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*ab*TEM: fast and flexible Python-based multislice simulation package for transmission electron microscopy

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Computer simulations have become an indispensable part of modern research, where careful comparison to theoretical models is often required to reliably interpret the data from experiments. The use of dynamical scattering simulations based on the multislice algorithm has, for several decades, been an invaluable aid for transmission electron microscopy (TEM) [1]. As a result, many excellent simulation codes exist; *ab*TEM is another one, but our approach differs in key aspects [2]. *ab*TEM is written exclusively in Python, making it easier for non-expert programmers to understand and extend the code.We show that the effective use of open-source libraries makes *ab*TEM highly competitive in terms of its performance compared to multislice codes based on compiled languages. The code uses NumPy arrays for CPU calculations and the NumPy-compatible CuPy arrays for fast GPU calculations, providing seamless integration with the full suite of tools in scientific Python and open-source electron microscopy packages, thus providing a single framework for simulation, analysis, and visualization. *ab*TEM is parallelized with Dask [3], which allows scaling the same code from a laptop to hundreds of nodes at high-performance computing facilities.

*ab*TEM is undergoing constant development and includes an expanding number of advanced algorithms. The code integrates directly with the GPAW density functional theory code for calculating electrostatic (or magnetic!) potentials that includes the effects of charge transfer due to chemical bonding [4]. A multi-GPU accelerated implementation of the PRISM algorithm allows efficient calculations of STEM images [5], and core-loss energy-filtered simulations are enabled by using GPAW to calculate ionization cross-sections for atoms of interest [6]. Most recently, we have been implementing the frequency-resolved frozen phonon multislice method of Zeiger and Rusz for simulating momentum-resolved phonon energy-loss spectra [7], and are working on the Pauli multislice method to simulate magnetic scattering based on first principles [8]. Preliminary results on both with live code examples will be shown during the seminar.
The code is openly available at https://github.com/abTEM/abTEM.

References:

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[8] Edström A., et al., *Phys. Rev. B* **94** (2016) 174414.

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