# FIRST IMAGING INITIATIVE WORKSHOP: TOMOGRAPHY AND PTYCHOGRAPHY
## SEPTEMBER 29 – 30, 2014
## ENERGY SCIENCES BUILDING 241, CONFERENCE ROOM D172
## ARGONNE NATIONAL LABORATORY

### *September 29, Monday 8:00-8:45 - Coffee and Registration*

8:45 - Amanda Petford-Long: Integrated Imaging Initiative Overview (context within Materials for Energy)

### *Session 1: Tomography 1*

9:00 - Begum Gulsoy (Northwestern) Tomography Across Length Scales: From Electron Tomography to Mechanical Serial Sectioning

9:30 - Xianghui Xiao (APS) microCT

10:00 – 10:20 Break

10:20 – Rowan Leary (University of Cambridge) Contemporary Electron Tomography for Materials Science

10:50 – Laurence Marks (Northwestern) Towards Atomic Resolution 3D Electron Tomography

11:20 – 1:00 Lunch (Boxed Lunches for those who ordered will be in break area**)**
11:30 - Tour of Mira (30 participants maximum – sign up sheet at registration desk)

### *Session 2: Ptychography 1*

1:00 – David Vine (ANL-APS) Ptychography combined with X-ray fluorescence
1:30 – Stefan Hruszkewycz (ANL-MSD) Nanoscale Materials Imaging with Bragg Ptychography
2:00 – David Shapiro (LBNL) Soft X-ray Microscopy with Wavelength Limited Spatial Resolution
2:30 – Youssef Nashed (ANL-MCS) PtychoLib: Parallel Ptychographic Reconstruction

3:00 - 3:30 Break

### *Software/Methods: Tomography 2*

3:30 - Doga Gursoy (ANL-APS) TomoPy: A Framework for the Analysis of Tomographic Data Abstract
4:00 - Charles Bouman (Purdue) Integrated Imaging: Creating Images from the Tight Integration of Algorithms, Computation, and Sensors
4:30 - Wendy Di (ANL-MCS) Optimization Approach for Tomographic Inversion from Multiple Data Modalities

### *5:00-6:30 Poster Session (Energy Sciences Building Foyer)*

**September 30, Tuesday**

*Session 1: Tomography 2*

8:30 - Stefan Vogt (ANL-APS) Hyperspectral Imaging in 3D
9:00 - Tom Kelly (CAMECA Instruments, Inc.) Ptychography and Atom Probe Tomography

9:30-10:00  Break

10:00 –Charudatta Phatak (ANL-MSD) Visualization of Three Dimensional Magnetization using Vector
        Field Electron Tomography
10:30 - Ross Harder (ANL-APS) Bragg Coherent Diffractive Imaging

11:00-12:15 Lunch

*Session 2: Visualization*

12:15 - Daniela Ushizima (LBNL) Visualization and Analysis of High Throughput Experiments.
12:45 - John Stone (UIUC) GPU-Accelerated Visualization and Analysis of Petascale Molecular Dynamics
        Simulations
 1:15  - Joe Insley(ANL-LCF) Scalable, Large-Scale Data Analysis and Visualization
 1:45  -  Francesco De Carlo (ANL-APS) Scientific Data Exchange

2:15-2:45  Break

*Session 3: Data Analysis*

2:45 -  Gordon Kindlmann (University of Chicago) Discovering Stable Features in Scientific Images
3:15 -  Tom Peterka (ANL-MCS) Imaging Meets HPC through Scalable Data Analysis
3:45 -  Stefan Wild (ANL-MCS) Nonnegative Matrix Analysis for Structured Feature Extraction
4:15 -  Nicola Ferrier (ANL-MCS) Image Analysis

5:00 - Tour of APS (30 participants maximum – sign up sheet at registration desk)

Abstracts Presented (in alphabetical order by last name)

Charles Bauman – Purdue University
*Integrated Imaging: Creating Images from the Tight Integration of Algorithms, Computation, and Sensors*
Integrated Imaging systems tightly integrate novel sensor design, algorithms, and computation to create new imaging modalities with dramatically new capabilities. This talk presents some examples of state-of-the-art integrated imaging systems based on computed tomography (CT), transmission electron microscopy (STEM), synchrotron beam imaging, optical sensing, and scanning electron microscopy (SEM). For each of these examples, we also explore their use and potential impact in applications ranging from healthcare to material science. We conclude with some speculation on where integrated imaging might be going; where it might have greatest impact; and what will be the greatest challenges ahead.

