10TH ANNUAL OAK RIDGE POSTDOCTORAL ASSOCIATION RESEARCH SYMPOSIUM

IN-PERSON WITH VIRTUAL OPTION AT

OAK RIDGE National Laboratory

JULY 14–15, 2022

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Acknowledgements

The Oak Ridge Postdoctoral Association (ORPA) and research committee would like to thank lab leadership, all volunteers, administrative assistants, Information Technology Services Division, and the ORNL community as a whole for their continued support of our annual Research Symposium. This event would not be possible without your continued commitment!

We are honored to have Dr. Alan McGaughey, (Carnegie Mellon University), Dr. Leslie Greengard (New York University) and Dr. Madhavi Martin (Oak Ridge National Laboratory) as keynote speakers for this year's symposium.

Our special thanks go to Moody Altamimi and Lynn Kszos for their guidance and support for the Postdoctoral Program and ORPA over this past year. We would further like to thank Caitlyn Wakefield, Laurie Varma, Douglas Edwardson, April Denning, Jeffery Cornett, and John Bui for their contribution to the success of this event.

Organizing Committee

Moody Altamimi	Xun Li	Aparna Annamraju
Mani Awale	Himel Barua	Shuvo De
Swarnava Ghosh	Hector Hernandez Corzo	Darren Hsu
Gerry Knapp	Jayanthi Kumar	Guru Madireddy
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Keynote Speakers

Leveraging High-Resolution Laser Spectroscopy for Solutions to Bioengineering, Biomass and Environmental Characterization Needs

Madhavi Martin

Group Leader,
Biomaterials and Biomass Characterization Group,
Biological Sciences Division,
Oak Ridge National Laboratory

Time: 9:30 – 10:30 am, July 14 (Thursday)

Abstract

A plethora of laser-based techniques are employed to understand the chemistry of biological and environmental matrices. In this seminar, the research that has been conducted in the last 10 years will be presented. The focus will be on the application of laser-induced breakdown spectroscopy (LIBS), which has been used for the elemental analysis of a number of biological and environmental samples. This laser-based technique has been successfully used at ORNL for the following applications:

- Quantification of soil carbon using MVA analysis
- Elemental characterization of 73 samples of switchgrass for ash characterization and poplar hardwood samples where elements of interest that were detected included silicon, potassium, calcium, magnesium, phosphorus and sulfur
- Forest fire events identified by scanning fire-affected wood to detect the changes in dendro-chemistry
- Detection of weather conditions at the treatment plots at throughfall displacement experimental site at ORNL

Combination of ionomics with new genotyping technologies to provide a rapid way to identify genes that control elemental accumulation in plants. It is very important to find the genes that control accumulation and distribution of each element by understanding the complex regulation of the ionome. Hierarchical models using principle component analysis and partial least square analysis was used to determine the presence of the specific elements mentioned above to (1) determine the characteristic spectra of switchgrass containing different amounts of these elements and (2) examine the viability of this technique for determining the quality of the feedstock in terms of the chemical composition.

Previous work in climate change applications has shown that LIBS is an accurate and reliable approach to measuring critical nutrients in woody biomass for a 13-year weather treatment study. We obtained the LIBS validation prediction for the micronutrient elements. Furthermore, these examples demonstrate an advance in LIBS-based techniques to determine the viability of switchgrass as a biomass in the production of biofuels and in the determination of climate change.

Speaker's Bio

Dr. Madhavi Martin holds a Ph.D. in solid-state physics from the University of California, Los Angeles. She focuses on research and development in the design, fabrication and testing of environmental sensors specifically for chemical and biological applications. Her work supports analysis of metabolite data from BESC poplar transgenics and helps characterize the performance of different BESC microbes degrading the transgenic biomass. Dr. Martin's work also supports metabolomics data analysis for plant–microbe interaction SFA. Results are applied to the advanced development of bioenergy crops, to understand soil carbon cycle processes (e.g., carbon storage research) and to correlate the environmental response to fire and climate. Forensic applications have led to solving murder cases and criminal lawsuits.

Fast and Adaptive Methods for the Simulation of Physical Processes in Complex Geometry

Leslie Greengard

Silver Professor of Mathematics and Computer Science,
Courant Institute of Mathematical Sciences,
New York University

Time: 2:00 – 3:00 pm, July 14 (Thursday)

Abstract

I will review the state of the art in integral equation methods for the solution of ordinary and partial differential equations. With suitable fast algorithms and quadrature techniques, such methods achieve optimal complexity and high-order accuracy. They are particularly well suited to problems requiring adaptivity in space or space-time.

Speaker's Bio

Leslie Greengard received his B.A. degree in mathematics from Wesleyan University in 1979, and his M.D/Ph.D. degree from Yale University in 1987, with his Ph.D. being in computer science. He has been a member of the faculty at the Courant Institute of Mathematical Sciences, NYU, since 1989, and was director of the Institute from 2006–2011. He is also Professor of Electrical and Computer Engineering at NYU's Tandon School of Engineering and presently serves as director of the Center for Computational Mathematics at the Flatiron Institute, a division of the Simons Foundation. With V. Rokhlin, Greengard developed the Fast Multipole Method for problems in gravitation, electrostatics and electromagnetics. Much of Greengard's research has been aimed at the development of high-order accurate integral equation based methods for partial differential equations in complex geometry. He is a member of the National Academy of Sciences, the National Academy of Engineering and the American Academy of Arts and Sciences.

Integrating Theory, Simulation, Machine Learning, and Experiments to Solve Heat Transfer Problems

Alan McGaughey

Trustee Professor of Mechanical Engineering,
Carnegie Mellon University

Time: 9:50 – 10:50 am, July 15 (Friday)

Abstract

I will describe my group's efforts and collaborations to solve two challenging heat transfer problems using a tight integration of modeling and experimentation.

The first part of my seminar will explore the evaporation from a water meniscus, which is relevant for designing heat pipes and understanding evaporation from a nanostructured surface. Frequency-domain thermoreflectance (FDTR) experiments are used to probe the meniscus, whose spatial extent is on the order of microns. Because this length scale is comparable to the FDTR laser spot size, standard analysis approaches that assume a uniform thickness cannot be applied. Instead, a neural network model trained on finite element simulations is built to extract the spatial dependence of the evaporation heat transfer coefficient with submicron resolution. At ambient conditions with a 20 K superheat, the maximum value is on the order of 1 MW/m^2-K.

The second part of my seminar will analyze the metal cap–metal contact–dielectric junction on the top of a transistor. Increasing its thermal boundary conductance (TBC) may enable top-side heat removal. Two-temperature model molecular dynamics (MD) simulations are applied to recreate the experimental observation that the junction TBC increases as the contact thickness increases. The MD simulations reveal a correlation between the junction TBC and the electron–phonon coupling in the contact. This correlation is combined with an analytical solution to the two-temperature model to propose a model that predicts how TBC varies with contact thickness. The model is validated against more than 100 measurements, which collapse onto a single curve. Through physically motivated approximations, the model reduces to a simple thermal circuit that maintains high predictive ability.

Speaker's Bio

Dr. Alan McGaughey is the Trustee Professor of Mechanical Engineering at Carnegie Mellon University with a courtesy appointment in Materials Science & Engineering. He holds B.Eng., M.A.Sc. and Ph.D. degrees in mechanical engineering from McMaster University, the University of Toronto and the University of Michigan. His research group has been supported by National Science Foundation, US Department of Energy, Air Force Office of Scientific Research, Army Research Office and Defense Advanced Research Projects Agency. He is a fellow of the American Society of Mechanical Engineers and the American Physical Society. He won the AFOSR Young Investigator Program award, was a Harrington Faculty Fellow at the University of Texas at Austin and won the Teare Teaching Award at CMU. He has been voted Professor of the Year by the CMU mechanical engineering senior class three times. He has given invited talks and seminars on modeling nanoscale transport phenomena across the United States and in Canada, Chile, China, France, Japan, Korea and Singapore.

Industry session

To foster collaborations and networking with industries, this year, we are pleased to announce an Industry Session from 12:50 – 13:50 on July 15, 2022 (Friday).

The industry panel discussion will feature two panelists from NOVONIX and LIRIO. Each panelist will have 20 mins to introduce the company and discuss any research that may be of interest to our postdocs. Then there will be 20 mins of Q&A.

More information about the companies can be found at NOVONIX and LIRIO.

