9TH ANNUAL OAK RIDGE POSTDOCTORAL ASSOCIATION RESEARCH SYMPOSIUM

VIRTUALLY AT

JULY 28–29, 2021

Contents

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. L. Mahadevan (Harvard University), Dr. Jeffrey S. Vetter (ORNL) and Dr. Julia A. Kornfield (California Institute of Technology) 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 Cydne Albers, Jeffrey Cornett, Douglas Edwardson, Dionne Harper, Tina Snyder, and Laurie Varma for their contribution to the success of this event.

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Keynote Speakers

Dr. L. Mahadevan

Prof. L. Mahadevan

Lola England de Valpine Professor of Applied Mathematics, of Organismic and Evolutionary Biology, and of Physics,
Harvard University
Title Predicting and Programming Shape: Geometry, Physics and Biology

Abstract

Shape enables and constrains function. In the first part of the talk, I will discuss aspects of how functional shape arises in living systems - one of the grand problems in biology. Using experiments, theory and computation allows us to describe the morphogenesis of tissue shape using examples such as the (1d) growth and form of a shoot, the (2d) rippling of a leaf, the (2+ d) coiling of the gut and the (3d) folding of the brain. In the second part of the talk, I will switch to the inverse problem of how to program and design shape, inspired by artists. I will describe how science and mathematics is slowly beginning to catch up with the remarkably imaginative ways of using sharp folds and cuts to create complex shapes from a simple sheet of paper. Using a combination of experimental, computational and theoretical approaches, I will discuss 2d (and 3d) kirigami tilings for planar shapes, 3d (and 4d) origami tessellations for complex surfaces, and 4d printing and growing strategies for flowers and faces. Along the way, I will indicate how these pan-disciplinary problems enrich their roots in mathematics, physics and biology, with potential implications for technology.

Biography

Following his undergraduate studies at the Indian Institute of Technology, Madras, L. Mahadevan moved to the US and received his PhD at Stanford. He started his independent career as a faculty member at MIT and then moved to Cambridge University before returning to Cambridge, this time to Harvard, where he is the de Valpine professor of applied mathematics, physics, and organismic and evolutionary biology. His work attempts to understand motion and matter at the observable scale of “middle earth” by integrating experiments, theory and computation. Areas of interest include the patterns of shape and

flow of inanimate matter and the dynamics of sentient living matter that can self-organize, perceive and act. Mahadevan is a MacArthur Fellow and a Fellow of the Royal Society.

Dr. Jeffrey S. Vetter

Corporate Fellow and Head for Advanced Computing Systems Research Section, Oak Ridge National Laboratory
Title Preparing for Extreme Heterogeneity in High Performance Computing

Dr. Jeffrey S. Vetter

Abstract

While computing technologies have remained relatively stable for nearly two decades, new architectural features, such as heterogeneous cores, deep memory hierarchies, non-volatile memory (NVM), and near-memory processing, have emerged as possible solutions to address the concerns of energy-efficiency and cost. However, we expect this 'golden age' of architectural change to lead to extreme heterogeneity and it will have a major impact on software systems and applications. Software will need to be redesigned to exploit these new capabilities and provide some level of performance portability across these diverse architectures. In this talk, I will survey these emerging technologies, discuss their architectural and software implications, and describe several new approaches (e.g., domain specific languages, intelligent runtime systems) to address these challenges.

Biography

Jeffrey Vetter, Ph.D., is a Corporate Fellow at Oak Ridge National Laboratory (ORNL). At ORNL, he is currently the Section Head for Advanced Computer Systems Research and the founding director of the Experimental Computing Laboratory (ExCL). Previously, Vetter was the founding group leader of the Future Technologies Group in the Computer Science and Mathematics Division from 2003 until 2020. Vetter earned his Ph.D. in Computer Science from the Georgia Institute of Technology. Vetter is a Fellow of the IEEE and AAAS, and a Distinguished Scientist Member of the ACM. In 2010, Vetter, as part of an interdisciplinary team from Georgia Tech, NYU, and ORNL, was awarded the ACM Gordon Bell Prize. In 2015, Vetter served as the SC15 Technical Program Chair. His recent books, entitled *Contemporary High Performance Computing: From Petascale toward Exascale (Vols. 1 and 2),* survey the international landscape of HPC. Learn more information at https://ft.ornl.gov/ vetter/.

