Enhanced Information Retrieval from Electron Microscopy Data Using Advanced Computational Techniques

Dr. Ivan Lobato
The Rosalind Franklin institute
Didcot, OX11 0FA, UK- Oxford

Abstract

Recent advancements in electron microscopy technology have significantly enhanced our capability to capture multidimensional data, accumulating at rates of several terabytes per hour. This wealth of experimental data holds the potential to reveal intricate details about the sample, such as three-dimensional atomic positions, atomic compositions, and valence states. However, the complex interactions between electrons and the specimen, governed by quantum mechanics, obscure this critical information within the experimental data. To effectively extract this information, we need to employ several computational techniques.

In this presentation, I will first discuss the fundamental physics of image formation in an electron microscope. This discussion will include a quantum mechanics description of the electron-specimen interaction, the impact of microscope aberrations, and the effects of the detection process. This will be followed by an introduction to the open-source C++ CUDA program called MULTEM (available on GitHub), which facilitates fast and precise simulations of electron diffraction and imaging on NVIDIA GPUs. This program can perform these simulations approximately a hundred times faster than typical desktop CPUs.

Subsequently, I will demonstrate methods for processing experimental data to compensate for distortions that arise during the detection process. This includes employing machine learning for data restoration and traditional programming for data alignment. Finally, the presentation will explore how to utilize these corrected datasets with various algorithms to retrieve detailed information about the sample, thereby enhancing our understanding and capabilities in electron microscopy.