NOVONIX

LIRIO

Agenda

Day 1 (July 14, 2022)

Event Contact: Xun Li (lix2@ornl.gov)
Event Location: 202B & 202C (Tennessee Room), 5200, ORNL main campus
Note: All times are in EDT (UTC-4)

Time	Event	Speakers
09:00 – 09:30	Welcome Remarks	Dr. Thomas Zacharia, Laboratory Director, Oak Ridge National Laboratory (ORNL); Dr. Moody Altamimi, Director, ORNL Office of Research Excellence; Dr. Rinkle Juneja, Vice President of ORPA
09:30 – 10:30	Keynote Lecture 1	Dr. Madhavi Martin, Oak Ridge Nationa Laboratory
10:30 – 10:40	Break	
10:40 – 11:20	Oral Session 1 – Bio and environmental sciences	**Speakers:** Yi-Syuan Guo, Muneeba Khalid, Bin Wang, Tomas Grejtak **Chair:** Duncan Moseley **Moderator:** Darren Hsu
11:10 – 11:20	Break	
11:30 – 12:10	Oral Session 2 – Neutron and nuclear sciences	**Speakers:** Francisco Gonzalez, Kristel Ghoos, Duncan Moseley, Alexander Laminack **Chair:** Xun Li **Moderator:** Gerry Knapp
12:10 – 13:10	Lunch break	
13:10 – 13:50	Oral Session 3 – Modeling, simulation, and AI - 1	**Speakers:** Matthew Krupcale, Vaidyanathan Sethuraman, Darren Hsu **Chair:** Hector Corzo **Moderator:** Biva Talukdar
13:50 – 14:00	Break	
14:00 – 15:00	Keynote Lecture 2	Dr. Leslie Greengard, New York University
15:00 – 15:10	Break	

15:10 – 15:50	Oral Session 4 – Quantum and condensed matter physics	**Speakers:** Vasudevan Iyer, Xun Li, Sang Yong Song, Hao Ma **Chair:** Duncan Moseley **Moderator:** Gerry Knapp
15:50 – 16:00	Break	
16:00 – 16:40	Oral Session 5 – Materials, manufacturing, and characterization	**Speakers:** Blane Fillingim, QQ Ren, Mitchell L. Rencheck, Aaron Werth **Chair:** Guru Madireddy **Moderator:** Biva Talukdar
16:40 – 16:50	Break	
16:50 – 17:30	Oral Session 6 – Energy and environment	**Speakers:** Xingang Zhao, Rachel Pilla, Nasir Ahmad **Chair:** Xun Li **Moderator:** Jayanthi Kumar

Day 2 (July 15, 2022)

Time	Event	Speakers
09:00 – 09:40	Oral Session 7 – Bio sciences	**Speakers:** Kyle Sullivan, Kevin R. Cope, Jaclyn Noshay, Charles Hodgens **Chair:** Guru Madireddy **Moderator:** Jayanthi Kumar
09:40 – 09:50	Break	
09:50 – 10:50	Keynote Lecture 3	Dr. Alan McGaughey, Carnegie Mellon University
10:50 – 11:00	Break	
11:00 – 11:40	Oral Session 8 - Modeling, simulation, and AI – 2	**Speakers:** Phani R V Marthi, Min-Tsung Kao, Arpan Biswas, Ayana Ghosh **Chair:** Hector Corzo **Moderator:** Darren Hsu
11:40 – 12:50	Lunch break	
12:50 – 13:50	Industry Session	NOVONIX and LIRIO
13:50 – 14:00	Break	
14:00 – 16:00	Poster Session (**Session Chair:** Xun Li)	
16:00 – 16:30	Closing Remarks and People's Choice Awards Announcement	Dr. Moody Altamimi, Director, ORNL Office of Research Excellence; Dr. Rinkle Juneja, Vice President of ORPA

Notes & FAQ

Notes for remote participants

- Please mute your mike while attending the talk.
- You can ask questions to the speaker during the talk in the chat box. At the end of the talk, the session chair will ask your question depending on the availability of time.
- If you have questions at the end of a given talk, please use the “Hands” feature in Microsoft Teams. If the Session Chair allows, please unmute yourself and ask the question.

FAQ

- Is there a registration fee?

  The symposium is funded through financial support from the ORNL Office of Research Excellence. There is no cost to presenters or attendees.
- What will be the length of the oral presentation slots?

  This year, each oral presentation slot will be **10 minutes** in length with 8 minutes for the presentation and the remaining time for Q & A.
- What will be the format of the symposium?

  The symposium will be a hybrid event with both in-person and virtual components. For the oral presentation and keynote sessions, presenters and attendees can attend in-person at ORNL main campus or join virtually through Microsoft Teams. The poster sessions will be in-person only.
- I have been assigned a talk. However, I will be unable to attend. Can I send a prerecorded video of my talk/poster?

  Yes. Please send the prerecorded video by **July 7, 2022** to your assigned session chair. Participants can use Zoom or Microsoft Teams to record their presentation. Please provide your E-mail contact information in the last slide so that the attendees can contact you if they have any question. Please note that, if you are using the Auto-Caption feature, make sure they show exactly what you are saying. Here are a few useful links on “How to prerecord”: Zoom, Teams 1, Teams 2.
- I will be unable to attend the symposium. Will the sessions be recorded?

  Unfortunately, the sessions will not be recorded.
- What will be the size of the poster?

  The poster size is 42” (width) x 36” (height). Please bring your printed poster and arrive at least half an hour before the poster session.

If you have any other questions, feel free to contact the organizers at orpex@ornl.gov.

List of Abstracts – Talks

Organizer's note: Only the speaker of the talk is listed. Please refer to the presentations for author lists, affiliations, and acknowledgements of funding sources, if available.

Talk Schedule for Day 1 (July 14, 2022) – Sessions 1 – 6

Session 1: Bio and Environmental Sciences

Schedule	Speaker	Title
10:40 – 10:50	Yi-Syuan Guo	Engineered habitats for understanding fungal growth in soil
10:50 – 11:00	Muneeba Khalid	Engineered habitats enable in situ visualization of bacterial movement and growth to understand plant-microbe interactions
11:00 – 11:10	Bin Wang	Complex systems, soil microbiomes, and global climate change
11:10 – 11:20	Tomas Grejtak	Enhancing performance and durability of a knife mill for biomass preprocessing by applying advanced blade materials

Session 2: Neutron and Nuclear Sciences

Schedule	Speaker	Title
11:30 – 11:40	Francisco Gonzalez	Experimental Searches for Neutron Oscillations at the Spallation Neutron Source
11:40 – 11:50	Kristel Ghoos	An automated optimization workflow to design the brightest cold-neutron source at the Second Target Station
11:50 – 12:00	Duncan Moseley	Giant doping response of magnetic anisotropy in MnTe
12:00 – 12:10	Alexander Laminack	β-decay of ^{104}Nb Studied via Total Absorption Spectroscopy

Session 3: Modeling, Simulation, and AI – 1

Schedule	Speaker	Title
13:10 – 13:20	Matthew Krupcale	Reintegration of the DELFIC Precipitation Scavenging Module
13:20 – 13:30	Vaidyanathan Sethuraman	Simulation of Branched Polydisperse Lignin Melts
13:30 – 13:40	Darren J. Hsu	High-throughput Pose Refinement Through Induced Fit Ligand Docking

Session 4: Quantum and Condensed Matter Physics

Schedule	Speaker	Title
15:10 – 15:20	Vasudevan Iyer	Understanding material properties at nanometer-length and picosecond-time scales
15:20 – 15:30	Xun Li	Phonons and phase symmetries in bulk CrCl3 from scattering measurements and theory
15:30 – 15:40	Sang Yong Song	Toward control and manipulation of superconducting vortex lattices from nano to mesoscales
15:40 – 15:50	Hao Ma	High Phonon Scattering Rates Suppress Thermal Conductivity in Hyperstoichiometric Uranium Dioxide

Session 5: Materials, Manufacturing, and Characterization

Schedule	Speaker	Title
16:00 – 16:10	Blane Fillingim	Hybrid DED Process Parameter Development across Spot Sizes
16:10 – 16:20	Qing-Qiang Ren	Sigma Phase Evolution and Nucleation Mechanisms Revealed by Atom Probe Tomography in a 347H Stainless Steel
16:20 – 16:30	Mitchell L. Rencheck	Mechanisms for Mechanical Property Degradation from Mechanical Recycling of Carbon Fiber Based Hybrid Composites
16:30 – 16:40	Aaron Werth	EmSense: A High-Resolution Emulated Sensor for Experiments with the DarkNet Infrastructure

Session 6: Energy and Environment

Schedule	Speaker	Title
16:50 – 17:00	Xingang Zhao	Net-zero pledges are not enough: a call for voluntary climate-positive actions from a carbon handprint perspective
17:00 – 17:10	Rachel Pilla	Understanding Temporal Variability in Greenhouse Gas Emissions from Hydropower Reservoirs in Tennessee
17:10 – 17:20	Nasir Ahmad	Infrastructure Failure Cascades in Interdependent Synthetic Networks in the City of Phoenix

Talk Schedule for Day 2 (July 15, 2022) – Sessions 7 & 8

Session 7: Biosciences

Schedule	Speaker	Title
9:00 – 9:10	Kyle Sullivan	Multi-omic network analysis identifies key neurobiological pathways in opioid addiction
9:10 – 9:20	Kevin R. Cope	Exploring the role of lysin motif receptor-like kinases in Populus-microbe interactions
9:20 – 9:30	Jaclyn Noshay	Quantum biological insights into CRISPR-Cas9 sgRNA efficiency from explainable-AI driven feature engineering
9:30 – 9:40	Charles Hodgens	Maximizing the information content of biological experiments: Systems modeling as a tool for learning molecular mechanisms from phenotype

