APS Workshop 9: Using Synchrotron Light to Probe Earth and Environmental Systems (EES)

Wednesday, May 8, Morning

8:00 – 8:05	Workshop Organizers *Welcome and Opening Remarks*

Session I: Instrumental/eBERlight/FICUS

8:05 – 8:20	Zou Finfrock (Argonne National Laboratory) *eBERlight: An Integrated User Program for Earth and Environmental Science at the APS*
8:20 – 8:50	Tamas Varga (Pacific Northwest National Laboratory) *Molecular Observation Network (MONet) and an eBERlight-MONet Collaboration*
8:50 – 9:10	Joanne Stubbs (University of Chicago) *GeoSoilEnviroCARS: Synchrotron X-ray Resources for the Earth and Environmental Science Community*
9:10 – 9:30	Andrei Smertenko (Washington State University) *MAP20-dependent Pit Architecture in Vascular Cells is Essential for Drought Survival*
9:30 – 10:00	Break

Session II: Earth and Environmental Science (Soil, Biogeochemistry, Atmospheric)

10:00 – 10:30	Alexandra Kravchenko (Michigan State University) Workshop Keynote *Examples of Using X-ray Computed Microtomography when Studying Soil Biochemical Processes*
10:30 – 10:50	Sharon Bone (SLAC, Stanford University) *Combining Synchrotron X-ray Fluorescence Microprobe Imaging with Conventional Microscopies to Obtain Multimodal Datasets for Biogeochemical Systems*
10:50 – 11:10	Viktor Nikitin (Argonne National Laboratory) *Tomographic Imaging of Methane Hydrate Formation in Porous Media*
11:10 – 11:30	Lucie Stetten (Argonne National Laboratory) *X-ray Absorption Spectroscopy to Unravel Iron Redox Biogeochemistry in Marine and Freshwater Coastal Environments*
11:30 – 1:30	Lunch Break

Wednesday, May 8, Afternoon

Session III: Plant and Rhizosphere Science

1:30 – 2:00 Joseph Jakes (USDA Forest Service, Forest Products Laboratory)
Workshop Keynote
Multiscale Multimodal Analysis of Brown-rot Fungal Decay Mechanisms for Improved Biomimetic Lignocellulosic Biorefinery Processes

2:00 – 2:20 Gyorgy Babnigg (Argonne National Laboratory)
Multimodal Imaging to Measure the Chemical Exchange and Physical Interactions in the Rhizosphere

2:20 – 2:40 Gosia Korbas (Argonne National Laboratory)
From Oats to Mangroves: Using Multiresolution X-ray Fluorescence Microscopy to Understand Processes in Plants

2:40 – 3:00 Tom Regier (Canadian Light Source)
Mail-in Operations for Soft X-ray Absorption Spectroscopic Analysis of Soils at the Canadian Light Source

3:00 – 3:30 Break

Session IV: Data Processing, Integration, and Automation

3:30 – 3:50 Arthur Glowacki (Argonne National Laboratory)
Automation and the Data Analysis Process for XRF at the APS

3:50 – 4:10 Neil Getty (Argonne National Laboratory)
AI-driven Bioimaging Analysis for Rhizosphere Interactions

4:10 – 4:30 Maksim Yakovlev (University of Chicago)
Feature-specific Segmentation Approaches for Highly Variable Microcomputed Tomography Datasets in Earth Science

4:30 – 5:00 Round Table Discussion

5:00 Adjourn

eBERlight: An Integrated User Program for Earth and Environmental Science at the APS

Zou Finfrock[1]

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Synchrotron-based techniques offer highly valuable insights for characterizing earth and environmental systems, yet these methods remain largely underutilized by many communities. The Advanced Photon Source (APS) facility is undergoing a soon-to-be-completed generational upgrade that capitalizes on a new light source design, improved instrumentation, and innovative methods. The upgraded APS is poised to become one of the world's brightest light sources, delivering x-rays up to 500 times brighter than those currently available.

