Ada Lovelace Centre - Scientific Computing Showcase event

Ada Lovelace Centre

Report of Contributions

https://indico.stfc.ac.uk/e/1554

Contribution ID: **3** Type: **not specified**

Materials Highlight - Machine learned interatomic potential for high-throughput phonon calculations of metal-organic frameworks

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

Speaker Alin-Marin Elena
 Join via Zoom: https://ukri.zoom.us/j/92256378528

Metal-organic frameworks (MOFs) are promising materials for applications like carbon capture, but predicting their phonon-mediated properties (e.g., thermal expansion, mechanical stability) is difficult using traditional DFT due to their complex structures. Existing machine learning models, such as MACE-MP-0, accurately predict MOF structures but fall short on phonon properties.

We have developed MACE-MP-MOF0, a fine-tuned machine learning model, and a new workflow to address this. Trained on a diverse dataset of 127 MOFs, MACE-MP-MOF0 significantly improves phonon density of states accuracy and corrects imaginary phonon modes, enabling precise, high-throughput phonon calculations. The model successfully predicts thermal expansion and bulk moduli consistent with DFT and experimental data, demonstrating its potential for guiding MOF design in energy storage and thermoelectrics.

Contribution ID: **4** Type: **not specified**

Maths highlight - Reducing acquisition and dose in spectral imaging

Thursday, 19 June 2025 11:00 (20 minutes)

Speakers: Maike Meier & Lorenzo Lazzarino
 Join via Zoom: https://ukri.zoom.us/j/92256378528

Spectro-microscopy is an experimental technique used to understand differences in chemical state across a sample. This can, for example, be used to understand changes variations across a battery material, corrosion near an an interface or the location ad state of drugs within a cell.
While this is a powerful method, the technique is often limited by factors such as long acquisition times and radiation damage. Here we present two data driven measurement strategies that exploit properties of the experimental data to significantly shorten experiment times and doses applied, in some cases reducing the amount of data required for a measurement to less than 5% of a conventional measurement.

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.

Contribution ID: **6** Type: **not specified**

Engineering Highlight - A Particle-in-Cell Study of Space Charge Compensation for ISIS H- Ion Sources

Thursday, 19 June 2025 13:00 (20 minutes)

Speaker: Benzi John
 Join via Zoom: https://ukri.zoom.us/j/92256378528

Negative hydrogen ion sources are extensively used in particle accelerators worldwide for a variety of applications (e.g. for high-energy particle physics in CERN and in spallation neutron source facilities like ISIS) and also in magnetic fusion experiments utilising neutral beam injection for plasma heating and diagnosis. A typical problem encountered in the low energy beam transport (LEBT) region of particle accelerators is beam divergence and transport losses due to space charge effects. Space Charge Compensation (SCC) is a process that lowers the space charge of the ion beam and helps to minimise transport losses. The SCC occurs when the H- beam ionises the background gas and traps positive ions to the beam potential forming a peculiar low-density "beam-plasma". An experimental-simulation campaign is currently underway jointly with the ISIS Low Energy Beam Group to study the space charge compensation process to support operations and upgrades to the facility in the negative H- ion source region. High-fidelity particle-in-cell (PIC) simulations considering a multi-reaction framework have been used to investigate the SCC process for a range of operating conditions using the open-source PIC code, PICLas. The effect of key parameters, such as external magnetic fields, secondary electron emission, and boundary conditions on the space charge compensation time and degree, are being investigated. Simulation results will be compared to diagnostic data from experiments to correlate the beam transport and light emissions with the space charge compensation process.

Contribution ID: **7** Type: **not specified**

Platforms highlight - The Ada platform for data analysis

Thursday, 19 June 2025 13:20 (20 minutes)

Speaker: Jeremy Spencer
 Join via Zoom: https://ukri.zoom.us/j/92256378528

The Ada platform, formerly, Data-Analysis as a service, connects scientists to their data, the right analysis tools and the appropriate computing resources to support their science.
It already plays a vital role at CLF and ISIS, supporting experimental science and is being increasingly used to deliver training activities.
Here we will provide an overview of the platform and some of the new developments which are coming online to meet new needs and challenges.

Contribution ID: **8** Type: **not specified**

AI Highlight -Learning Fully Semantic Representations across 1D, 2D, and 3D Scientific Data

Thursday, 19 June 2025 13:40 (20 minutes)

Speaker: Jaehoon Cha
 Join via Zoom: https://ukri.zoom.us/j/92256378528

Applying AI to the interpretation of scientific data often requires learning representations that are invariant to symmetries such as shifts, translations, and rotations. In this talk, I will present the Disentangling Autoencoder, an encoder–decoder framework designed to extract fully semantic and interpretable features from scientific data. The model is built on the principle that different symmetry transformations can be independently modeled and disentangled. Its architecture is easily adaptable to 1D, 2D, and 3D data, demonstrating its flexibility and generality. We validate the model on diverse datasets, including 1D optical absorption spectra, 2D protein and galaxy images, 4D-STEM data, and 3D crystal morphologies. The results show that the model enables interpretable representation learning and enhances downstream tasks such as classification, clustering, and semantic feature discovery across scientific domains.

Contribution ID: **9** Type: **not specified**

Ada Lovelace Centre - Year in review and next steps

Thursday, 19 June 2025 14:00 (20 minutes)

Contribution ID: **11** Type: **not specified**

Materials Highlight - Machine learned interatomic potential for high-throughput phonon calculations of metal-organic frameworks

Speaker Alin-Marin Elena
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Contribution ID: **12** Type: **not specified**

Maths highlight - Reducing acquisition and dose in spectral imaging