Joint NSRC Workshop

Big, Deep, and Smart Data Analytics in Materials Imaging

Jointly organized by the five DOE Office of Science Nanoscale Science Research Centers and held at Oak Ridge National Laboratory, Oak Ridge, TN
June 8-10, 2015
(www.cnms.ornl.gov/JointNSRC2015/)

Abstract Deadline: May 17, 2015
Registration Deadline: May 26, 2015

Organizing Committee:
Eric Stach, Center for Functional Nanomaterials, Brookhaven National Laboratory
Jim Werner, Center for Integrated Nanotechnologies, Los Alamos National Laboratory
Dean Miller, Center for Nanoscale Materials, Argonne National Laboratory
Sergei Kalinin, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory
Jim Schuck, Molecular Foundry, Lawrence Berkeley National Laboratory

Scope: This workshop will bring together researchers from different imaging disciplines (electron microscopy, scanning probe microscopy, focused x-ray, neutron, atom probe tomography, chemical imaging, optical microscopies) as well as experts in mathematical/statistical/computational approaches **to discuss opportunities and future needs in the integration of advanced data analytics and theory into imaging science**. It will provide a forum to present achievements in the various imaging disciplines with emphasis on acquisition, visualization, and analysis of multidimensional data sets, the corresponding approaches for theory-experiment matching, and novel opportunities for instrumental development enabled by the availability of high speed data analytic tools.

Background: Understanding and ultimately designing improved functional materials that possess complex properties will require the ability to integrate and analyze data from multiple instruments designed to probe complementary ranges of space, time, and energy. Recent advances in imaging technologies have opened the floodgates of high-veracity information in the form of multidimensional data sets. These high-resolution images and spectra conceal unexamined information on atomic positions and local functionalities, as well as their evolution with time, temperature, and applied fields. To gain the full benefits of such data sets, we must be able to effectively interrogate them for a variety of physically and chemically relevant

information, develop pathways for probing local structure-property relationships, and to synergistically link these results to atomistic theories (e.g., "deep" data analysis for scientific inference). The traditional simple graphical representation and visual inspection of such data sets are no longer sufficient to extract the most meaningful information. Advanced mathematical and computational methods are increasingly being incorporated into imaging sciences to deal with such deep data sets, and to combine data streams from different imaging techniques. However, many of the required mathematical or numerical tools are either lacking or not generally accessible to the imaging sciences community.

Outcomes: The workshop aims to identify areas where advanced data analytics approaches will significantly increase the quality of information extracted from imaging data, and identify the role to be played by the NSRCs to make such approaches accessible to the user community. At the same time, the workshop will identify areas in which enhanced interaction with researchers in applied mathematics, statistics, theoretical and computational sciences will be most beneficial to the imaging and materials sciences community in particular, and nanosciences in general.

Format: The workshop will consist of plenary lectures to introduce the key areas of interest, contributed talks and posters, as well as panel discussions and/or breakout sessions to discuss the needs and opportunities in the various areas.

Tentative Topics include:

- Unsupervised learning for image analysis, classification, and information extraction
- Harnessing structural and functional imaging for materials development and discovery, for soft/hybrid as well as for hard materials
- Deep learning in imaging: Bayesian inference, parameter space compression, exploring unstructured data
- Integrating data sets from different imaging modalities and different length and time scales

Any questions about this workshop should be directed to:
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