The upgrade project includes the construction of new feature beamlines to fully take advantage of the increased brightness and coherence of the x-ray beams, alongside various technical enhancements to almost all existing beamlines. High-energy x-ray will enable users to probe unaltered large bulk samples with scientific relevance. Increased brightness will allow macroscopic fields of view with nanometer resolution, while enhanced coherence will provide the highest spatial resolution even in highly heterogeneous environments. These characteristics position the APS as one of the premier x-ray light sources for imaging applications across many scientific disciplines.

Introducing an innovative initiative, eBERlight, which provides an integrated platform with dedicated support from experts in the field. It offers a multimode approach to studying earth and environmental systems. The program will also leverage additional Argonne resources, assisting users with sample preparation, data collection, and data analysis.

Molecular Observation Network (MONet) and an eBERlight-MONet Collaboration

Tamas Varga[1], Yuri E. Corilo[1], Emiley Eloe-Fadrosh[2], Emily B. Graham[3], Satish Karra[1], Sarah Leichty[1], Odeta Qafoku[1], Qian Zhao[1], Zou Finfrock[4], Lucie Stetten[5], Gyorgy Babnigg[5], Kenneth M. Kemner[5], Karolina M. Michalska[4], John Bargar[1], and Douglas Mans[1]

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Soils contain 75% of the Earth’s carbon, with more carbon residing in soils than in the atmosphere and in plants combined. The role of soil carbon in the global carbon cycle is a crucial one. However, the ecological processes that govern whether carbon remains in soils or is released into the atmosphere are complex making it difficult to predict and mitigate climate change. Standardized soil molecular and microscale data – at regional and larger scales – is needed to improve biogeochemical process representations, provide model inputs, and reduce uncertainty in Earth System and climate predictions. To address this need, the Environmental Molecular Sciences Laboratory (EMSL) has developed and launched the Molecular Observation Network (MONet). Scientists participating in the Soil Function open science user call by submitting soil cores from sites across the continental US will have access to premier analytical methods at EMSL and the Joint Genome Institute, and soon the Advanced Photon Source, to support their research. Advanced molecular and microscale data produced from analyses of these cores will be available in a searchable open database. This database will allow for the conversion of traditionally labor-intensive molecular analysis methods into a high-throughput workflow, providing key molecular and microscale information to climate scientists, modelers, and experimenters. In this presentation, the Molecular Observation Network will be introduced and ongoing efforts to develop an eBERlight-MONet collaboration will be discussed.

GeoSoilEnviroCARS: Synchrotron X-ray Resources for the Earth and Environmental Science Community

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GeoSoilEnviroCARS (GSECARS) is a national user facility for frontier research in the Earth and environmental sciences (EES) using synchrotron radiation, operating Sector 13 at the Advanced Photon Source (APS) for the benefit of the EES community. Experiments in five stations on four beamlines are distributed among five broadly-defined scientific programs: (1) high-pressure/high-temperature diffraction, scattering, and spectroscopy using the laser heated diamond anvil cell (DAC); (2) high-pressure/high-temperature diffraction, scattering, and imaging using the large-volume press (LVP); (3) surface, interface, and ambient-pressure diffraction (SIAD); x-ray fluorescence microprobe analysis, micro-diffraction and micro-x-ray absorption fine structure spectroscopy (Microprobe); and x-ray computed microtomography (Tomography). The DAC and LVP programs primarily serve the high-pressure Earth science and rock deformation communities; the SIAD program primarily serves the ambient-pressure/temperature geochemistry, mineralogy, and environmental science communities; and the Microprobe and Tomography programs serve broad cross-sections of environmental scientists, (bio)geochemists, mineralogists, petrologists, and *in-situ* rock deformation specialists. After the APS-Upgrade is complete, the GSECARS beamlines will leverage the power of APS-U with new and upgraded x-ray optics that will preserve the enhanced x-ray coherence and focus more photons into smaller spots. Upgrades to end station instrumentation will enhance and add new measurement capabilities across all the GSECARS scientific programs.

