doi:10.1017/S1431927617007632
Microsc. Microanal. 23 (Suppl 1), 2017

Tutorial: Processing of Atomic Resolution Images and Multispectral Data

Stephen Jesse[1,2], Alex Belianinov[1,2]

[1.] Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831.
[2.] Institute for the Functional Imaging of Materials, Oak Ridge National Laboratory, Oak Ridge, TN 37831

Understanding and designing functional materials with customized properties relies on the ability to integrate and analyze data from multiple characterization tools designed to probe complementary ranges of space, time, and energy. Recent advances in hardware, algorithms, and imaging technologies have made large volumes of high veracity materials data easy to acquire, store, and process. However, these typically mixed, hyperspectral data sets conceal unexamined information that is difficult to tease out, co-register, and interpret when the data size is large, complex, and corrupted by noise and/or artifacts.

This tutorial will showcase analysis strategies, and how-to approaches in processing of images, hyperspectral images, as well as time-series, and time-frequency spectral data using unsupervised multivariate methods, Bayesian inference and machine learning algorithms. A focus of this tutorial is to go beyond presenting the data and describing the algorithmic outcomes, and further to showcase how to load, preprocess, analyze, and visualize the data, while maintaining a record of the analysis steps undertaken. The instructors will rely heavily on open source, freely accessible Python libraries NumPy, SciPy, OpenCV, Pycroscopy, *etc.* The information presented in this tutorial will be made available to download throughout the presentations and afterwards in the form of Python Jupyter notebooks. **Figure 1** illustrates some of the concepts and methods covered during the tutorial.

Furthermore, the instructors will utilize and demonstrate the use of Bellerophon Environment for Analysis of Materials – BEAM, as a part of the analysis workflow. BEAM, is computational workflow managing software, available on Apple, Linux, and Windows. This lightweight Java application is designed to make High Performance Computing (HPC) platforms easy to use by offering an intuitive graphical-user-interface, a choice of scalable data analysis algorithms, simulation packages, input and output data storage - all with a click of a button.

This tutorial will bring together expertise from various fields (ion and electron microscopies, scanning probes, atom probe tomography, chemical imaging, *etc.*) to discuss strategies for the analysis of multidimensional hyperspectral data. Relating extracted parameter fields to underlying physics will also be discussed.

As an outcome of this tutorial, we aim to identify a set of approaches that will significantly increase the quality of information extracted from imaging data, discuss their implementation, and highlight the strengths and weaknesses of various methods when dealing with a particular type of a problem. At the same time, we hope to spark potential collaborations and discussions amongst researchers in the area of statistics, computational sciences, and materials and build a community for sourcing and sharing analysis methods in the future.

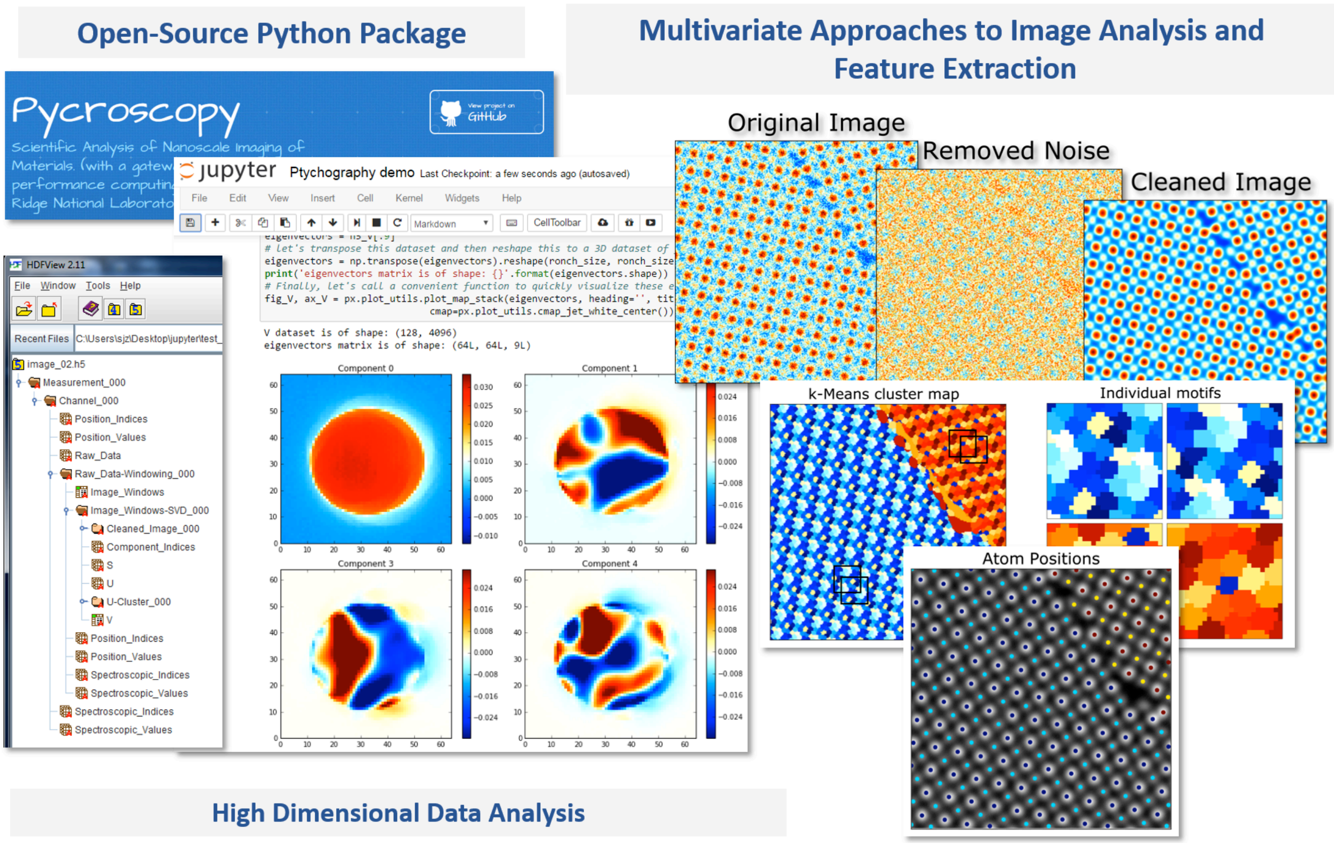

Figure 1. As part of this tutorial, we will utilize open-source and freely available python-based packages for the analysis of multidimensional data sets. All examples will be in the form of interactive Jupyter notebooks. Among the topics to be discussed are: i) the use of data structures based in hierarchical data formats and translating to and from the formats, ii) navigation, viewing, and processing of large, high dimensional data sets such as those captured during ptychography, EELS mapping, and movies of dynamic processes, and iii) the use of multivariate and machine learning methods for de-noising and feature extraction of images.

[1] This research was supported partially conducted (AFM, ToF-SIMS) at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Scientific User Facilities Division, Office of Basic Energy Sciences, US Department of Energy. Research was partially sponsored (STEM, HIM) by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U. S. Department of Energy.

https://doi.org/10.1017/S1431927617007632 Published online by Cambridge University Press