Dr. Julia A. Kornfield

Elizabeth W. Gilloon Professor of Chemical Engineering,
California Institute of Technology
Title Flow, Structure and Function

Prof. Julia A. Kornfield

Abstract

My research weaves together the flow, structure, and function of polymers, and over the years, I have come to appreciate the unexpected ways that those three themes are woven into my life and work. The projects I've worked on may seem unrelated, but they are connected by my love of seeing how molecules move, the flow. I enjoy using the knowledge gleaned from these projects to then design polymers to fulfill new functions. Looking back, I see that the polymeric systems I decided to study and the methods I chose to use from NMR methods to observing dynamics in polymers to x-ray and neutron scattering methods to watch structure emerge, were influenced by my desire to work with people who inspire me. This lecture celebrates the flow of thoughts, ideas and inspiration and reflects on the structure of our intellectual community and its function of perpetuating traditions of mutual support. For me, this pursuit of the unexpected and finding inspiration within this community is a recipe for finding joy in doing science. After my talk, I look forward to hearing about your accomplishments, questions and plans.

Biography

Julia A. Kornfield, Elizabeth W. Gilloon Professor of Chemical Engineering at the California Institute of Technology (Caltech), is an expert in polymer science. She has applied small angle neutron and x-ray scattering to diverse systems, including end-associative polymers for aviation safety and security (Wei *et al.*, Science 2015), flow-induced crystallization of polymers (e.g., Science 2007) and the effects of flow on polymer self-assembly (e.g., Science 1997). Since she joined the Caltech faculty in 1990, Kornfield has received the Dillon Medal of the American Physical Society, been elected Fellow of the American Physical Society and the American Association for the Advancement of Science and received the Bingham Medal of the Society of Rheology, among other honors. She holds 39 patents and is a co-founder of Calhoun Vision, which uses polymers developed at Caltech to customize vision by noninvasively optimizing a lens after it is implanted into a

patients' eye (FDA-approved 2017). Thus, her work spans from fundamental research on the molecular basis of polymer structure and properties, to commercialization of polymers that improve sustainability health and safety.

Industry Session

To foster collaborations and networking with industries, this year, we are pleased to announce an Industry Session from 11:10 – 12:20 on July 29, 2021 (Thursday). The representatives from each industry will give a 5-7 minute presentation and will be followed by a breakout session for each industry. The breakout session is aimed at having an interactive session between the symposium attendees and the industrial representatives.

The following companies are expected to be present at the Industry Session:

Choice Spine

HEVO Inc.

NellOne Therapeutics

PlayCore, Inc.

Timetable

WR: Welcome Remarks, KL: Keynote Lecture, OS: Oral Session
PS: Poster Session, IS: Industry Session, CR:Closing Remarks
Note: all times are EDT

Day-01: Wednesday, July-28-2021

Event contacts	Xingang Zhao, zhaox2@ornl.gov; Vaidyanathan M. Sethuraman, v0e@ornl.gov		
Location	Online via Teams (WR, KL, OS, IS, and CR) and iSeeVC (posters)		
09:00–09:30	WR	Welcome Remarks	Dr. Thomas Zacharia, Director, ORNL; Dr. Moody Altamimi, Director, Office of Research Excellence, ORNL; Dr. Phil Lotshaw, President, ORPA
09:30–10:18	OS	Oral Session 1: Materials & Neutron Sciences	Wellington Claiton Leite, Matthew Heath, Manjula Senanayake, Tao Xie, Duncan H. Moseley, Hui Li **Session Chairs:** Nikhil Sivadas, Zach Liu
10:18–10:30	Break		
10:30–11:18	OS	Oral Session 2: Materials & Additive Manufacturing	Matthew Bryan, Shree Ram Acharya, Nikhil Sivadas, Gerry Knapp, Matthew Korey, Yiyu Wang **Session Chairs:** Zach Liu, Nikhil Sivadas
11:18–11:30	Break		
11:30–12:18	OS	Oral Session 3: Bio & Environmental Sciences, Part - I	Jia Wang, Fernanda Santos, Kuntal De, Debjani Pal, Tomasz Krzysztof Bednarski, Leobarda Robles-Martinez **Session Chairs:** Duncan Moseley, Joseph Chapman
12:18–13:00	Break		

13:00–13:40	OS	Oral Session 4: Bio & Environmental Sciences, Part - II	Zheng Cui, Siru Liu, Tao Yao, Courtney Walton, Spencer J. Washburn **Session Chairs:** Marie Romedenne, Dhruba Chowdhury
13:40–13:50	Break		
13:50–14:38	OS	Oral Session 5: Modeling & Simulation, Computing, and AI, Part - I	Nicholson Konrad Koukpaizan, Adam Spannaus, Paul Eller, Arnab Kumar Paul, N. S. Harsha Gunda, Arpan Sircar, **Session Chairs:** Nicholson Koukpaizan, Murali Gopal Muraleedharan
14:38–15:00	Break		
15:00–16:00	KL	Keynote Lecture	Dr. L. Mahadevan, Harvard University
16:00–16:10	Break		
16:10–16:58	OS	Oral Session 6: Modeling & Simulation, Computing, and AI, Part - II	Dhrubajit Chowdhury, Philipe Ambrozio Dias, Satarupa Bal, Kubra Yeter-Aydeniz, Andre Sieverding, Rinkle Juneja **Session Chairs:** Murali Gopal Muraleedharan, Nicholson Koukpaizan