GeoSoilEnviroCARS is supported as a national user facility by the National Science Foundation – Earth Sciences via SEES: Synchrotron Earth and Environmental Science (EAR –2223273). Further support is provided by NASA's Planetary Science Enabling Facilities (PSEF) program (grant number 80NSSC23K0196) and DOE BES Geosciences (DE-SC0020112 and DE-SC0019108) for the Microprobe, Tomography, and SIAD programs, respectively. This research uses resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

MAP20-dependent Pit Architecture in Vascular Cells Is Essential for Drought Survival

Andrei Smertenko[1], Tania Smertenko[1], Rhoda A.T. Brew-Appiah[2], Glenn Turner[1], Adam Denny[3], Anil Battu[3], Zou Finfrock[4], Gyorgy Babnigg[4], Karolina Michalska[4], Changsoo Chang[4], Tanya Winkler[3], Chase Akins[4], Viktor Nikitin[4], Pavel Shevchenko[4], Alex Lavens[4], Andrzej Joachimiak[4], Tamas Varga[3], and Karen Sanguinet[2]

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Evolution of drought resiliency in flowering plants is accompanied by changes in morphology of specialized structures within the walls of vascular cells, known as pits. Pits facilitate the transport of solutes between vascular cells under mesic environmental conditions and restrict spread of air pockets (embolisms) during arid conditions. Conductivity of pits for both water and embolisms depends on pit membrane thickness; thicker membranes restrict movement of both water and embolism, whereas thinner membranes are more permeable. Plants adapted to arid environments have smaller vascular pits with thicker membranes. Genes that determine pit membrane morphology and thickness remain poorly understood. It has been shown that microtubules play a key role in pit development. Specifically, microtubule depolymerization in the pit construction sites define the pit shape and size. However, our knowledge of proteins governing microtubule stabilization outside pit construction sites and role of these proteins in drought adaptation remain limited. Here we report that the borders of the pit construction sites in the model grass *Brachypodium distachyon* recruit a TPX2-like angiosperm-specific microtubule protein MAP20, which is expressed during late stages of metaxylem and phloem differentiation. *In vitro*, MAP20 promotes microtubule nucleation and inhibits microtubule depolymerization. *In vivo*, MAP20 suppresses microtubule depolymerization. Knockdown of MAP20 causes increase of pit size, thinner pit membranes, perturbed vasculature development, and higher drought susceptibility. We imaged embolism formation in stems of wild type and MAP20 knockdown *B. distachyon* lines using x-ray computed microtomography (2-BM) and Thermo Fisher Heliscan MicroCT Mark II. The imaging data shows differences of embolism onset in these lines. We conclude that MAP20 functions in drought adaptation by regulating pit membrane architecture.

Examples of Using X-ray Computed Microtomography when Studying Soil Biochemical Processes

Alexandra Kravchenko[1] and Andrey Guber[1]

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Micro-scale physical structure of soil matrix plays a major role in driving water and air fluxes, transport of chemicals, and movement of soil micro- and meso-biota. Biological and chemical processes take place within this physical-hydrological continuum and understanding and quantification of connections between microbial activities and physical/chemical flows require direct assessment of microbial compositions and functioning within undisturbed soil with flow-carrying and water-holding pore structure being kept intact. At present, x-ray computed microtomography (μCT) is the only tool that enables comprehensive assessment of the soil physical structure in intact soil samples ranging from few mm to few cm sizes. Combining the knowledge of the intact soil physical structure with experiments targeting soil biochemical processes and with measurements of soil biological and biochemical characteristics is a promising and exciting way forward in better understanding of soil functioning. Here we will present several examples of such studies where information from μCT soil images about pore size distribution, characteristics of pores of biological origin, and soil particulate organic matter is used for exploring processes of plant residue decomposition, soil C gains, and greenhouse gas (N_2O) emissions.

