



Science and
Technology
Facilities Council

Ada Lovelace Centre

Contribution ID: 5

Type: **not specified**

Biology Highlight - Modernising Macromolecular Diffraction Analysis with DIALS and DiffraView

Thursday, 19 June 2025 11:40 (20 minutes)

Speaker: David McDonagh

Macromolecular diffraction analysis is now a mature field with established (X-ray) and newer (neutron, electron) communities. These communities have historically developed separately, with distinct software, despite significant overlap in the problems being addressed. This no longer reflects the needs of the modern researcher, as it is now increasingly common for users to have diffraction data from multiple sources. Additionally, recent years have seen significant disruptions to the field, such as machine learning and cloud services impacting how diffraction analysis can be done, and STFC Net Zero targets presenting an imminent challenge to a field rapidly expanding to higher throughput. Here I will show how the DIALS software package is being expanded to address these challenges, including enabling polychromatic sources in DIALS, a new way of visualising data in the browser with DiffraView, and how machine learning methods can be embedded to help improve results and computational efficiency.