Day-02: Thursday, July-29-2021

09:00–09:40	OS	Oral Session 7: Fuel & Nuclear Engineering	Matthew Krupcale, Richard Reed, Erik Nykwest, Erin Creel, Yeonshil Park **Session Chairs:** Allen Scheie, William Meier
09:40–10:00	Break		
10:00–11:00	KL	Keynote Lecture	Dr. Jeffrey S. Vetter, ORNL
11:00–11:10	Break		

11:10–12:20	IS	Industry Session	ChoiceSpine, Knoxville, TN HEVO Inc., Brookyln, NY NellOne Therapeutics, Knoxville, TN PlayCore, Chattanooga, TN
12:20–13:00	Break		
13:00–14:00	KL	Keynote Lecture	Dr. Julia A. Kornfield, California Institute of Technology
14:00–14:10	Break, switch from Teams to iSeeVC for poster session		
14:10–15:50	PS	Poster Session	**Session Chairs:** Allen Scheie, Joseph Chapman, Dhruba Chowdhury
15:50–16:00	Break, switch from iSeeVC to Teams		
15:50–16:00	Break		
16:00–16:30	CR	Closing Remarks	Dr. Moody Altamimi, Director, Office of Research Excellence, ORNL; Phil Lotshaw, President, ORPA

Notes & FAQ

Notes

- 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 upon 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

- **Q**: What will be the length of the oral presentation slots?
  This year, each oral presentation slot will be 8 minutes in length with 6 minutes for the presentation and the remaining time for Q & A. The oral presentation sessions will be presented through Microsoft Teams.
- **Q**: 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.
- **Q**: I have been assigned a poster/talk. However, I will be unable to attend. Can I send a prerecorded video of the talk/poster?
  Yes. Please send the prerecorded video by 11:59 pm on **July-25-2021** to the organizers at v0e@ornl.gov or zhaox2@ornl.gov. 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 questions. Please note that, if you are using the Auto-Caption feature, please make sure they show exactly what you are saying. Below are a few useful links on "How to prerecord?"

  Zoom: https://www.youtube.com/watch?v=GjhHsTmXCKg
  Microsoft Teams: https://www.youtube.com/watch?v=ymnTVkIGtAY
  Microsoft Teams: https://office365itpros.com/2020/05/15/recording-screen-output-microsoft-stream/amp/

- **Q**: I will be unable to attend the symposium. Will the sessions be recorded? Unfortunately, the sessions will not be recorded.

iSeeVC Poster Presentation Platform

- **Q: How will you hold a virtual poster session?**

  We will be using a software called iSeeVC for the virtual poster session. The environment is built like a video game - everyone will have an avatar which can be moved about the virtual environment. Posters will be put on the walls and the attendees can walk up and interact with the poster presenter and others nearby, using the **spatial audio** feature to limit conversations a user hears to those spatially nearby in the environment.

- **Q: Where can I download the iSeeVC platform from?**

  For information about downloading iSeeVC (please use the **iSee2020** version) and some basic functionality, please review this PowerPoint presentation. Below are some additional tips which may enhance your user experience. Please note that only Windows and macOS support this platform. Linux OS does **NOT** support iSeeVC.

- **Q: [For Presenters Only] What is the recommended poster size?**

  The recommended size of the poster is **A1 landscape (W: 33.1 in x H: 23.4 in)**. Note that this size is much smaller than the traditional physical poster presentation boards. Please **DO NOT** make the poster size bigger than this as it will not be visible. Please adjust the font size accordingly. A font size of 12-18 points will be appropriate as opposed to 18-36 points in the physical poster presentation boards. Note that you can zoom-in to a particular part of the poster while presenting.

- **Q: [For Presenters Only] In which format should I upload my poster file?**

  Please upload the poster file in PDF format ONLY.

- **Q: [For Presenters Only] How should I name my poster file?**

  Name of the file should be Lastname_FourKeywords.pdf. The four keywords should summarize the contents of the poster. Make sure the keywords are separated by a space. While the attendees walk along the poster presentation room, this will be the title they will see on top of each poster. Please note that the four keywords in

the filename is DIFFERENT from the poster title that you will be putting *inside* the poster.