Combining Synchrotron X-ray Fluorescence Microprobe Imaging with Conventional Microscopies to Obtain Multimodal Datasets for Biogeochemical Systems

Sharon Bone[1]

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A grand challenge in the study of environmental systems lies in understanding how organisms modify and are modified by their host environment. This interplay has a profound influence on carbon and nutrient cycling, as well as creating suitable environmental conditions for the proliferation of other organisms. Synchrotron-based x-ray fluorescence (XRF) microprobe imaging is a powerful tool to study the complex interplay between plants, microorganisms, and their soil environment; synchrotrons provide both high brightness and tunability of the incident x-ray energy to provide both unique sensitivities and the ability to perform spectroscopy to obtain chemical species information. However, the x-ray microprobe is not suitable for imaging numerous biological processes (e.g., enzymatic activities, metabolites, etc.), nor is it suitable for imaging organic materials. When combined quantitatively with complimentary methods, such as optical/fluorescence light microscopy, FTIR microscopy, or mass spectrometry, XRF microprobe imaging has the potential to provide wholistic insight into soil biogeochemical processes. Our ability to utilize this multimodal approach depends on proper registration of images, which, for disparate data types presents a challenge.

Herein, we present a multimodal data collection and analysis approach that is being implemented at the Stanford Synchrotron Radiation Lightsource. Imaging data from optical/fluorescence light microscopy, FTIR microscopy, and XRF imaging can be collected, with some datasets collected contemporaneously and some datasets as separate experiments, and then processed in a data pipeline as a coherent multimodal set of data, where each pixel of the data image stack contains information from each of the data modalities. Various statistical methods, including clustering and principal component analysis, can then be applied to the full set of data types to aid interpretation. Applications of this approach to biogeochemical systems will be discussed.

Tomographic Imaging of Methane Hydrate Formation in Porous Media

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Gas hydrates, resulting from the intricate bonding of water and gas molecules under precise pressure and temperature conditions, play a pivotal role in energy generation, climate dynamics, and environmental equilibrium. Understanding the dynamic evolution of gas hydrates within porous media is imperative for refining extraction methods and assessing associated risks. This presentation unveils outcomes from computed tomography (CT) experiments focusing on methane hydrate formation and dissociation within an environmental cell filled with porous media. Synchrotron micro-CT imaging has delivered remarkable spatial and temporal resolution scans, unraveling insights into water dynamics and various gas hydrate formation morphologies. Further exploration via nano-CT measurements has probed deeper into water extraction mechanisms through micro-channels within grains. The environmental cell for the hydrate growth was also equipped with acoustic sensors, which facilitated correlating CT with acoustic data for further analysis and using the results during real seismic surveys. By combining multiple imaging modalities available with the APS-U, we aim to enrich our understanding of gas hydrate formation processes and their implications for energy exploration and environmental management.

X-ray Absorption Spectroscopy to Unravel Iron Redox Biogeochemistry in Marine and Freshwater Coastal Environments

Lucie Stetten[1], Maxim I. Boyanov[1,2], Edward J. O'Loughlin[1], Roberta Bittencourt Peixoto[3], Donnie Day[3], Matthew Kovach[3], Fausto Machado-Silva[3], Allison Myers-Pigg[3,4], Opal Otenburg[4], Stephanie Wilson[5], Elena Shevchenko[6], Nicholas Ward[4], Patrick Megonigal[5], Michael N. Weintraub[3,4], Vanessa Bailey[3,4], and Kenneth M. Kemner[1]