Session 8: Modeling, Simulation, and AI – 2

Schedule	Speaker	Title
11:00 – 11:10	Phani R V Marthi	Advanced PLL-Less Grid-Forming Control Algorithm for MARS
11:10 – 11:20	Min-Tsung Kao	CFD Modeling Supports Developing the Target Segment Conceptual Design for the Second Target Station
11:20 – 11:30	Arpan Biswas	A Latent Bayesian Optimization Approach for High Dimensional Hyperparameter Tuning of Autoencoder: Towards Better Insight of Microscopic Data
11:30 – 11:40	Ayana Ghosh	Building frameworks to bridge electron microscopes with atomistic simulations using machine learning and causal relations

Session 1: Bio and Environmental Sciences

Engineered habitats for understanding fungal growth in soil

Yi-Syuan Guo

Oak Ridge National Laboratory

Measuring microbiome assembly and formation within the developing rhizosphere is essential to reveal the key physical and chemical drivers of this dynamic process. Microfluidics-based engineered habitats provide a window through which this process can be visualized and quantified to assess the response of microbiome members to specific physical and chemical signals. In this study, we have used engineered habitats to measure the impact of spatial confinement and network complexity on fungal growth. These microfluidic environments were fabricated using photo-and soft lithography and assembled onto glass slides. Two-dimensional microfluidic networks were designed to imitate the structure of the soil ,using a Voronoi-tessellation of grid points that can be randomly offset to generate networks with systematically varied complexity and dimensions. Fungal growth of selected soil fungi (*Linnemannia elongata*, *Podila minutissima*, *Fusarium falciforme*, *Laccaria bicolor*, and *Morchella sextalata*)was recorded using time-lapse microscopy. Rates of hyphal penetration and expansion through soil networks were compared and revealed the impact of network complexity and pore size on penetration and expansion rates. Our results demonstrate the utility of using microfluidics to systematically control spatial parameters for understanding fungal migration and point towards the use of such platforms to comprehend microbiome assembly within the rhizosphere.

Engineered habitats enable *in situ* visualization of bacterial movement and growth to understand plant-microbe interactions

Muneeba Khalid

Oak Ridge National Laboratory

Predicting the function of dynamic biological systems requires understanding how the biosystem responds to and alters its physical and chemical environment over time. Here, we describe efforts to develop a platform for tracking eleven species of rhizosphere bacteria through space and time in engineered habitats. A microfluidic device featuring a microchannel design that integrates physical barriers of deterministic shape and size distribution is sealed with a glass slide to provide access for online imaging of bacterial motility. The bacteria are introduced into the device using a plug from an agar plate and images are collected as the bacteria release from the plug and move into the channel. We are examining how the physical architecture, fluid flow, and initial placement influences motility (speed, direction), distribution, and growth of bacteria within the device in the presence or absence of chemoattractants. These experiments are being compared to co-cultures of plants and microbes grown in the same microfluidic devices with a similar architecture. Future work includes correlating bacterial distribution along the roots with the chemical environment to better understand how the plant helps to shape its microbiome.

Complex systems, soil microbiomes, and global climate change

Bin Wang

Oak Ridge National Laboratory

The Nobel Prize in Physics 2021 was awarded to "groundbreaking contributions to our understanding of complex systems," including major advances in understanding and predicting climate change. It is encouraging to see the recognition given to complex systems and climate. However, the Biosphere, integral to the complex climate system, is also a complex adaptive system; predicting the complex Biosphere is equally (if not more) important. In this talk I will focus on modelling soil microbiomes, a tremendously complex component in the Biosphere regarded as the engine driving the Earth's biogeochemical cycles. Using plant litter microbiome as an example system, I model complex microbial systems explicitly by bridging across scales of metabolism, community, and system using a trait-and individual-based approach by implementing eco-evolutionary tradeoffs. Using this model, I revealed a 3-way tradeoff among resource acquisition, drought tolerance, and growth yield to explain microbial systems memory of climatic disturbances, especially drought, manifested in organic matter decomposition. Also, this fine-grained mechanistic model confirms coarse-grained modelling of organic matter decomposition using the Equilibrium Chemical Approximation approach. These exercises highlight the importance of complex systems in understanding microbiomes and shed light on building a predictive understanding of the Biosphere under global climate change.

Enhancing performance and durability of a knife mill for biomass preprocessing by applying advanced blade materials

Tomas Grejtak

Oak Ridge National Laboratory

Biomass size reduction using specialized preprocessing machines such as knife mill, hammer mill or rotary shear is a crucial step in converting biomass into biofuel. However, critical tools of preprocessing equipment are susceptible to excessive wear due to inorganic components of biomass feedstock. These inorganics are typically in a form of silica particles which cause rapid edge blunting and wear of the cutting tools when processing feedstock. Blunt and worn blades significantly reduce the ability to properly grind biomass feedstock which can lead to increased particle size, reduced throughput, higher cost of operation due to more frequent tool replacement and higher energy consumption. In this work we show through extensive experimental testing and characterization that the knife mill performance can be significantly improved by applying proper wear resistant material. Knife mill experiments demonstrated significant improvement in the wear resistance of the blades and enhanced efficiency of the biomass size reduction process by applying tungsten carbide and iron borided blades when compared to commonly used tool steel blades. Techno-economic analysis revealed that these advanced wear resistant materials improve the overall economics of knife milling operation.

Session 2: Neutron and Nuclear Sciences

Experimental Searches for Neutron Oscillations at the Spallation Neutron Source

Francisco Gonzalez

Oak Ridge National Laboratory

The theory of "mirror matter" restores parity to the Standard Model of Particle Physics by hypothesizing an identical copy of Standard Model particles and interactions except with right-handed weak interactions. Since mirror matter would rarely interact with normal matter, particles predicted by this theory provide one potential candidate for dark matter. A version of this theory attempts to explain the $> 4\sigma$ discrepancy between the neutron lifetime τ_n measured in two ways: either counting neutrons remaining in a trap, or counting decay products produced by a cold neutron beam. In the event of a small mass difference Δm between normal and mirror neutron states, the presence of a large magnetic field in the beam lifetime experiment could enhance the probability of oscillations and cause an increase in the measured τ_n. An experiment at the Spallation Neutron Source probed this theory by searching for the hypothesized disappearance and reappearance of neutrons passing through an absorber in-side a magnetic field. Here we present new limits on neutron oscillations into non-degenerate mirror matter. We will also discuss efforts to improve these limits and new searches for other models of n oscillations at neutron scattering facilities.

An automated optimization workflow to design the brightest cold-neutron source at the Second Target Station

Kristel Ghoos

Oak Ridge National Laboratory

The Second Target Station is being designed to become the world's brightest cold neutron source. By bombarding a solid tungsten target with high-energy protons, a large number of neutrons is produced and are subsequently slowed down in the moderators: small vessels with liquid hydrogen surrounded by a beryllium reflector. The more concentrated the region of neutron production, the brighter the neutron beams, but also the larger the dynamic mechanical stresses in the target. Therefore, two competing objectives need to be balanced.

We developed a fully automated optimization workflow that selects the most favorable designs considering both neutronics output and target lifetime. The backbone of the optimization is provided by Dakota, a state-of-the-art optimization toolkit. For each set of design parameters, a new solid geometry is automatically built in Creo and SpaceClaim, exported in Attila4MC to generate the meshed model for MCNP6, evaluated for neutronics output as well as heating rates in MCNP6 and analyzed for target fatigue lifetime in Sierra. This innovative tool enables cutting-edge analysis of new target-moderator designs on the road to world-leading brightness.

Giant doping response of magnetic anisotropy in MnTe

Duncan H. Moseley

Oak Ridge National Laboratory

Developing simple ways to control spin states in spintronic devices is a crucial step towards increasing their functionality. MnTe is a room-temperature antiferromagnet with promising spintronic properties, including thermospintronics and magnon-based devices. Here, we show that incorporating less than 1% Li in polycrystalline MnTe results in a dramatic spin reorientation as observed by neutron diffraction. The behavior of the [0001] magnetic Bragg peak reveals a significant reorientation of the Mn spins from planar in the pure material to almost completely axial with minimal Li-doping. Temperature dependence of the magnetic peaks in Li-doped samples indicates that axial spins shift back to planar suddenly upon approaching the Néel temperature (T_N = 307 K). DFT calculations support the idea that the shift in the Fermi level caused by doping is responsible for switching the material between two competing magnetic ground states. These results pave the way for developing easy switching of magnetic states in functional materials such as spintronic devices and topological insulators.