- **Q: [For Presenters Only] When and how should I upload my poster?**

  Make sure the posters are uploaded to this LINK by 11:59 pm on **July-25-2021**. We will upload it in the software platform and the presenters will be able to view their posters on July-27-2021. Please note that, NO changes to the posters will be allowed once uploaded.

- **Q: Why is the installation unsuccessful? Why is my iSeeVC screen simply grey after logging in?**

  Make sure that you have disabled any VPN application (such as GlobalProtect, Cisco Connect) or security software (such as Netskope Client) while downloading, installing, and running iSeeVC.

- **Q: Can I run Teams in parallel?**

  Please avoid doing so. Occasionally, it messes up the iSeeVC platform.

- **Q: Where can I get the meeting ID to join iSeeVC?**

  The meeting ID will be provided to all registered external participants and distributed within ORNL. Please use "Join as a Guest" and give that meeting ID.

  Additional tips: Please make sure you read the following.

- Close all other apps while using iSeeVC. Because of the computer load needed to render the graphics, iSeeVC can be a bit intense. Closing all other apps can increase performance.

- If you have trouble reading the poster, right click on the poster and select **"Overlay View"**. This will allow the poster to fill your iSeeVC screen. If you want to switch your view back, right click and select "3D view". In our experience, the "Overlay View" is the optimal way to present the poster.

- Want to check out iSee before the poster sessions? The rooms will be live soon. Use the meeting ID to access the rooms at any time leading up the poster session. The posters will be available on both July 28 and July 29, in case you cannot make it to all the posters you would like to visit during the poster session. However, presenters will only be available during the poster session.

List of Abstracts – Talks

Wednesday (July 28)

>>Timetable

Oral Session 1, Materials & Neutron Sciences

Time	Presenter	Title
9:30-9:38	Wellington Claiton Leite	Studies of DMPC/CHAPSO Bicelles by Small-angle neutron scattering (SANS) and Contrast Variation
9:38-9:46	Matthew Heath	A Portable Pixelated Fast-Neutron Imaging Panel
9:46-9:54	Manjula Senanayake	Structure and Morphology of Plant Polymers in Transgenic Poplar Stems used for Production of Advanced Biofuels
9:54-10:02	Tao Xie	Dynamical spin excitations in an Yb-based delafossite
10:02-10:10	Duncan H. Moseley	Doping-Controlled Spin Reorientation in MnTe
10:10-10:18	Hui Li	Adsorption and oxidative degradation of organic compounds on structurally diverse Mn-oxides

Oral Session 2, Materials & Additive Manufacturing

Time	Presenter	Title
10:30-10:38	Matthew Bryan	Nonlinear Propagating Modes in Fluorite Structured Crystals
10:38-10:46	Shree Ram Acharya	The Phase stability and tuning of magnetism of layered $SrFeO_2$ with Hydrogen from topochemical reduction
10:46-10:54	Nikhil Sivadas	Anharmonic stabilization of ferrielectricity in $CuInP_2Se_6$
10:54-11:02	Gerry Knapp	Applied process modeling to meet additive manufacturing challenges
11:02-11:10	Matthew Korey	Big Area Additive Manufacturing of Recycled Carbon Fiber-Filled ABS
11:10-11:18	Yiyu Wang	Residual Lifetime Assessment of Service-Aged Dissimilar Forge 91-Pipe 91 Steel Header Welds with High Temperature Digital Image Correlation.

Oral Session 3, Bio & Environmental Sciences, Part I

Time	Presenter	Title
11:30-11:38	Jia Wang	Formation, characterization, and modeling of emergent synthetic microbial communities.
11:38-11:46	Fernanda Santos	Interactive effects of manganese availability and warming on CO_2 fluxes from soils during decomposition

11:46-11:54	Kuntal De	The Plasminogen-Apple-Nematode (PAN) domain suppresses plant immunity
11:54-12:02	Debjani Pal	PAN domain of proteins regulates immunosuppression
12:02-12:10	Tomasz Krzysztof Bednarski	Investigating the ability of SERCA2b activation to mitigate hepatic lipotoxicity
12:10-12:18	Leobarda Robles-Martinez	Role of nSMase-2 in the onset of glucocorticoid hypersensitivity in hepatocytes

Oral Session 4, Bio & Environmental Sciences, Part II

Time	Presenter	Title
13:00-13:08	Zheng Cui	Discovery and Characterization of Pyridoxal-5'-Phosphate-Dependent Alkyl Transferase in Nucleoside Antibiotic Muraymycin Biosynthesis
13:08-13:16	Siru Liu	Leveraging Transfer Learning to Analyze Behavioral Intentions Toward COVID-19 Vaccines
13:16-13:24	Tao Yao	A trans-eQTL, PtrXBAT35, regulates root architecture and shoot stature in Populus
13:24-13:32	Courtney Walton	Chemical Imaging of Microbial and Plant Systems via Liquid-Extraction Mass Spectrometry
13:32-13:40	Spencer J. Washburn	Understanding the Effects of Nutrient Concentration on Mercury Cycling within Fluvial Periphyton

