LiberTEM: An open software platform for pixelated scanning transmission electron microscopy

Weber, D.[1], Clausen, A.[1] and Dunin-Borkowski, R.[1]

[1] Forschungszentrum Jülich, Germany

Recently, pixelated detectors have been introduced for scanning transmission electron microscopy (STEM) with fields of view of 256 × 256 pixels and better, frame rates above 1000 frames per second, and exceptional dynamic range and radiation hardness. For the first time, such detectors allow efficient capture of complete frames of the scattered electron beam intensity for all scanned pixels. However, the resulting files are very large, already reaching 64 TB when scanning 1024x1024 pixels with 4096x4096 pixel detector resolution, the highest detector resolution available today.

Instead of changing settings or image forming conditions on the microscope and performing a new acquisition, such rich datasets can now be re-analyzed after acquisition, in order to extract new information about the sample. However, working with such files requires a paradigm shift in electron microscopy because storage and processing has to move from personal computers to more powerful processing infrastructure for interactive work on large scans.

Furthermore, open science requires that data and metadata generated during experiments can be accessed and supplemented during analysis. In order to achieve this goal, data formats should ideally be standardized and open, and processing algorithms should be documented and accessible, so that processing steps between raw data and results can be reproduced and analysed in detail. The use of undocumented file formats and the closed source nature of current software for electron microscopy are major obstacles to advances in electron microscopy and quantitative data analysis.

Currently, software support for pixelated detectors is still in its infancy, with image capture and basic analysis capabilities provided by vendors of detectors, and experimental data analysis scripts developed by individual users. The goal of the LiberTEM project is to combine the efforts of both the user community and willing vendors, in order to create full, open software support for pixelated STEM. A key aim is to establish a standardized file format with rich metadata for seamless data exchange, as well as a processing architecture that allows convenient interactive work on large files with very high throughput and scaling from personal computers to supercomputing infrastructure.

Within the framework of the LiberTEM project, we will apply collaborative, open development and standardization concepts, which are common and successful in large information technology infrastructure projects such as the Linux kernel, the Apache web server, and almost all programming languages, in order to address the challenges of interoperability and extensibility.

In this presentation, we will summarize the project, introduce the current status of a NeXus-based file format[1] for pixelated STEM, showcase the user-friendly interactive processing of large datasets with a lightweight local graphical user interface that controls a remote high-performance cluster backend, present future plans, and discuss how LiberTEM can best help our community.

References

[1] M. Konnecke, F. A. Akeroyd, H. J. Bernstein, A. S. Brewster, S. I. Campbell, B. Clausen, S. Cottrell, J. U. Hoffmann, P. R. Jemian, D. Mannicke, R. Osborn, P. F. Peterson, T. Richter, J. Suzuki, B. Watts, E. Wintersberger and J. Wuttke, "The NeXus data format," *J. Appl. Cryst.*, no. 48, pp. 301-305, 2015.

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 780487).