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Coastal terrestrial-aquatic interfaces are dynamic environments with spatial variability and hydrological fluctuations that impact the geochemical behavior of redox sensitive elements such as iron (Fe), that is directly implicated in the biogeochemical cycles of carbon, nutrients, and contaminants. This talk will present a collaborative study conducted within the Coastal Observations, Mechanisms, and Predictions across Systems and Scales - Field, Measurements, and Experiments project, which aims to understand Fe redox biogeochemistry across coastal sites and to improve the predictions of biogeochemical responses to hydrological disturbances. Soil cores were collected across upland to shoreline gradients from coastal locations in the Western Lake Erie Basin and the Chesapeake Bay regions, chosen as model systems to represent freshwater and saltwater environments, respectively. Using x-ray absorption spectroscopy, the oxidation state and molecular environment of Fe were determined with depth along the undisturbed soil profiles. We show that Fe occurs mainly in its oxidized form, Fe(III), in cores collected from unsaturated upland and transition locations, with variable proportions of Fe(III)-oxyhydroxide, Fe(II,III)-phyllosilicate, and Fe(III)-organic species depending on the soil characteristics (e.g., mineral and organic carbon contents). In water-saturated soils (i.e., wetlands and some upland-wetland transition zones), varying Fe(III)/Fe(II) ratios and reduced Fe(II) species revealed diverse redox and biogeochemical conditions. At the Lake Erie wetlands, Fe reduction was identified as a dominant process responsible for the release of Fe(II) to the pore waters. Nevertheless, the extent of Fe(III) reduction was limited by the presence of recalcitrant Fe(III) in phyllosilicates. In the Chesapeake Bay wetlands and one transition site, the pore water sulfide concentrations, and the abundance of pyrite (FeS_2) indicate that Fe cycling is controlled by sulfur-driven redox dynamics. In contrast, some transition sites at both Lake Erie and Chesapeake Bay showed predominantly oxidized Fe(III) despite water-saturated conditions. At these sites, the pore water chemistry was indicative of little to no reduction of Fe(III) and of sulfate, suggesting water inputs that may have impacted microbial redox processes. These results demonstrate the advantage of combining classic solid and pore water chemistry analyses with advanced techniques such as x-ray spectroscopy for determining elemental distribution and speciation at the atomic and microscopic scales and for improving our understanding of biogeochemical cycling in natural environments.

Multiscale Multimodal Analysis of Brown-rot Fungal Decay Mechanisms for Improved Biomimetic Lignocellulosic Biorefinery Processes

Joseph E. Jakes[1], Katie Ohno[1], Grant Kirker[1], Nayomi Plaza[1], Daniel Yelle[1], Sam Zelinka[1], Christopher Hunt[1], Carl Houtman[1], and Peter Ciesielski[2]

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An improved understanding of non-enzymatic brown-rot decay mechanisms in lignocellulosics, such as wood, could inspire improved biomimetic biorefinery processes to elevate lignocellulosic materials as important renewable resources for meeting a sustainable energy future. Lignocellulosic polymers in secondary cell walls are too tightly packed for direct enzymatic deconstruction. Like biorefineries, fungi can first “pretreat” the cell walls using non-enzymatic mechanisms before enzymatic access is possible. The main non-enzymatic mechanisms used by brown-rot are generally understood to include chelator-mediated Fenton (CMF) reactions that involve Fe(II)/Fe(III) redox reactions, a wide range of metabolites, such as oxalic acid and catecholate/hydroxyquinone chelators, and trace elements like Fe, Mn, Ca, Zn, and K. However, to mimic the full decay process, details about the decay mechanisms are still needed. Nearly all previous work studying brown-rot decay mechanisms relied on bulk wood characterization techniques. A major shortcoming of these previous studies is that decay in wood is inhomogeneous across the wood cellular structure in decaying wood. Even neighboring cells may be at different stages of decay. Therefore, bulk wood characterization results are the agglomeration of various decay stages. Mechanistic study of different decay stages requires multiple characterization techniques that can probe across relevant cellular and cell wall length scales.