Oral Session 5, Modeling & Simulation, Computing and AI, Part I

Time	Presenter	Title
13:50-13:58	Nicholson Konrad Koukpaizan	A Comparison of OpenACC and OpenMP Target Offload for NVIDIA and AMD GPUs: Application to Computational Fluid Dynamics
13:58-14:06	Adam Spannaus	Topological Interpretation of Deep-Learning Models
14:06-14:14	Paul Eller	Parallel Accelerated 1-bit Dense Matrix Multiplies for Large-scale Correlation Analysis
14:14-14:22	Arnab Kumar Paul	Analyzing Machine Learning Workloads on Leadership Scale HPC Storage Systems
14:22-14:30	N. S. Harsha Gunda	High performance computing and modern data analytics to develop accurate ReaxFF interatomic potentials.
14:30-14:38	Arpan Sircar	Coupled multi-physics simulations using preCICE

Oral Session 6, Modeling & Simulation, Computing and AI, Part II

Time	Presenter	Title
16:10-16:18	Dhrubajit Chowdhury	Optimization of Water Systems through Model Free Controllers
16:18-16:26	Philipe Ambrozio Dias	Towards generalizable, scalable & explainable AI methods for satellite imagery analysis
16:26-16:34	Satarupa Bal	Comprehensive Evaluation of Semi-Conductor Technology for Solid-State Circuit Breaker Application
16:34-16:42	Kubra Yeter-Aydeniz	Continuous Variable Quantum Imaginary-Time Evolution Algorithm for Quantum Field Theories
16:42-16:50	Andre Sieverding	Nucleosynthesis with Modern Supernova Simulations
16:50-16:58	Rinkle Juneja	Symmetry consequences on phonons and thermal transport

Thursday (July 29)

Oral Session 7, Fuel & Nuclear Engineering

Time	Presenter	Title
9:00 - 9:08	Matthew Krupcale	Overview of the DELFIC atmospheric transport model for nuclear fallout modeling
9:08 - 9:16	Richard Reed	Reactor modeling and simulation to underpin the science of safeguarding thorium fuel cycles
9:16 - 9:24	Erik Nykwest	Role of lattice dynamics in the structural stability of uranium Laves phasess
9:24 - 9:32	Erin Creel	Effects of Ink Concentration and Mixing on Fuel Cell Catalyst Layers.
9:32 - 9:40	Yeonshil Park	Impact of fuel chemistry and distillation temperature on emissions from a single-cylinder multimode engine.

Wednesday

Oral Session 1

Studies of DMPC/CHAPSO Bicelles by Small-angle neutron scattering (SANS) and Contrast Variation

Wellington Claiton Leite

ORNL

Bicelles provide a versatile nanostructured fluid environment that can be used as a model system and platform for studies of membrane proteins. They represent a middle ground between micelles and environments such as lipid bilayer membranes. Nature has evolved ways to structure its lipid bilayers and to organize them into continuous systems that facilitate transport and metabolism. On the other hand, human designed systems are still a far cry from such intricately controlled structures. It may however be speculated that by selection of lipid and cosurfactant molecules, similarly sophisticated bilayer structures could be generated and their morphology be controlled. In this contribution we will present new data on the DMPC/CHAPSO bicelle system. We have studied the influence of temperature and of added co-surfactant DDM on the DMPC/CHAPSO assembly. Small-angle neutron scattering (SANS) data, measured on a series of different isotope contrast scenarios provide a detailed picture about the distribution of the different molecules in different domains of the bicelle. Our data suggests that increased temperature and added co-surfactant may increase mixing of the primary bilayer constituents and thereby can alter the nanoscale dimensions of bicelle membrane channels as well as drive larger scale assembly into an extended worm-like bicelle system.
Oak Ridge National Laboratory is managed by UT-Battelle, LLC for the U.S. Department of Energy under contract no. DE-AC05-00OR22725. This research is supported by the Office of Biological and Environmental Research in the DOE Office of Science. This research used resources at the High Flux Isotope Reactor, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.

A Portable Pixelated Fast-Neutron Imaging Panel

Matthew Heath

ORNL

Oak Ridge National Laboratory is developing a portable, pixelated fast-neutron imaging panel for associated particle imaging (API). The panel is intended to be capable of both transmission and induced reaction imaging, allowing for a full 3-dimensional density map of an object without requiring 360° access. Unlike the current generation of API-based neutron imaging systems, this panel is intended to be field deployable. The panel is composed of an array of optically-isolated pulse-shape discriminating plastic scintillator pixels which are optically coupled to an array of position sensitive photomultiplier tubes in a hand-carryable package. Each quadrant of the panel is read out with a resistive charge-division network allowing it to be read out with only 4 channels that preserve the average position of detected light. This provides the fast timing and modest spatial resolution required for high-quality images. The design of the panel and initial testing of the light collection and position encoding electronics is presented herein.

