STEM

Development of Electron Microscopy Analysis and Simulation Tools for nanoHUB

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Electron microscopy has a crucial role in the field of materials science and structural biology. Although electron microscopy provides many important results and findings, additional simulations and image processing/reconstruction are required to obtain more information from the data collected from the experiments. For this purpose, researchers are using IMOD and QSTEM for electron microscopy analysis and simulation.

IMOD is a set of programs used for tomographic reconstruction and 3-D visualization, and QSTEM is used for quantitative simulations of transmission electron microscope (TEM) and scanning transmission electron microscope (STEM) images. However, IMOD and QSTEM are hard to install or use for beginners without advanced computational skills. To overcome this issue, online IMOD and QSTEM tools were developed. Both tools were built with the graphical interface builder Rappure toolkits available on the nanoHUB website (<https://nanoHUB.org>). The first tool, IMOD online (<https://nanohub.org/resources/imod>), enables electron tomography simulation. Users can apply this tool to reconstruct 3-D volume images using data from an electron microscope. The IMOD command line interface was replaced by a graphical interface. Moreover, hardware (memory, CPU) limitation is no longer an issue when using this tool on the nanoHUB website. The second tool, QSTEM online (<https://nanohub.org/tools/>

qstem), which enables TEM and STEM simulations, also contains atomic modeling functions. Users can construct an atomic model by specifying crystal structure. As of April 2015, both tools had supported more than 600 simulations by 58 users.

Research advisor Volkan Ortolan writes, "Electron microscopy has a critical role in the field of materials science and structural biology. However, fundamental understanding of material properties requires tools to explore them at the atomic scale in three dimensions. Mingxuan worked with great enthusiasm and dedication to develop online tools used for tomographic reconstruction and quantitative simulations of TEM/STEM images and made them ready to use and accessible to the world."

The images show the graphical user interfaces as well as two simulation results for IMOD online and QSTEM online.