The project scope, which is funded through the Facilities Integrating Collaborations for User Science (FICUS) program, will therefore be centered on multiscale (from molecular to cellular) compositional and structural characterization of wood at different stages of decay using a combination of techniques at Environmental Molecular Sciences Laboratory (EMSL) at Pacific Northwest National Laboratory, Joint Genome Institute (JGI) at Lawrence Berkeley National Laboratory, and the Advanced Photon Source (APS) at Argonne National Laboratory. Experiments at EMSL will include mass spectrometry imaging (MSI), atom probe tomography (APT), nano-FTIR, and AFM Raman. Experiments at JGI will include transcriptome experiments and liquid-chromatography tandem mass spectrometry (LC-MS/MS). Experiments at APS will include multiscale x-ray fluorescence microscopy (XFM), micro-x-ray absorption near edge spectroscopy (μXANES), wide angle x-ray scattering (WAXS), and ptychography. Experiments will be designed such that multiple techniques can be performed on the same wood tissue. Combined JGI, EMSL, and APS results will include gene expression during different decay stages, multiscale maps of metabolites and trace elements, trace element oxidation states, changes in polymer chemistry in individual wood cell walls, and characterization of 0.1-100 nm structure in wood cell walls. Mechanical properties of the same cell walls will also be measured by nanoindentation at FPL. The accumulative transcriptomic, chemical, composition, structural, and mechanical data will be used to identify different decay stages with their associated decay mechanisms and cell wall modifications.

This FICUS project began in October 2023 and is still in its early stages. This presentation will give an overview of the project. Relevant past experiments performed at the APS to study wood

decay fungi will also be presented, as well as updates on preliminary results from EMSL and JGI.

Multimodal Imaging to Measure the Chemical Exchange and Physical Interactions in the Rhizosphere

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Root-microbe interactions in the rhizosphere are highly complex, leading to recognizable spatial structure variations. The identity of specific factors that lead to their development and sustain them for plant health and productivity is poorly understood. We are developing a unique functional imaging technique that exploits native sense-and-respond circuits of plant growth-promoting rhizobacteria (PGPR) to monitor chemical exchange between the plant root and microbe during the different phases of colonization. Several native PGPRs have been turned into biosensor cells, and root colonization is monitored with Arabidopsis, Camelina, and poplar plants. Genetic variants of Arabidopsis with gain or loss of function provides drastically altered local environments, resulting in colonization patterns that differ from those observed previously. An orthogonal x-ray imaging approach provides high resolution elemental analysis of the local environment as well as structural insights into root and soil interface. The capability under development combining HTP-AI bioimaging capability, along with advanced analytical techniques offered by APS and EMSL, will help understanding the dynamic chemical shifts and formation of colonization patterns in the rhizosphere.

Results from biosensor development and characterization, poplar root rhizosphere imaging at the Advanced Photon Source will be discussed.

From Oats to Mangroves: Using Multiresolution X-ray Fluorescence Microscopy to Understand Processes in Plants

Gosia Korbas[1]

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The distribution of elements in plants changes in response to many factors, including physiological stimuli or environmental conditions. It is crucial to determine these changes at the tissue, cellular, and subcellular levels to adequately understand processes controlling plant growth, plant adaptability to changing climates, or its resistance to diseases. Knowledge of the element's distribution is also helpful in guiding the biofortification of food products.

Synchrotron-based x-ray fluorescence microscopy (XFM) provides critical spatial information on various elements simultaneously and without sample pre-processing. Depending on the setup, the intact plant and its root system could be imaged. If scanning is performed suHiciently fast, radiation damage and drying of the imaged live plant tissue can be minimized. Rapid scanning also allows proper biological replication.

Here, I present three applications of multiresolution XFM to study: (1) micronutrient distribution in early-maturing and high-yielding Arborg oat species, (2) nitrogen fixation eHiciency in root nodules of various genotypes of soybean plants, and (3) phytoremediation potential of black and red mangroves.