β-Decay of ^{104}Nb Studied via Total Absorption Spectroscopy

Alexander Laminack

Oak Ridge National Laboratory

Using the Modular Total Absorption Spectrometer (MTAS), β-decay properties of the A=104 decay chain were measured. MTAS is a 1 ton array of NaI that uses its near 100% efficiency to defeat the Pandemonium effect. I will focus on the decay of ^{104}Nb as it is of particular importance to resolving the reactor anti-neutrino anomaly, a deficit of observed anti-neutrinos generated by a nuclear reactor compared to prediction. In this measurement, I update the half-life of ^{104}Nb in the literature, perform the first measurement of the ^{104}Nb β-feeding intensity, as well as present evidence that the previously-assigned spin-parity arrangement for ^{104gs,m}Nb is incorrect.

Session 3: Modeling, Simulation, and AI – 1

Reintegration of the DELFIC Precipitation Scavenging Module

Matthew J. Krupcale

Oak Ridge National Laboratory

The Defense Land Fallout Interpretive Code (DELFIC) is a local nuclear fallout prediction code designed for research and to serve as a standard against which less-capable production codes can be judged. The Precipitation Scavenging Module (PSM) was originally written for DELFIC in the mid-1970s to model the wet scavenging and deposition of fallout particles, but it was removed from DELFIC by 1979. We present a summary of the PSM, which has been reintegrated to the modern version of DELFIC. Fundamentally, the PSM consists of four parts: storm cloud kinematics, hydrometeor microphysics, below- and in-cloud wet scavenging, and transport of the scavenged fallout particles for wet ground deposition. The output of each part is discussed for a test-case input.

Simulations of Branched Polydisperse Lignin Melts

Vaidyanathan Sethuraman

Oak Ridge National Laboratory

Understanding the conformational and dynamical properties of lignin melts is imperative for biofuel production. We developed a software SPRInG (Simple Polydisperse Residue Input Generator), for generating initial configurations of lignin copolymer melts at the atomistic level. We identify the glass transition temperature for lignin melts to be approximately 435 ± 10 K. We demonstrate that these melts behave as Gaussian polymers with a scaling parameter for the segmental radius of gyration that varies between 0.42 and 0.45. Further, we show that the mean squared displacements are independent of molecular weight below the glass transition temperature and they vary inversely with the molecular weight above the glass transition temperature.

High-throughput Pose Refinement Through Induced Fit Ligand Docking

Darren J. Hsu

Oak Ridge National Laboratory

Structure-based drug discovery has become a fundamental step in the pharmaceutical R&D. It aims at predicting whether and how a candidate molecule binds toa model of a therapeutic target. However, current screening methods, such as docking, are incapable of accurately predicting the conformations and require expensive refinement to produce viable candidates. To improve the quality of the predicted structures, and facilitate more accurate downstream modeling, a workflow incorporating accurate physics-based modelstailored for such a data-rich regime is required. Here, we present the development of a high-throughput and flexible ligand pose refinement workflow based on molecular dynamics (MD) simulations. The workflow involves (1) parametrizing candidate ligands, (2) truncating the receptor to the active site core for specialized high-throughput, small-system MD simulation code, (3) assembling the complexes, (4) performing MD simulations, and (5) passing the features calculated from the sampled conformations to a classifier to judge the quality of the refinement. The entire workflow is tailored to large-scale computing facilities, where individual refinement tasks can be trivially parallelized. We show the application of this workflow on a large test set of diverse protein targets. Finally, we discuss the performance and time-to-solution for small and large datasets.

Session 4: Quantum and Condensed Matter Physics

Understanding material properties at nanometer-length and picosecond-time scales

Vasudevan Iyer

Oak Ridge National Laboratory

Technologies needed to solve problems in climate change, energy security, and quantum information rely on a fundamental understanding of novel nanomaterials. Next-generation tools that can probe and manipulate the optical, electronic, and physical properties of nanomaterials at sub-picosecond time scales and nanometer length scales will enable new nanodevice architectures. We have developed a laser coupled scanning ultrafast electron microscope that incorporates cathodoluminescence, photoluminescence, and electron-beam-induced deposition in a single user tool. This tool provides the required high spatial and temporal resolutions and meV spectral resolution at temperatures from 8-300 K. I will describe our recent explorations of near-field plasmon interactions in nanopatch antennas and plasmonic oligomers. Further, I will present the nanoscale energetics of grains and defects in hybrid perovskites and CdSe photovoltaic devices. Lastly, I will describe combined picosecond-pulsed electron and laser beam experiments that enable nanometer scale investigations of carrier diffusion and dynamics, greatly surpassing the optical diffraction limit associated with conventional time-resolved spectroscopies.

Phonons and phase symmetries in bulk $CrCl_3$ from scattering measurements and theory

Xun Li

Oak Ridge National Laboratory

Phonon-derived behaviors are important indicators of novel phenomena in transition metal trihalides, including spin liquid behavior, two-dimensional magnetism, and spin-lattice coupling. However, phonons and their interactions with other quasiparticles have not been adequately explored. In this work, we probe and critically examine the vibrational properties of bulk $CrCl_3$ using inelastic neutron scattering and density functional theory. We demonstrate that magnetic and van der Waals interactions are essential to describing the structure and phonons in $CrCl_3$; however, the specific spin configuration is unimportant. This provides context for understanding thermal transport measurements as governed by dynamical spin-lattice couplings. More importantly, we introduce an efficient 'slide' dynamics for large conventional unit cells that builds insights into phonon dispersions, interactions, and measured spectra in terms of quantum phase interference conditions. This work opens new avenues for understanding phonons in layered magnets and more generally in conventional cell geometries of a variety of materials.

Toward control and manipulation of superconducting vortex lattices from nano to mesoscales

Sang Yong Song

Oak Ridge National Laboratory

In this talk, we will explore in detail the mechanism of superconducting vortex manipulation using a scanning tunneling microscope (STM). The results of vortex manipulation by using STM and its analysis show that the STM tip induces strain on the surface and current density begins to locally heat the area around the tunneling junction. Local weakening of the order parameter in the thermal and strain field around the STM probe lowers the energy of the vortex and attracts the vortex line, allowing the STM tip to become a direct and effective way to arbitrarily manipulate vortices. We suggest that precise control over the high tunneling current can translate into an effective vortex manipulation approach without destruction of the superconducting state, with the possibility of one or several driving mechanisms depending on specific conditions. Our result establishes an understanding of vortex manipulation in STM geometry toward quantitative nanoscale probe of vortex dynamics and a platform to explore vortex manipulation in the context of topological quantum computing.

High Phonon Scattering Rates Suppress Thermal Conductivity in Hyper stoichiometric Uranium Dioxide

Hao Ma

Oak Ridge National Laboratory

Thermal transport in nuclear fuels used for nuclear energy applications is directly tied to performance and reliability. Uranium dioxide (UO_2), one of the most important nuclear fuels, can accumulate excess oxygen atoms as interstitial defects, which significantly impacts thermal transport properties. In this study, thermal conductivities and inelastic neutron scattering (INS) measurements on UO_{2+x} were performed at low temperatures (2-300 K). The thermal conductivity of UO_{2+x} (x = 0, 0.03, 0.04, 0.11) is significantly suppressed compared to UO_2 except near the Néel temperature T_N = 30.8 K, where it is independent of *x*. INS measurements demonstrate that the heat capacities and phonon group velocities of UO_2 and $UO_{2.08}$ are similar and that the suppressed thermal conductivity results from smaller phonon lifetimes. These new insights advance our understanding of thermal transport properties in advanced nuclear fuels and guide safe and economic utilization of nuclear energy.

Session 5: Materials, Manufacturing, and Characterization

Hybrid DED Process Parameter Development across Spot Sizes

Blane Fillingim

Oak Ridge National Laboratory

Directed Energy Deposition (DED) systems now allow for variable laser spot size potential. However, a method should be developed for easier parameter development and translation across a range of spot sizes. A strategy was formed to produce 316L stainless steel walls for beam diameters ranging from 1.5mm – 3.5mm. The developed method keeps energy density constant while varying power, speed, and powder flow rates. Starting with a known 3.5mm spot size parameter set, scan speed and powder flowrate are modified proportionally to the decrease in spot size. Five walls at different beam diameters produced acceptable porosity and hardness values, giving validation to the proposed rule of thumb. Time, material, and net shape considerations are discussed from a DED hybrid manufacturing context. This method is applied to the production of thin walls with voids using DED, a design necessary for damping applications.