Francesco De Carlo - Argonne National Laboratory
*Scientific Data Exchange*
As different research teams and techniques have grown at various facilities, they have often developed local data storage formats based on instrument hardware specificity and expediency rather than rational planning, often drawing upon the particular preferences of a scientist or engineer writing software at the project's outset. The Data Exchange is a simple data model that is designed to interface, or "exchange" data among different instruments, and to enable sharing of data analysis tools. In this talk we will describe the successful application of the Data Exchange model to a variety of synchrotron-based techniques, including X-ray tomography, X-ray fluorescence spectroscopy, X-ray fluorescence tomography, coherent diffraction imaging and X-ray photon correlation spectroscopy.

Wendy Di – Argonne National Laboratory
*Optimization Approach for Tomographic Inversion from Multiple Data Modalities*
Fluorescence tomographic reconstruction can be used to reveal the internal elemental composition of a sample. On the other hand, transmission tomography can be used to obtain the spatial distribution of the absorption coefficient inside the sample. In this work, we integrate both modalities and formulate an optimization approach to simultaneously reconstruct the composition and absorption effect in the sample. The result is demonstrated on a simple sample.

Nicola Ferrier - Argonne National Laboratory
*Image Analysis*
An overview of some imaging techniques applicable for imaging of materials will be presented.

Begum Gulsoy - Northwestern University
*Tomography Across Length Scales: From Electron Tomography to Mechanical Serial Sectioning*
Tomographic methods span multiple length scales ranging from nano scale using electron tomography, to micro scale using FIB-SEM serial sectioning and X-Ray tomography and to macro via mechanical serial sectioning. This talk will provide examples of scientific problems addressed at each length scale as well as highlight our current efforts in building a mechanical serial sectioning system coupled with a desktop scanning electron microscope. Common obstacles in fusing and analyzing data will also be briefly discussed.

Doga Gursoy – Argonne National Laboratory
*TomoPy: A framework for the Analysis of Tomographic Data*
In this talk, I will describe an attempt to provide a collaborative framework for the analysis of tomographic data that has the potential to unify the effort of different facilities and beamlines performing similar tasks. The proposed Python based framework is open-source, platform and data format independent, has multiprocessing and grid computing infrastructure that many iterative techniques demand.

Ross John Harder - Argonne National Laboratory
*Bragg Coherent Diffractive Imaging*

Stephan Hruszkewycz - Argonne National Laboratory
*Nanoscale Materials Imaging with Bragg Ptychography*
In recent years, new tools for materials characterization based on Bragg diffraction of coherent hard x-rays have been developed with sensitivity to mesoscale atomic structure. In this talk, I will focus on recent progress and future applications of nanoscale coherent x-ray Bragg ptychography imaging. By applying the ptychography techniques we have been developing at the APS, we successfully imaged nanoscale strain and polarization distributions in single crystal thin film systems in two dimensions, and we have recently developed new promising methods for 3D structural imaging of lattice properties in nanoscale crystals.

Joseph A. Insley - Argonne National Laboratory
*Scalable, Large-Scale Data Analysis and Visualization*
The scale of scientific datasets, both collected and simulated, routinely exceed the capabilities of a single workstation. This necessitates the use of parallel resources and software for analyzing and visualizing such large-scale data. This presentation will highlight several tools currently used for these purposes, as well as efforts underway for improved interactive analysis of data at scale. Use of simulation/acquisition-time analysis will also be discussed.

