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Reimagining the Data-Driven Microscopy Paradigm

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Scanning / transmission electron microscopy (S/TEM) has grown to become a cornerstone of the physical and biological sciences, underpinning some of the most important discoveries about the nature of matter and the behavior of chemical systems. While decades of development have culminated in a powerful experimental platform, the *ad hoc*, disconnected nature of such development has multiplied the complexity of the microscope so that it is now often difficult to quickly and effectively extract knowledge across a full range of techniques. With the emergence of ultra-high-speed detectors for *in situ* experimentation, diffraction imaging, and spectroscopy, there is an urgent need to reevaluate how data is collected and analyzed. Hidden in this challenge is the opportunity for the community to radically rethink how experiments are planned, executed, interpreted, and shared.[1]

Here I will discuss our efforts to reimagine the microscopy paradigm, leveraging low-level system automation, domain-grounded data pre-processing, and emerging machine learning methods to rapidly extract statistical information from a variety of systems. As shown in Figure 1, the heart of our platform consists of a customizable automation application (AutoEM) that acts a centralized TEM controller. The application interfaces with instrument components, including the beam, stage, and various detectors, enabling remote, automated data collection, montaging, and predictive tilting. Data streams collected by AutoEM are pre-processed by a second application (Nanocartographer), which uses information about the stage orientation and sample to construct a detailed crystallographic map. In this way, it is possible to derive crystallographic features to act as signposts for automation. Finally, rapid and flexible feature classification can be performed in near-real-time using a customizable classification engine (WizEM) based on few shot machine learning. In contrast to other deep learning methods, few shot learning relies on generalized offline network pre-training, followed by online tailoring using aggressively augmented, limited training data. We show that few shot is highly adaptable and capable of classifying a range of features in noisy, incomplete data sets. Importantly, this approach scales favorably with additional data types and volumes, providing closed-loop feedback for autonomous decision making. I will discuss the current and future potential of this new paradigm to both unlock experimentation at scale and derive richer, more meaningful physical models for important systems.

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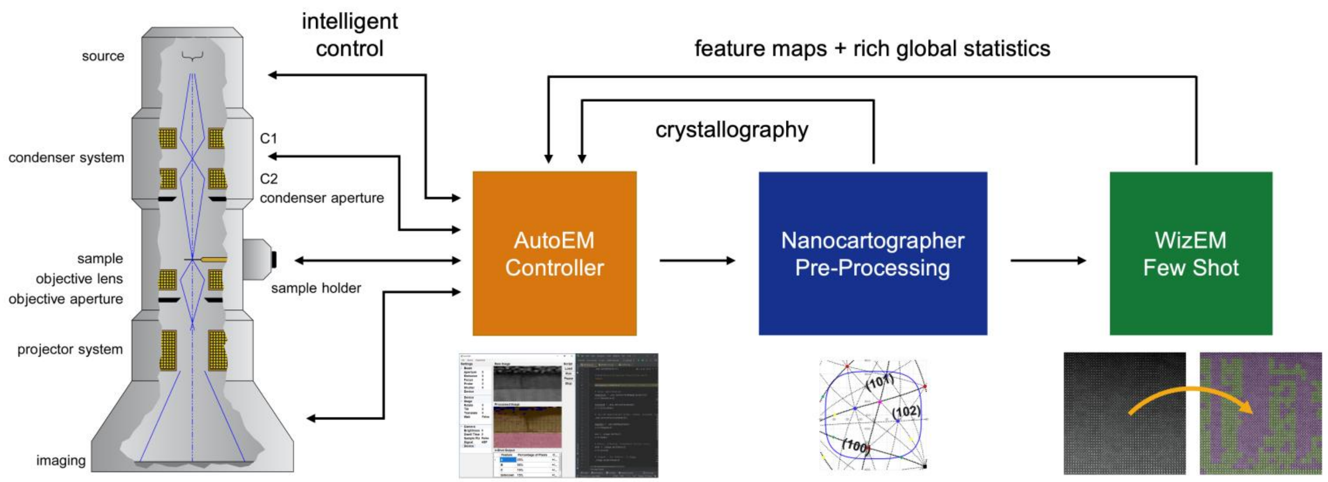

Figure 1. Schematic of a scalable, data-driven platform for TEM automation, domain-grounded pre-processing, and rapid, flexible feature classification.

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