Sigma Phase Evolution and Nucleation Mechanisms Revealed by Atom Probe Tomography in a 347H Stainless Steel

Qing-Qiang Ren

Oak Ridge National Laboratory

The size evolution and phase composition of sigma phases were investigated for a 347H stainless steels subject to isothermal aging at 750 °C for up to 10,000 h. Scanning electron microscopy reveals that the sigma phases are present after 336h aging and continue to grow all aging times studied. Atom probe tomography reveals that the sigma phase C content is ~0.14 at.% C after a short 336h aging time, which decreases to ~0.05 at.% after >1,000h aging. The high C concentration for short aging times clarifies its nucleation mechanism, suggesting that the sigma phase nucleates around dissolving metastable M23C6 carbides. Based on the experimental results and thermodynamic simulations, the desirable Nb concentration is discussed to reduce the kinetics of sigma phase growth, and possible design directions are suggested to improve 347H. APT was performed at ORNL's CNMS, a US DOE office of science user facility.

Mechanisms for Mechanical Property Degradation from Mechanical Recycling of Carbon Fiber Based Hybrid Composites

Mitchell L. Rencheck

Oak Ridge National Laboratory

Carbon fiber (CF) reinforced composites are a high-performing and highly utilized material system historically used in aerospace. As the cost of CF decreases, other industries, such as automotive and energy generation, seek to adopt CF composites into their applications. A sudden increase in CF demand may create supply chain issues if the adoption happens without scaling up CF production. A primary solution for reducing the reliance on the CF supply chain, that also enables sustainable manufacturing practices, is to utilize mechanically recycled feedstocks. Here, the effects of utilizing mechanically recycled feedstocks on the mechanical properties of injection molded samples are explored. After establishing the mechanical properties, the mechanisms that caused the change in mechanical properties were analyzed through change in fiber length, fiber content, and molecular weight of the polymer. By determining the mechanical properties and mechanisms in which the properties change through varying recycled content, the assessment of how the material will perform in other manufacturing processes can be inferred. As a result, industry will gain better insight into utilizing mechanically recycled feedstocks to reduce their reliance on the CF supply chain.

EmSense: A High-Resolution Emulated Sensor for Experiments with the DarkNet Infrastructure

Aaron Werth

Oak Ridge National Laboratory

EmSense ("Emulated Sensor") is a device that emulates a high-resolution sensor for a power grid. The device collects raw current and voltage sensor data from ORNL's signature library, which is a dataset derived from various electric utilities. The EmSense packages the data in the form of IEC 61850 Sampled Value (SV) packets and then broadcasts the packets on the network. The purpose of the EmSense is to allow for experimentation with the DarkNet Infrastructure where a variety of power line sensors must be represented along where their typical communication traffic. The EmSense supports the development of the software for receiving and processing the packets in the Distributed Ledger Technology (DLT) framework of the DarkNet Project. This receiving software must be able to process information of high velocity, variety, and volume. The results show that the DLT framework and the trust-anchoring approach can process a large flow of traffic even with six instances of the EmSense device. This was achieved without overfilling packet queues in the memory of the actual hardware of the DLT devices or causing the Computer Processing Unit (CPU) of the hardware to be overwhelmed. The DLTs could also store the data compactly for later analysis.

Session 6: Energy and Environment

Net-zero pledges are not enough: a call for voluntary climate-positive actions from a carbon handprint perspective

Xingang Zhao

Oak Ridge National Laboratory

Signatories of the Paris Agreement are set to miss their climate targets. The net-zero pledges announced to date are insufficient to achieve carbon neutrality, which requires implementation of far-reaching deep decarbonization and carbon removal action plans. In addition to governmental policy support, every company/organization must take voluntary climate-positive actions that can be measured with the concept of carbon handprint. This presentation will introduce a carbon handprint perspective to characterize the environmental benefits of hybrid energy systems (HESs)—a widely applicable solution to a carbon neutral energy future leveraging the capabilities of multiple low-carbon energy sources—that provide heat and electricity to industrial processes. First, carbon handprint and its assessment methods are described. The state of the art of HES-enabled industrial cogeneration is then briefly surveyed. Next, drawing on a case study about a US chemical facility's voluntary initiative to explore replacing its fossil fuel–based cogeneration infrastructure with a clean energy–powered HES, several technically viable scenarios are evaluated to illustrate how the positive-thinking handprint approach informs search for widespread influence pathways. Finally, current knowledge gaps are identified, and opportunities to scale up the handprint-based analysis are outlined with consideration of an expanded role of HESs in fulfilling climate objectives.

Understanding Temporal Variability in Greenhouse Gas Emissions from Hydropower Reservoirs in Tennessee

Rachel Pilla

Oak Ridge National Laboratory

Hydropower reservoirs provide "green" power generation and often many other services, such as drinking water, irrigation, flood control, and recreation. As with most aquatic ecosystems, reservoirs play an important role in global carbon processing and have biogenic carbon emissions that influence their net carbon footprint as renewable energy sources. Anthropogenic pressures such as climate and land-use changes can alter reservoir water quality and biogeochemistry and thereby influence their carbon dynamics and emissions. We sampled multiple hydropower reservoirs in Tennessee at different time points and compared the temporal changes and seasonal variability in emission rates of both CO_2 and methane via different pathways to understand their variability as carbon sources or sinks. Some sites varied between net sinks vs. sources of CO_2 due to altered primary productivity, while other sites showed minimal change in CO_2 emissions. In contrast, methane emissions generally increased over the 10-yeartime period by 1.1 to130 times, which is of particular concern due to its 34 times greater global warming potential compared to CO_2. The balance of CO_2 sink-source dynamics plus the increased methane emissions contributes to understanding the net carbon footprint of these hydropower reservoirs and how it may vary over different temporal scales.

Infrastructure Failure Cascades in Interdependent Synthetic Networks in the City of Phoenix

Nasir Ahmad

Oak Ridge National Laboratory

The acceleration of the Anthropocene demands robust analysis of infrastructure weaknesses and interdependencies towards resilience, especially the cascading failures, how small disruptions can cascade to large-scale outages. Detailed information of infrastructures are publicly unavailable, either due to security or privacy concerns. The dearth of fine-scale infrastructure network data is inimical to resilience analysis. Synthetic networks are promising alternative methods to analyze urban infrastructure networks, their interdependencies, and their propensity for cascading failures. For this study, we build synthetic water and power networks couple them, and simulate disturbances (i.e., water and power failures) for the city of Phoenix. With 10,000 iterations, the results demonstrated that 41% of the time power failures did not lead to water outages. However, the results also revealed a small subset (2%) of power outage scenarios also involved catastrophic water outages, often referred to as "Black Swan" events. We explore dynamics of these outages based on cascade behavior and network configuration. Additionally, we discuss how synthetic networks can guide infrastructure managers in analyzing interdependent urban infrastructure systems to build resilience. Ultimately this study shows potential for expansion of synthetic interdependent network analysis to other infrastructure, such as critical services, transportation networks, communications, and ecological systems.

Session 7: Biosciences

Multi-omic network analysis identifies key neurobiological pathways in opioid addiction

Kyle A. Sullivan

Oak Ridge National Laboratory

Recent genome-wide association studies and omic-wide gene dysregulation studies in postmortem human brains have begun to robustly identify variants and genes associated with opioid addiction (OA). Linking these genes to neurobiological pathways will help to elucidate the biological drivers underlying the observed associations and provide hypotheses for experimental studies. Here we connected OA-associated genes using 15 multiplex network layers from distinct types of biological experimental evidence, including four brain region-specific networks constructed using explainable-AI and RNA-seq expression data. Our analysis focused on 15 OA-associated genes: five GWAS-derived genes (*OPRM1*, *FURIN*, *KDM4A*, *PPP6C*, and *PTPRF*), five differentially expressed genes (*DUSP4*, *DUSP6*, *EGR4*, *ETV5*, and *NPAS4*) from postmortem dorsolateral prefrontal cortex (dlPFC), and five genes from opioid-related epigenetic alterations to the dlPFC, including H3K27 hypoacetylation by ChIP-seq (*ASTN2*, *DUSP4*, *ENOX1*, *GABBR2*, *KCNMA1*) and DNA hypermethylation (NTN1). Using network mining algorithms, we identified a tight network of only 96 additional genes needed to connect all 15 OA-associated genes. Novel OA gene connections were observed, including functional links in the MAPK signaling pathway (*DUSP4*, *DUSP6*, and *PPP6C*) that is modulated by morphine exposure in animal models. Together, we identify a conceptual model underlying OA-associated genes by integrating multi-omic datasets with a systems-level approach.

Exploring the role of lysin motif receptor-like kinases in *Populus*-microbe interactions

Kevin R. Cope

Oak Ridge National Laboratory

For plants, discriminating mutualistic and pathogenic microbes is a matter of survival. All microbes contain microbe-associated molecular patterns (MAMPs) that are perceived by plant pattern recognition receptors (PRRs). Lysin motif receptor-like kinases (LysM-RLKs) are PRRs attuned for binding and triggering a response to specific MAMPs, like chitin oligomers (COs) from fungi and lipo-chitooligosaccharides (LCOs) from fungi and some bacteria. Several LysM-RLKs have been well characterized in several herbaceous model plants, but not in the bioenergy crop *Populus trichocarpa*. As such, we performed a sequence analysis of 18 LysM-RLKs in the *Populus* genome and predicted their function based on phylogenetic analysis with known LysM-RLKs. Using AlphaFold models and molecular dynamics for comparative structural analysis with previously characterized CO and LCO plant receptors, we identified probable ligand binding sites in multiple *Populus* LysM-RLKs. We then used several machine learning-based algorithms to predict consistent binding affinity rankings of *Populus* LysM-RLKs to CO. Finally, we used a modified Random Walk with Restart network-topology based approach to identify a subset of *Populus* LysM-RLKs that are functionally related and propose a corresponding signal transduction cascade. Using these several lines of evidence, we have constructed a model for testing the role of select LysM-RLKs in *Populus*-microbe interactions.