Tom Kelly - CAMECA Instruments, Inc.
*Ptychography and Atom Probe Tomography*
The ability to locate atoms accurately in 3D space in atom probe tomography depends on accurate knowledge of the projection law. The shape of a specimen apex is the principal determinant of the projection, i.e., the trajectories of ions from the specimen to the detector. Simple assumptions about the specimen apex shape are often used but these are known to be inaccurate. Images of the specimen apex at the nanometer scale should provide the information needed to improve the projection law. In-situ ptychography is being explored as a means to obtain this information and greatly improve the projection law.

Gordon Kindlmann - University of Chicago
*Discovering Stable Features in Scientific Images*
Researchers who acquire images as part of their research often want to perform some kind of feature detection and quantitation to answer their scientific questions. Not all users know, however, exactly which image features are the most reliable representatives of the physical or anatomical structures of interest. A tool that surveys a palette of possible features (e.g. ridge and valley lines or surfaces, edges, isosurfaces), and visually indicates which features are stable at which scales, could help the researcher find which features correspond to structure of interest, as well as help discover new structures revealed by the advanced imaging.

Rowan Kendall Leary – University of Cambridge
*Contemporary Electron Tomography for Materials Science*
Electron tomography (ET) is now firmly established in the physical sciences for 3D morphological characterisation at the nanoscale. Recent years have seen considerable efforts to extend ET capabilities, seeking to achieve higher-fidelity 3D reconstructions that can be analysed quantitatively; to address hitherto inaccessible beam-sensitive specimens; to reach new length-scales; and to obtain information-rich multi-dimensional data by coupling ET with, for example, spectroscopic or crystallographic signals. This talk will focus on recent progress in these areas by our research group, with particular highlights being the use of compressed sensing in ET reconstruction and 3D imaging of localized surface plasmon resonances.

Laurence Marks - Northwestern University
*Towards Atomic Resolution 3D Electron Tomography*
Electron tomography is a well established technique at the 1nm scale for morphology, local chemical or electronic structure information. To achieve 0.1nm resolution one has to dynamical diffraction, which complicates the linear approximations often invoked in tomography. However, the problem is really a feasible set reconstruction of the representation rather than an image. This distinction is standard in crystallographic direct methods, and integration over angles is known to damp dynamical diffraction effects, as well established for Precession Electron Diffraction. As a consequence we are approaching true atomic resolution 3D tomography with electrons.

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Youssef S G Nashed - Argonne National Laboratory
*PtychoLib: Parallel Ptychographic Reconstruction*
Ptychography is a phase retrieval technique for reconstructing a specimen's image from its diffraction patterns in light, X-ray, and electron microscopes. Despite the potential for ptychography there is a lack of tools for data online analysis while it is being acquired. PtychoLib is a library for real-time ptychographic phase retrieval. It uses a hybrid parallel strategy to divide the computation between multiple graphics processing units then merge partial reconstructions into one coherent phase contrast image.

Tom Peterka - Argonne National Laboratory
*Imaging Meets HPC through Scalable Data Analysis*
From use cases in data analysis of scientific HPC applications, I will derive common patterns for analyzing very large spatiotemporal data. Then, I will present one example applicable to materials science, the problem of converting discrete point data into a continuous field using Voronoi and Delaunay tessellations, and doing so in parallel at very large scale.

Charudatta Phatak - Argonne National Laboratory
*Visualization Of Three Dimensional Magnetization using Vector Field Electron Tomography*
With advances in fabrication and lithography, magnetic nanostructures can be made in complex, confined three-dimensional (3D) geometries as well as patterned into a variety of interacting lattices. In order to control their behavior, it is necessary to understand the fundamental physics of their magnetic interactions along with the influence of physical shape of the nanostructures in 3D. In this talk, I will present our work on 3D visualization of magnetization of such nanostructures using vector field electron tomography (VFET). I will present a brief introduction to the VFET technique and demonstrate its application to a variety of complex magnetic structures.