Structure and Morphology of Plant Polymers in Transgenic Poplar Stems used for Production of Advanced Biofuels

Manjula Senanayake

ORNL

Lignocellulosic biomass is sustainable, carbon dioxide neutral and non-competitive energy sources to produce advanced biofuels and biproducts. However, deconstruction of lignocellulose into its simple building blocks by simple hydrolysis process is constrained by the strong inter chain packing of cellulose fibrils and the associated lignin and the hemicellulose polymers. Regulation of lignin biosynthesis in the plant cell wall will reduce secretion of lignin and ultimately results in the packing of microfibrils. Here, we studied the effects of QsuB expression level, which regulate the lignin biosynthesis pathway, in three transgenic species of poplar trees, and compared with the wildtype (WT). The level of the expression of QsuB varies as Q1 > Q15 > Q5 > WT. The biochemical characterization shows Q1 and Q15 has 15% less lignin and higher hemicellulose than Q5 and WT. Small-Angle Neutron Scattering (SANS) results show that the cross-sectional radius of the cellulose microfibrils varies as Q5 = Q15 = WT < Q1. With increasing levels of QsuB expression, the inter microfibril distances increases and at highest expressed QsuB mutant, Q1, no ordering of microfibrils was observed. These molecular-level structural knowledge will particularly help understand the mutants best suited for conversion into efficient biofuels productions.

Dynamical spin excitations in an Yb-based delafossite

Tao Xie

ORNL

We present a systematic neutron scattering study on a perfect two-dimensional triangular magnet, $CsYbSe_2$, which is a member of the large quantum spin liquid candidate family rare-earth chalcogenides. The inelastic neutron scattering spectra evolve from highly damped continuum-like excitations at zero field to relatively sharp spin wave modes at higher fields. The spin excitation spectra can be well described by the dynamical spin structure factors obtained from dynamical density-matrix renormalization group calculation with a nearly isotropic Heisenberg model considering the nearest-neighbor magnetic coupling. Our work provides a reasonable Hamiltonian that is appropriate for the different quantum phases in this ideal S = 1/2 triangular-lattice antiferromagnet.

Doping-Controlled Spin Reorientation in MnTe

Duncan H. Moseley

ORNL

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 future spintronic materials.

Adsorption and oxidative degradation of organic compounds on structurally diverse Mn-oxides

Hui Li

ORNL

Soil is a major carbon (C) reservoir. Much of this soil C is intimately associated with minerals. A vast body of literature has investigated the stability of C associated with Fe-(hydr)oxides, whereas the role of Mn-oxides in regulating soil C storage is relatively unexplored. As an essential trace metal with strong redox potential, Mn may play multiple competing roles in regulating C cycling in soils by adsorbing and/or oxidizing soil organic matter. In the present study, seven aromatic/aliphatic organic carbon (OC) compounds were reacted with three common Mn(III/IV)-oxides comprised of layer or tunnel structures to study reaction kinetics and interaction mechanisms. Effects of mineral crystallinity and structure, solution pH, and C:Mn ratios on Mn–C interaction mechanisms were investigated, using TOC, ICP-OES, XAS, XRD, FTIR and HPLC. Results indicated that different Mn-oxides possessed different sorption and/or oxidation capacities under different pH conditions, while OC compounds varied in their binding mechanisms. Cryptomelane, a tunnel-structured Mn-oxide with high specific surface area and point of zero charge, showed stronger reactivity with OC than layer-structured hydrous Mnoxide and birnessite. Lower pH and higher C:Mn ratios favored adsorption and/or redox reactions between OC and Mn-oxides. Phthalate and propanol primarily sorbed on Mn-oxides with no detectable mineral dissolution. However, citrate, pyruvate, ascorbate, catechol, and hydroquinone dissolved appreciable amounts of Mn-oxides and/or induced phase transformation. The average oxidation state of Mn in the solid phase did not change during reaction with citrate but decreased significantly during reaction with the other compounds, suggesting ligandpromoted and reductive dissolution mechanisms, respectively. Together, these results provided more detailed fundamental insights into reactions happening at organo-mineral interfaces in soils.