Quantum biological insights into CRISPR-Cas9 sgRNA efficiency from explainable-AI driven feature engineering

Jaclyn M. Noshay

Oak Ridge National Laboratory

CRISPR-Cas9 tools have transformed genetic manipulation capabilities in the laboratory. Despite these advances, CRISPR-Cas9 is prone to error and increased uncertainty exists when this system is applied beyond model organisms or stringently-controlled conditions. While empirical rules-of-thumb have been established for a narrow range of model organisms, mechanistic underpinnings for sgRNA efficiency remain poorly understood. Further, with the extraordinary variation in genomic and epigenomic architectures across species and kingdoms, mammalian data alone are insufficient to generate accurate and predictive models in other organisms. This work establishes a novel feature set and new public resource, created with quantum chemical tensors, that provides a quantitative view of nucleotide positioning and mechanistic interactions. Notably, these features can be applied to any species. These novel encodings of sgRNAs greatly enhance our understanding of the elaborate quantum biological processes involved in CRISPR-Cas9 machinery. We perform feature engineering using an explainable-artificial intelligence model—iterative Random Forest (iRF)—to identify key features influencing the efficiency of a sgRNA. By encoding quantitative attributes of position-specific sequences for *E. coli* sgRNAs, we identify important traits for sgRNA design in bacterial species. We also show that expanding positional encoding with both quantum and one-hot encoded nucleotide base-pair, dimer, trimer and tetramer sequences captures intricate interactions in local and neighboring nucleotides. Additionally, we observe striking variation in highly-influential features between *E. coli* and *H. sapien* genomes. These advances provide avenues for improving the safety and reliability of biosystem design and ecosystem engineering for non-model organisms.

Maximizing the information content of biological experiments: Systems modeling as a tool for learning molecular mechanisms from phenotype

Charles Hodgens

University of Tennessee, Knoxville

Plant leaf pores, or stomata, are important organs for a diverse set of biological processes such as gas exchange and temperature regulation. However, we lack a full understanding of the regulatory events which govern these organs, which has resulted in seemingly paradoxical observations. For example, if we chemically deplete a critical molecular component of the stomatal opening machinery, we initiate opening rather than block it. To better understand this system, we have developed an ordinary differential equation model that describes the subcellular behavior of key proteins in the stoma opening process. However, we face a challenge common in biological modeling. We lack detailed, time-resolved observations of the proteins involved, as these quantitative data would be difficult and expensive to acquire. Instead, we have defined several qualitative constraints that reflect experimentally observed emergent properties of plant stomata. Using these constraints as a guide, we have leveraged methods from Bayesian inference and variational sensitivity analysis to define regions in multi-dimensional parameter space which are consistent with our biological observations. This provides a platform to iteratively propose experiments and hone in on the regions of parameter space most representative of the biological reality.

Session 8: Modeling, Simulation, and AI – 2

Advanced PLL-Less Grid-Forming Control Algorithm for MARS

Phani R. V. Marthi

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Integration of power-electronic (PE)-based resources has been on the rise in the past decade due to factors such as drastic reduction of levelized cost of energy (LCOE), and clean energy initiatives. The hybrid PE-based solar resources might occupy the major share in the integration process and can continue to grow. One such novel application is integrated development of large-scale photovoltaic (PV) systems, energy storage systems (ESS), and high-voltage direct current (HVdc) systems connected through alternating current (ac) transmission systems called Multi-port Autonomous Reconfigurable Solar (MARS) plant. With higher penetration of such PE-based resources, the major chunk of synchronous generation will get replaced leading to drastic unforeseen changes that can affect the system stability. One of the key aspects of this change would be: reduction in grid's capability to recover from frequency disturbances. Therefore, one of the vital objectives of any new grid integrated PE-based resource is to provide advanced control functions like voltage and frequency support to the grid during disturbances. In this research work, advanced phase-locked loop (PLL)-less model predictive control (MPC)-based control algorithm for MARS is proposed. Furthermore, the proposed algorithm is evaluated on Opal-RT real-time platforms through control-hardware-in-the-loop (cHIL) tests.

CFD Modeling Supports Developing the Target Segment Conceptual Design for the Second Target Station

Min-Tsung Kao

Oak Ridge National Laboratory

The second target station (STS) at the Spallation Neutron Source (SNS) is designed to produce the world's highest peak brightness neutron source with a short pulse 700 kW proton beam at 15 Hz using solid rotating tungsten target segments. The tungsten is hipped with tantalum clad to minimize corrosion. Advanced CFD Models were developed in STAR-CCM+, and multiple cooling channel arrangements were studied to improve heat transfer performance for different proton beam profiles, including normal, off-center, peaked, and diffuse proton beams.

The energy depositions in the target segments were calculated from neutronic analysis. The results from transient heat sources that model all proton pulses and equivalent steady state heat sources will be compared and discussed. The impact of Coriolis and centrifugal forces in the rotating target will be discussed. The results from reduced thermal conductivity in tungsten due to irradiation damage will also be compared with that from unirradiated tungsten. The temperature profiles, velocity distributions and pressure drops will be presented.

A Latent Bayesian Optimization Approach for High Dimensional Hyperparameter Tuning of Autoencoder: Towards Better Insight of Microscopic Data

Arpan Biswas

Oak Ridge National Laboratory

With the rapid advancement in material science through ML methods, it is also a challenging task to select and best train a ML model to provide the balance between better physical insights and computational cost. One popular ML technique is joint-rotationally-invariant-Variational-Auto-Encoder (jrVAE) which performs unsupervised classification and disentangle relevant continuous factors of variation at the same time. However, for optimal performance, such model needs proper tuning which can be exhaustive, given the expensive training and some hyperparameters are high dimensional. The performance of jrVAE highly depends on the high-dimensional trajectory of Kullback–Leibler (KL) scale factors. Though Bayesian optimization (BO) is well suited for an expensive optimization problem, it is generally unstable for any high-dimensional parameter optimization. To mitigate this, we present a latent Bayesian optimization (LBO), integrated to the jrVAE model. Here, we first project the N-dimensional KL trajectories into a 2D latent representation through a standard VAE model from a defined ensemble of trajectories. Then, a constrained BO is implemented where the acquisition function samples from the 2D latent space, which can be easily decoded into the N-dimensional trajectory. This workflow has been applied to MNIST data set and plasmonic nanoparticles material system. This approach allows for any high dimensional hyperparameter tuning of other ML models.

Building frameworks to bridge electron microscopes with atomistic simulations using machine learning and causal relations

Ayana Ghosh

Oak Ridge National Laboratory

With the emergence of efficient algorithms and advancement in electron microscopes, there is a scope to utilize theoretical models to guide, perform experiments while refining the parameters in both spaces, to establish a continuous feedback-loop. Instrument specificity, implementation complexity, information transferability by addressing fundamentally different latencies of imaging and simulations, remain the primary challenges. Hence, there is a need to connect this gap to allow for co-navigation of theory and experiment to develop comprehensive physics of materials. This talk will focus on examples of such open-source workflows aiming at establishing a bridge environment between the instrument-specific libraries and general physical analysis. These enable seamless deployment of several deep learning algorithms on-the-fly for appropriate feature finding, property predictions in combination with atomistic simulations to explore underpinning causal mechanisms. Investigations of dynamic evolution of graphene under the electron beam and cation ordering occurring in double perovskite oxides are considered as example case studies to showcase the efficacy of machine learning frameworks combined with casual relations.

List of Abstracts – Posters

Organizer's note: Only the presenter of the poster is listed. Please refer to the posters for author lists, affiliations, and acknowledgements of funding sources, if available.

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Jia Wang	Formation, characterization,and modeling of emergent synthetic microbial communities

The effect of complex macromolecular architecture on the morphology and feature dimensions of block copolymers with highly immiscible blocks

Polyxeni Angelopoulou

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Block copolymers can microphase separate in the bulk or thin film state leading to periodical structures with dimensions scaling down to the sub-5-nm regime. These structures can find multiple applications in pattern transfer, nanoporous materials, as nanotemplates, and more. The versatility and processability of block copolymers and the low cost of the technique have drawn much scientific and industrial interest the last decade. However, in order to attain ultra-small features, low molecular weight block copolymers with highly immiscible blocks have to be used. Macromolecular architecture can play a crucial role, as well, allowing for morphology tuning, and lower dimensions, while providing an additional variable to manipulate the microphase separation process. Not much work has been done on this topic due to inherent synthetic challenges. In this work, the synthesis and characterization of A-*b*-B, A-*b*-B-*b*-A and AB_n block copolymers with highly immiscible blocks are discussed. Promising results regarding domain miniaturization and morphology tuning can be observed.