David Alexander Shapiro – Lawrence Berkeley National Laboratory
*Soft X-ray Microscopy with Wavelength Limited Spatial Resolution*
The development of soft x-ray ptychography at the Advanced Light Source (ALS) has pushed the spatial resolution of our microscopes significantly closer to the wavelength limit by imaging isolated 5 nm structures. The use of soft x-rays offers sources with high coherent flux, high absorption and phase contrast, high penetration, and sensitivity to electronic/magnetic states and bond orientation. The ptychographic microscopes at the ALS are based on custom high performance scanning systems, high speed CCD detectors, and massively parallel reconstruction code. I will present the details of these microscopes and their application to the study of chemical composition at the nanoscale.

John Stone - University of Illinois at Urbana-Champaign
*GPU-accelerated Visualization and Analysis of Petascale Molecular Dynamics Simulations*
State-of-the-art molecular dynamics simulations augment and refine structural data produced by experimental imaging techniques, giving access to the dynamics of cellular machines at spatial and temporal timescales that are not accessible to experimental methods alone. Petascale computers enable simulation of large biomolecular complexes such as the HIV capsid, but they produce vast quantities of simulation output that must be carefully visualized and analyzed. VMD addresses the computational challenges posed by such simulations using GPUs, solid state disks, and parallel computers, thereby enabling researchers to perform detailed analyses on petascale molecular simulations, while retaining the ease-of-use and analytical capabilities it is known for.

Daniela Ushizima – Lawrence Berkeley National Laboratory
*Scaling Scientific Image Analysis*
Research laboratories store images as part of experimental records. Limitations in scientific image analysis hamper ability to understand the acquired data. This talk will describe our current research on general and domain-specific pattern recognition methods that exploits mathematical and statistical image analysis techniques and brings knowledge about known structures as constraints, in which we apply priors to find scientifically relevant constructs and allow agile software for the use in everyday analysis.

David Vine - Argonne National Laboratory
*Cryo X-ray Fluorescence and Ptychographic Microscopy*
The combination of ptychography with fluorescence microsocpy yields a unique method with elemental and electron density contrast. In this presentation I will present the latest results from the BioNanoProbe where we have been developing two and three-dimensional imaging of biological cells at cryogenic temperature.

Stefan Vogt - Argonne National Laboratory
*Data Analysis for X-ray Fluorescence Microscopy: Unique Challenges and Opportunities*
X-ray fluorescence microscopy (XFM) is a powerful technique to map and quantify trace element distributions in applications ranging from biology to material science. Advances in instrumentation, such as faster detectors, better optics, and improved data acquisition strategies are fundamentally changing the way experiments can be carried out, with unique challenges and opportunities. We will identify unique challenges and opportunities brought about by instrumentation advances, and discuss steps we have taken to exploit these opportunities through advances in data analysis.

Stefan Wild – Argonne National Laboratory
*Nonnegative Matrix Analysis for Structured Feature Extraction*
Nonnegative matrix approximation (NMA; also called NMF) is a data reduction methodology that has proved popular for determining parts-based representations in classical image processing domains. We review algorithms for NMA and modifications to enforce desired structure in the approximation. We show how NMA-based approaches can be powerful tools in the physical sciences, especially given the additive nature of the densities of materials, nonnegativity of energy absorption, etc. We
illustrate our approach on biological data from a scanning transmission x-ray microscope at Stony Brook and on fluorescence microscopy data from Argonne's APS.

Xianghui Xiao - Argonne National Laboratory
*X-ray Fast Tomography and its Applications in Dynamical Phenomena Studies in Geoscience at APS*
Synchrotron radiation based fast tomography can provide high spatial and temporal resolutions that is suitable in dynamical phenomena studies in geoscience. This presentation aims at reviewing the potential of Synchrotron radiation based micro-tomography for research applications in structural geology and experimental rock mechanics. Besides outlining the technical capabilities of the latest generation of microtomography beam lines at the Advanced Photon Source (USA), we will present our workflow for the analysis of large time-resolved tomographic datasets. We will conclude with an outlook on a next generation of in-situ studies on fluid-rock interaction and rock deformation.