Wednesday

Oral Session 2

Nonlinear Propagating Modes in Fluorite Structured Crystals

Matthew Bryan

ORNL

The vibrational energy of crystals is known to propagate in a fixed number of phonon branches allowed by symmetry. In the realm of nonlinear dynamics, however, additional nonlinear propagating modes are possible. Nonlinear propagating modes have unique properties that are important in many disciplines including optical communications, conducting polymers, biology, magnetism, and nuclear physics. Yet, despite the crucial importance of crystal lattice vibrations in fundamental and applied science, such additional propagating modes have not been observed in ordinary crystals. Here, we show that propagating modes exist beyond the phonons in fluorite-structured crystals as observed by neutron scattering. These modes are observed at temperatures ranging from 5 K up to 1200 K, extend to frequencies 30–40% higher than the maximum phonon frequency, and travel at velocities comparable to or higher than the fastest phonon. Unlike anharmonicity-driven intrinsic localized modes (ILMs), the modes observed here are robust and not sensitive to small changes in the system. The geometry of the nonlinear mode in reciprocal space is often, but not always, shared with an optic phonon. The existence of these waves in three-dimensional crystals may have ramifications for material properties.

The Phase stability and tuning of magnetism of layered $SrFeO_2$ with Hydrogen from topochemical reduction

Shree Ram Acharya

ORNL

The infinite layer structure type has been known to host high temperature superconductivity since the discovery of $Ca_{0.86}Sr_{0.14}CuO_2$, yet little progress has been made to synthesize many analogs. Here, using $SrFeO_x$ as a prototype system, we demonstrate that the conventionally reported topochemical reduction results in hydride incorporation into $SrFeO_2$. First-principles simulations confirm that the incorporation of H enhances the stability of the $SrFeO_x$, reduces the thermodynamic cost, and is the driving factor behind changes in the magnetic exchange interactions that ultimately offers tuning of the Neel temperature (T_N) depending on its site occupancy. These results suggest that charge doping into the ABO_2 lattice may be a fruitful route for tuning the stability and magnetic properties of these materials, with potential consequences for their superconducting behavior.

Anharmonic stabilization of ferrielectricity in $CuInP_2Se_6$

Nikhil Sivadas

ORNL

Using first-principles calculations and group-theoretical methods, we study the origin and stabilization of ferrielectricity (FiE) in $CuInP_2Se_6$. We find that the polar distortions of metal atoms create most of the polarization in the FiE phase. Surprisingly, the stabilization of the FiE phase comes from an anharmonic coupling between the polar mode and a fully symmetric Raman-active mode comprising primarily of the Se atoms. This coupling is large, and the degree of anharmonicity is comparable to improper ferroelectrics. Thus, the origin of polarization is different from the factors that stabilizes the FiE phase in $CuInP_2Se_6$, unlike conventional ferroelectrics. Our results open up possibilities for dynamical control of the single-step ferroelectric switching barrier by directly tuning the Raman-active mode.These finding has important implications not only for designing next-generation microelectronic devices that can overcome the voltage-time dilemma but also in understanding the emergent responses in these materials.

Applied process modeling to meet additive manufacturing challenges

Gerry Knapp

ORNL

Additive manufacturing presents exciting opportunities for producing novel alloys and parts due to the unique process conditions experienced by additively manufactured materials. Fast cooling rates, microscale segregation, directional solidification, repeated thermal cycling, and spatially varying composition are just some of the factors affected as-built material condition. At the Manufacturing Demonstration Facility, we are integrating process models, thermodynamic simulations, and microstructure models to better understand the relationship of processing parameters to materials outcomes. Applying these models to practical problems reduces the time to implement new materials for additive manufacturing processes and provides insight into experimental results. This talk will highlight my work on using process models and high-throughput thermodynamic simulations for laser hot-wire additive manufacturing of aluminum alloys. Both modeling methods and results, as well as initial experiments will be discussed.

Big Area Additive Manufacturing of Recycled Carbon Fiber-Filled ABS

Matthew Korey

ORNL

Additive manufacturing (AM) – also known as 3D printing - has enabled previously unseen and complex geometries in manufacturing to become a reality. Although often touted as a green manufacturing process, material extrusion printing generates a significant amount of waste, especially at the larger build volumes more recently achieved within the industry. Some of the most utilized composite materials for the emerging applications of BAAM are fiber-filled ABS, PESU, PA6, and others which are sourced from petroleum and are currently landfilled at extremely high rates – often more than 90% in the U.S. Thermoplastic composites can be ground up using a shredder and granulator or "chipper" to pieces on the millimeter scale which can be potentially re-compounded and put back into BAAM. Mechanical recycling, although limited to thermoplastic materials or materials which can be re-melted and re-processed using existing manufacturing equipment, enables an additional pathway for direct reintegration of waste material back into BAAM without additional processing steps. The goal of this work was to understand the impacts of recycling on the mechanical, thermomechanical, and rheological properties of CF-ABS waste from BAAM.