Optimized jet impingement based direct substrate cooling of Wide bandgap device

Himel Barua

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Thermal management of high-power density wide bandgap (WBG) devices requires high heat extraction which is critical for system reliability. Current study explores jet impingement-based cooling system which has been implemented for direct substrate cooling of two SiC device placed above Direct bonded copper (DBC) substrate. An initial comparison has been conducted to compare direct and indirect substrate cooling by jet impingement. Results show that removing the lower baseplate and corresponding thermal interface material (TIM) reduces the thermal resistance ~25%. Later the jet impingement-based cooling is compared with conventional horizontal liquid cooling for pin fin-based heat sink and GA optimized heat sink. Initial results show, jet impingement-based cooling has high local heat transfer coefficient (htc) but lower average value due to very small heat transfer area. A methodical approach has been undertaken to resolve the issue by increasing number of nozzles and modifying the nozzle design which increases the flow coverage. To lower the pressure-drop in the system, parametric optimization and GA based optimization algorithm has been implemented to get non uniform distribution of nozzle diameters which provides lowest junction temperature and minimum pressure drop.

Hyperledger fabric blockchain-enhanced remote attestation architecture for the electric grid

Raymond C. Borges Hink

Oak Ridge National Laboratory

Background: Resource-constrained intelligent electronic devices (IED) in the electric grid which lack trusted protected modules (TPM) or encryption modules make it difficult to verify data and device trustworthiness through traditionally established means. Aim: The goal is to provide an alternative means to enhance data integrity and device trustworthiness for IEDs in the electric grid within and between substations, control centers, distributed energy resources (DER), and other grid systems. Method: A pilot hyperledger fabric blockchain-based remote attestation framework was implemented on an electrical substation-grid testbed with real substation, control center, and metering components such as protection relays, meters, and human-machine interfaces (HMI). A series of experiments were conducted to test data and device integrity using standard challenge-response remote attestation protocol during emulated cyber events, electrical faults, and maintenance event grid operation. Results: 1) Cyber-induced event operation changes to device configurations were detected using the blockchain-enhanced attestation in near real-time with no negative effects on the operation of the testbed components. 2) During electrical fault and maintenance events non-optimal states were detected when deviating from established baseline signatures recorded in the blockchain. Conclusion: blockchain-enhanced attestation shows promise to increase data and device integrity and trustworthiness in electric grid devices and systems.

Understanding particle leakage for steady state fusion plasma

Kirtan Davda

University of Tennessee, Knoxville

Fusion energy offers carbon free, unlimited energy that has the potential to curb the climate change crisis. As of today, fusion plasma has been sustained today for at least 30 minutes, however, to make it a reliable energy source it needs to operate for 365 days 24x7. The fusion plasma – made up of charged ions and neutrals magnetically contained inside a vessel called the tokamak, tend to have temperatures higher than the core of the sun. These highly charged particles tend to leak from the plasma core and travel towards the walls of the tokamak. These leaked particles near the wall increases localized fueling which could lead to increased material degradation and loss in plasma confinement due to impurity production. The aim of this work is to understand the number of leaked particles needed to induce aforementioned processes that could lead to potential deterioration of plasma. Here we quantify the number of particles in different regions of the plasma vessel experimentally using radiometric, spectroscopic and probe measurements. Thus, comparing the magnitude of leaked particles in different regions will help us reduce plasma contamination and pave the way to steady state fusion plasma.

A Novel Acyclic Ligand for Precision Leaching of Rare Earth Elements

Janel M. Dempsey

Oak Ridge National Laboratory

The rare earth elements (REEs) possess concentrations within the earth's crust comparable to many transition metals, but their similar chemical and physical properties render them difficult to obtain in their pure forms. REEs are often isolated from minerals such as monazite following caustic cracking using sodium hydroxide, whereupon soluble sodium salts are filtered off, yielding an insoluble rare earth hydroxide cake ($RE(OH)_3$). Pure REEs are obtained from the hydroxide cake through multiple dissolution/reprecipitation steps involving large pH changes before conventional solvent extraction methods are employed, an expensive process generating large amounts of hazardous waste. Thus, an approach which facilitates REE separation directly following caustic cracking would be particularly advantageous.

In this work, we introduce acyclopa, an acyclic ligand with high affinity for the larger light REEs. The $RE(OH)_3$s composed of early lanthanides are more soluble than those containing the smaller late lanthanides, so we predict that acyclopa's higher affinity for light REEs will synergize with the higher solubility of light $RE(OH)_3$s to yield selective dissolution of light REEs over heavy REEs. Preliminary results indicate selective dissolution of light $RE(OH)_3$s from a synthetic mixed rare earth hydroxide cake, showing promise as a selective leaching agent for REE mineral processing.

Microgravity Crystallization and Neutron Diffraction of Perdeuterated Tryptophan Synthase

Victoria N. Drago

Oak Ridge National Laboratory

Pyridoxal 5'-phosphate (PLP)-dependent enzymes, present in all forms, are functionally diverse; catalyzing transamination, racemization, β-and γ-elimination, α-decarboxylation, replacement reactions, and phosphorylation. Due to their significance in metabolic pathways and amino acid synthesis, PLP-dependent enzymes are attractive targets for specific inhibitor design. Atomic-level structural studies are necessary to understand how PLP is modulated to perform specific chemistries. Because neutron diffraction provides the ability to directly visualize the position of hydrogens and assign protonation states, it is a favorable technique for studying PLP-dependent enzymes. To overcome the low fluxes of neutron sources, large crystals (≥ 0.5 mm^3) must be used. Microgravity crystallization provides the opportunity to grow large, well-ordered crystals by reducing gravity-driven convection currents that permit variable crystal feeding and impede crystal growth. We developed the Toledo Crystallization Box (TCB), a membrane-barrier capillary-dialysis device, to grow neutron diffraction quality crystals of perdeuterated tryptophan synthase (TS) in microgravity. Here, we present the design of the TCB and the results from Center for Advancement of Science in Space (CASIS) supported International Space Station (ISS) Missions Protein Crystal Growth (PCG)-8 and PCG-15. With microgravity-grown perdeuterated TS crystals, we collected a 2.1 Å neutron diffraction data set and solved the joint X-ray/neutron structure.

A Biomolecular Small Angle Neutron Scattering Contrast Match Point Calculator using 3D Structural Models and Explicit Deuteration

Alan Hicks

Oak Ridge National Laboratory

The contrast variation technique is a fundamental neutron scattering technique for determining structural correlations and shape distributions of macromolecular complexes and their components. Calculation of contrast match points of these complexes is critical for the preparation of SANS experiments. We present a 3D structure-based model with explicit deuteration and solvent for predicting contrast match points of protein, RNA, DNA and lipid nanodiscs as both monomers and complexes. Our method combines a structural model for hydrogen deuterium exchange and an empirical model for deuterium incorporation into non-exchangeable hydrogen sites from mass spectrometry. We demonstrate that this method accurately predicts contrast match points over a wide range of contrast variation conditions. In addition, we demonstrate how our models can investigate scattering vector dependent contrast effects.

SOLPS-ITER modelling of Liquid Lithium Divertor for Advanced Tokamaks

Md. Shahinul Islam

Oak Ridge National Laboratory

Divertors which are located near the x-point of the last closed magnetic surface in advanced tokamaks play an important role in exhausting the heat load from the core plasma .The energy flux to the divertor plates must be mitigated to prevent damage to the plasma facing components; a significant barrier to the success of fusion reactors such as ITER. Lithium (Li) is used as a plasma facing material shows feasibility to enhance the core plasma performance while mitigating the huge energy flux to the divertor. The SOLPS-ITER code is used to analyze the boundary plasma associated with fast flow Li divertor design in advanced tokamaks. Here, the impact of Li on the plasmas is investigated by sourcing Li uniformly along the divertor surfaces and scanning over a large range to understand (1) what level of Li emission is needed to influence the divertor and core plasma conditions, (2) Li-plasma interactions, and (3) to find the tolerable Li flux in terms of core and divertor plasma. In addition, the coupling between a liquid Li MHD heat transfer code and SOLPS is also performed, and the radial profile of evaporated flux is imposed according to the surface temperature calculated by the MHD code.