Mail-in Operations for Soft X-ray Absorption Spectroscopic Analysis of Soils at the Canadian Light Source

Tom Regier[1]

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Ongoing development of C and N K-edge measurement methods for soils has led to the creation of a standardized procedure that is now in use at the SGM beamline at the Canadian Light Source. Beamline automation, quality control and data handling methods have been developed to enable unsupervised collection and reduction of soft x-ray absorption datasets. Mail-in access methods, which had been under consideration even before 2020, were quickly implement during the pandemic and continue to be used by the user community. A description of the procedures, examples of large dataset capabilities, and a discussion of lessons learned will be provided. Future opportunities for improving through-put and sensitivity will be presented.

Automation and the Data Analysis Process for XRF at the APS

Arthur Glowacki[1]

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With the APS-Upgrade nearing completion, beamlines are expecting to increase their raw data collection by orders of magnitude. The ability to efficiently process and analyze vast amounts of data is crucial to keep up with the faster data acquisition rates. Automatic data analysis pipelines have been in production pre-upgrade, and we have been expanding its functionality, enabling the beamlines to extract valuable insights quickly and accurately. This talk will delve into the components of automatic data analysis of XRF pipelines, from data ingestion and preprocessing to modeling and visualization. We will explore the benefits of automation in reducing human error, improving scalability, and accelerating decision-making processes. Additionally, practical examples and a future roadmap will be shared to illustrate how the APS can leverage automatic data analysis pipelines to drive innovation, optimize operations, and enhance overall performance.

AI-driven Bioimaging Analysis for Rhizosphere Interactions

Neil Getty[1]

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We've developed an AI/ML vision pipeline for automated analysis of local environments from high resolution x-ray images. Given a roughly 2000 slice volumetric scan of a seedling root using traditional computer vision and deep learning methods, this pipeline detects and quantifies many thousands of nanoparticles and characterizes features such as location, volume, intensity, and distance from center. We further use this pipeline to bootstrap training of faster end-to-end deep learning segmentation model. Additionally, we explore foundation vision models for segmentation and image feature encoding. These generalizable approaches are accelerating and automating discovery across domains without the overhead of manual annotation as well as driving integration with large language models for complex visual and language understanding.

Feature-specific Segmentation Approaches for Highly Variable Microcomputed Tomography Datasets in Earth Science

Maksim A. Yakovlev[1], Timothy Officer[1], Tony Yu[1], Yanbin Wang[1], Geeth Manthilake[2], Tahar Hammouda[2], and Mark Rivers[1]

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Synchrotron microcomputed tomography (micro-CT) enables the rapid acquisition of large, highly detailed 3-dimensional (3D) datasets. However, as 3D images increase in size and number, they become less feasible and more prohibitive to manually segment and analyze while thoroughly probing all relevant elements. The need for robust automated analysis pipelines capable of interrogating the complexities of 3D image data beyond qualitative assessment of representative slices has given rise to multiple automated and semi-automated segmentation approaches. Image data processing tools such as intensity thresholding, watershed expansion, filtering, and edge detection have been assisting automated segmentation efforts for decades. Such methods have been explored to the point of creation of commercial and open-source software for easy use such as ImageJ, SimpleITK, Avizo, and Dragonfly. However, the need to segment complex or noisy datasets, such as those composed of multiple similar material types or acquired with difficult, artifact-prone techniques, prompted the development of new automated segmentation tools to deal with the varying differences in contrast levels, textures, and intensities. Combinations of traditional approaches with newer programs using machine learning algorithms such as Ilastik allow for solutions to specific image segmentation and classification problems containing highly varied volumes of interest. Here, we present our approach to such semi-automated segmentation methods as applied to image datasets acquired at GSECARS containing shear-induced faults, melt inclusions, and granular substrates. Such methods can save resources and standardize the process across multiple images, allowing downstream quantitative characterization based on attributes such as shape, texture, abundance, or location of the volumes of interest.