EPSRC CDT in Distributed Algorithms

PhD Project: Machine Learning to Identify Unique Events in Sparse Hyperspectral Datasets

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Project Description

This project has been developed by the University of Liverpool in partnership with STFC Hartree and Sivananthan Laboratories.

Many characterisation methods used in materials science and structural biology involve data intensive acquisitions that can be multi-dimensional in nature (3 spatial dimensions, time and any number of spectral bands). Often the limitation in the precision of the data analysis is the damage to the sample being investigated — for example, a protein structure being imaged in an electron microscope is often destroyed before enough signal is generated to form a high-resolution image. While each material being characterised optically, by X-rays, electrons, neutrons, or ions is in some way different from others, it must conform the well-established rules of chemistry — there are only a small number of possible atoms, crystal structure types and bonding mechanisms. By using existing structures that are more stable to the radiation being used to analyse them, we can provide a set of training data that could be used to interpret the much lower signals that are possible from the technologically more relevant, but thermodynamically less stable structures important for many current/future applications.

The goal of this PhD project is to investigate machine learning approaches that may permit images from stable materials, obtained from a wide variety of methods, to be used to increase the ability of methods such as hyperspectral imaging in electron microscopy and X-ray systems to observe thermodynamically unstable materials and processes on the atomic scale. Such advances have the potential to significantly impact the search for new personalized medicines, the development of new advanced energy storage systems, and our ability to directly see chemistry important for catalysing environmentally friendly processes.

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