Removing I/O bottleneck for large scale deep learning applications

Awais Khan

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Scientific communities are increasingly adopting deep learning (DL) models in their applications to accelerate scientific insights. However, with rapid growth in the computing capabilities of HPC supercomputers, large-scale DL applications spend a significant portion of training time performing I/O to a parallel storage system. Several researchers have investigated techniques to optimize DL applications by prefetching and caching. Unfortunately, there exist several challenges to adopting the existing solutions on HPC supercomputers for large-scale DL training applications. A few include failure to fully scale on large-scale HPC supercomputers, lack of portability and generality in design, complex deployment methodology, and being limited to a specific application or dataset. To address these challenges, we propose High-Velocity AI Cache (HVAC), a distributed read-cache layer that targets and fully exploits the node-local storage or near node-local storage technology. HVAC seamlessly accelerates read I/O by aggregating node-local/near node-local storage, avoiding metadata lookups and file locking while preserving portability in the application code. We evaluate HVAC on 1024 nodes of the Summit supercomputer. We compare HVAC with GPFS and XFS-on-NVMe. With four DL applications, we observe an average 25% performance improvement atop GPFS and 9% lower performance against XFS-on-NVMe.

Travel patterns and characteristics of elderly population in the state of New York

Yuandong Liu

Oak Ridge National Laboratory

The elderly population in the U.S. has steadily grown in recent years and is expected to continue growing significantly in the future. It is essential for policymakers to understand travel patterns of their senior citizens to make decisions that meet their growing travel demands. In this study, a detailed examination on travel behaviors and trends of elderly residents within New York State (NYS) was conducted. The 2017 National Household Travel Survey data was used to summarize social-demographic patterns and travel behaviors of the elderly population. The study found that, on average, an elderly NYS resident took fewer daily trips and traveled shorter distance than a non-elderly person from the same region. Such difference has decreased over the past 16 years (since 2001) however. Additionally, many factors were recognized to have affected travel behavior of the elderly population. These include gender, medical condition, driving status, household (HH) income, size, and vehicle ownership. As an example, within the rural NYS region, a typical zero-vehicle elderly HH (defined as a household with at least one person aged 65 or older) took about 40% fewer daily trips than the elderly HH that owned at least one vehicle.

Development of CRISPR based tools for examining microbial ecosystems

Michael Melesse Vergara

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The simplicity and flexibility of CRISPR/Cas offers unprecedented opportunities to rewrite genomes, yet the ubiquity of this technology introduces new challenges. As advances in CRISPR-based genomic engineering technologies continue to be made, the risks of introducing unintended or unwanted genomic alterations into a host cell are ever-present. We have undertaken efforts to perform detailed transcriptomic and proteomic characterizations of Cas9. We have also developed gRNA-based countermeasures that can be applied to inhibit genome engineering activity. These gRNAs, designed to redirect Cas9 specificity towards its own locus, effectively reduce Cas9 transcripts, proteins, and protect the genome.

The principle of adapting the naturally occurring molecular machines for other applications provides another avenue of research. One such tool under development is the use of the CRISPR adaptation machinery for recording transcripts into DNA arrays, called Record-seq. Record-seq uses an innate bacterial protein complex to acquire CRISPR spacers reverse-transcribed from RNA at a rate proportional to the transcript abundance. We are pursuing experiments to build on the current state of this technology and investigate its feasibility as an orthogonally expressed transcriptional recorder. The long-term goals are to optimize Record-seq to monitor transcriptional changes associated with microbial interactions within the plant microbiome.

Synthesis of Phenanthroline and Diglycolamide Ligands for Separation of Lanthanides

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Rare earth elements (REE) mainly lanthanides have important role in US economic, energy and national security grounds due to their prevalent applications in advanced technologies. The separation of lanthanides is a mammoth task due to exorbitant costly methods and environmental challenges. My present work involves the design and synthesis of multidentate, stimuli responsive and preorganized ligands for binding lanthanides. Our focus is to synthesize redox-active water-soluble compound as well as long aliphatic chain tethered highly non-polar ligand which could lead us to develop new environmentally friendly and efficient separation of lanthanides of different sizes. This presentation will highlight our recent results on unravelling the synthesis and selective methods to separate lanthanides.

Material Phase Prediction for Li-ion Battery using Curriculum Learning

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Li-ion Batteries (LIB), one of the most efficient energy storage devices, are widely adopted in many industrial applications. These batteries consist of electrodes that are put together with heterogeneous material compositions. Imaging data of these battery electrodes obtained from X-ray tomography and scanning electron microscopy (SEM) techniques can explain the distribution of material constituents and allow reconstructions to study these transport pathways. Therefore, it can eventually help quantify various associated properties of electrodes, e.g., volume specific surface area, porosity, tortuosity, which determine the performance of the batteries. However, these images often suffer from low image contrast between multiple material constituents (phase boundaries), making it difficult for humans to distinguish and characterize these constituents through visualization. A minor error in detecting a phase boundary instance can lead to a high error in the calculated parameters of material properties (e.g., porosity). Towards this, we present *MatPhase*, a deep-learning framework to identify material constituents and phase transitions from low contrast images of electrode samples. *MatPhase* works well with fewer samples, provide more spatially smooth prediction, hence identifies material constituents with complex phase boundaries than any nontrivial models. We implement a hierarchical curriculum learning technique to solve the task. *MatPhase* consists of three modules: (i) an uncertainty-aware global model trained to get a high-level overview about the distribution of material constituents, (ii) a local model to capture the fine-grained input signals, (iii) an aggregator model to incorporate local and global effects towards predicting chemical phases. On average our frameworks improve prediction upto 8.5% than other non-trivial competitors and state-of-the-arts (SOTA) object detection models.

Understanding zeolite deactivation mechanisms using advanced microscopy techniques

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Conventional liquid fuel is primarily dependent on petroleum and natural gas that both contribute to the emission of anthropogenic CO_2, and hence effect climate change. Consequently, tremendous efforts are being focused on searching for renewable sources to produce biofuels, including direct liquefaction of biomass by fast pyrolysis. Biomass, especially lignocellulose, has proven to be an efficient source for biofuel production. However, the biofuel generated by fast pyrolysis of lignocellulose is accompanied by oxygenates, which limit its practical use in a petroleum refinery. Therefore, reduction of oxygenates from biofuels is a necessary upgrading step. In the catalytic fast pyrolysis method, zeolite HZSM-5 (Si:Al=30) is used to convert the pyrolysis vapor to aromatic molecules. The major drawback with this method is zeolite deactivation by coke formation, causing possible blockage of the porous framework. Thus, it is necessary to study zeolite catalyst deactivation mechanisms. In the present work, we used X-ray photoelectron spectroscopy and advanced microscopy techniques to investigate changes in catalyst morphology due to coke formation, its distribution, and characteristics. Understanding the mechanisms of coke formation will guide process conditions and synthesis methods for industrial scale-up of catalytic fast pyrolysis.

Real-Time Control and Feedback of Hyperspectral Neutron Computed Tomography at the Spallation Neutron Source

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Hyperspectral neutron computed tomography (HSnCT) is a technique that can provide complementary information to X-ray CT. Generally, an HSnCT scan requires several days of measurements since several CT scans are performed simultaneously, each at a neutron wavelength band. Although advanced reconstruction methods, such as the modeled-based iterative reconstruction (MBIR), can reconstruct hyperspectral (HS) projections in less than an hour, the decision to acquire a new angle or stop the experiment is usually made without knowledge of the reconstructed data. Therefore, a highly effective measurement for which preferred projection angles or acquisition times are selected is one of the current challenges in performing an HSnCT. Theoretically, the quality of the reconstruction is the decision criteria to stop an HSnCT data acquisition. However, there is no previous high-quality reconstructed data that can serve as a reference for the quality assessment (QA) because of the uniqueness of each research sample and experiment configuration. This research project aims at providing real-time optimization of an HSnCT scanning strategy using machine-learning (ML) algorithms to make decision on what projection angle to acquire while providing real-time feedback of the state of reconstruction. Moreover, algorithms are developed to evaluate when a scan has reached the desired reconstruction quality set in place prior to starting the scan.

Formation, characterization and modeling of emergent synthetic microbial communities

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Microbial communities colonize plant tissues and contribute to host function. How these communities form and how individual members contribute to shaping the community structure are not well understood. Synthetic microbial communities composed of well-studied individual isolates can be valuable model systems for elucidating the organizational principles of communities. Using genome-defined strains, systematic analysis by computational modeling can lead to mechanistic insights about potential metabolic interactions among species. In this study, 3 bacterial strains isolated from the *Populus deltoides* rhizosphere were co-cultured in a complex medium environment and found to form stable microbial communities. The community stabilized to the same structure after several passages when starting with significantly different initial relative ratios. To unravel the underlying metabolic interactions within the community, dynamic flux balance analysis was used to model microbial growth during serial dilution process and predict metabolic interactions involved during the organization of the microbial communities. These analyses were complemented by metaproteomics of the community. Interrogating the mechanisms of interaction among plant-associated microorganisms provides insights into strategies for engineering microbial communities that can potentially increase plant growth and disease resistance. Deciphering the metabolic potentials and emergent properties of microbial communities will enable the design of synthetic consortia with desired biological functions.

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