4 One of the unsolved problems in this context is to match the simulated datasets that the ML algorithms are trained on to the experimental datasets. This has particularly been a problem for the analysis of inelastic neutron scattering (INS), where it is computationally expensive to ensure that simulated data correctly mimics the experimental signal and background.5 In our project, we are attempting to improve this state through better ML for helping us effectively analyse neutron datasets. More specifically, we are developing generative adversarial networks (GANs) that can learn to make simulated INS data that matches experimental INS dataset under a second. This GAN-based approach, once trained, will be deployed in a range of scenarios for analysing and understanding INS dataset. It can be used to help classify materials structures from the INS datasets and to work with other ML and non-ML (e.g. Spin-W6) algorithms which can estimate magnetic Hamiltonian parameters from INS data. Furthermore, the aim is to expand the algorithm to also match simulated and experimental datasets for other techniques than INS.

References

1. Wang, C.; Steiner, U.; Sepe, A., Synchrotron Big Data Science. Small 2018, 14 (46), e1802291.
2. Agrawal, A.; Choudhary, A., Perspective: Materials informatics and big data: Realization of the "fourth paradigm" of science in materials science. APL Materials 2016, 4 (5), 053208.
3. Butler, K. T.; Davies, D. W.; Cartwright, H.; Isayev, O.; Walsh, A., Machine learning for molecular and materials science. Nature 2018, 559 (7715), 547-555.
4. Hey, T.; Butler, K.; Jackson, S.; Thiyagalingam, J., Machine learning and big scientific data. Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences 2020, 378 (2166), 20190054.
5. Butler, K. T.; Le, M. D.; Thiyagalingam, J.; Perring, T. G., Interpretable, calibrated neural networks for analysis and understanding of inelastic neutron scattering data. J. Phys.: Condens. Matter 2021, 33 (19), 194006.
6. https://spinw.org/

Primary authors: Mr ANKER, Andy Sode (Department of Chemistry, University of Copenhagen, 2100 Copenhagen Ø, Denmark); Dr BUTLER, Keith Tobias (Scientific Computing Department, Rutherford Appleton Laboratory, OX11 0QX Harwell, United Kingdom); Dr LE, Duc (ISIS Neutron and Muon Source, Rutherford Appleton Laboratory, OX11 0QX Harwell, United Kingdom); Dr THIYAGALINGAM, Jeyan (Scientific Computing Department, Rutherford Appleton Laboratory, OX11 0QX Harwell, United Kingdom)

Presenter: Mr ANKER, Andy Sode (Department of Chemistry, University of Copenhagen, 2100 Copenhagen Ø, Denmark)

Session Classification: Poster session