Residual Lifetime Assessment of Service-Aged Dissimilar Forge 91-Pipe 91 Steel Header Welds with High Temperature Digital Image Correlation

Yiyu Wang

ORNL

Condition assessment of welded steam components is a crucial activity for power plant operation and maintenance. In this work, creep performance of an ex-service large girth weld between an SA-182 Forge 91 reducer to a SA-335 Pipe 91 header was tested with a specially designed high temperature digital image correlation (DIC) system.Feature cross-weld creep samples were assessed using full field creep strain monitoring with DIC which permitted for analysis of local strain accumulation. The results provide insight regarding creep failure in the heat affected zone (HAZ) in 9-12% Cr creep strength enhanced ferritic steel welds. The in-situ DIC strain measurements quantified a highly nonuniform creep strain distribution across the F91-P91 weld. The specimens eventually failed through the F91 HAZ exhibiting the so-called "Type IV failure" .The measured strain shows the nominal creep strain averaged over the gauge length is consistently below 3%, while the localized creep strain in the HAZ where failure occurs is $\sim$ 10%. Post-test characterization shows that creep failure occurred in the most pre-damaged region and this location is adjacent to, but not inside the documented soft zone prior to the test. Roles of underlying microstructure features are also discussed to further clarify the creep failure mechanism.

Wednesday

Oral Session 3

Formation, characterization, and modeling of emergent synthetic microbial communities

Jia Wang

ORNL

The microorganisms present in soil are recruited by the plant to form microbial communities in the rhizosphere. Although several important factors such as soil properties, plant genotype and agricultural practices have been studied for their effects in the construction of the rhizosphere microbiome, how these microorganisms contribute to shaping their own community is still poorly understood. An important challenge exists in elucidating the dynamics of interactions among microbial community members. Synthetic microbial communities can serve as valuable model systems for unraveling community organization principles. In this study, 10 bacterial strains isolated from the *Populus deltoides* rhizosphere were co-cultured in different media environments. The growth behavior of community members was tracked and compared with their individual cultures. A generalized Lotka-Volterra modeling approach was used to predict dynamical properties of the microbial community. Additionally, steady-state metabolic reconstructions were extended to dynamic flux balance analysis which performed transient modeling of cellular metabolism at genome-scale resolution. Meta-omics analysis also provided experimental evidence to support the dynamic modeling results. The approach of discovering the growth behavior of strains in the microbial community under laboratory-defined conditions will facilitate understanding of the formation and dynamics of natural communities and the rational design of synthetic consortia with desired biological functions.gradation of both receptors. Collectively, our results suggest that proteolytic degradation plays a role in sequestering receptors to impair downstream defense signaling cascades.

Interactive effects of manganese availability and warming on CO_2 fluxes from soils during decomposition

Fernanda Santos

ORNL

Manganese (Mn) participates in the microbial decomposition of organic matter by mediating the oxidation of lignin through fungal-produced Mn peroxidase. The positive relationship between litter Mn, ligninolytic enzyme activity,and mass loss during decomposition suggests that increased Mn availability may decrease soil carbon (C) storage. However, it is unclear how Mn availability affects C dynamics under a changing climate.To address these unknowns, we initiated a 1-year field incubation study at ORNL Walker Branch to test the interactive effects Mn availability and warming on the decomposition of the litter layer placed in nylon bags. For total soil CO_2 effluxes (g m^{-2} $hour^{-1}$)measured monthly up to Day 196, fluxes were significantly lower in the winter relative to fall and spring but were not affected by Mn and warming treatments. Fluxes estimated for the organic layer were faster in heated treatments relative to non-heated treatment from Day 77 to 196, suggesting that warming enhanced C losses from organic horizons regardless of Mn levels during the first 7 months of decomposition. We will also present data on mass loss, Mn concentrations, lignin, and C functional groups in litter layer at days 30 and 180 to discuss mechanisms that could explain these results.

The Plasminogen-Apple-Nematode (PAN) domain suppresses plant immunity

Kuntal De

ORNL

Hormonal pathways Jasmonic Acid and Ethylene are essential for plant defense against pathogens and parasites. The two hormones have been shown to mediating defense against necrotrophic pathogens and herbivorous insects. Negative regulation of these defense pathways to facilitate colonization by microbes has largely been attributed to microbial genetic systems that evolved to counteract plant defenses. However, emerging evidence suggests that plant G-type lectin receptorlike kinases can negatively regulate plant immunity by retarding Jasmonic acid and Ethylene signaling. In this study, we show that the Plasminogen-Apple-Nematode domain of the G-type lectin receptor-like kinases is essential for this phenomenon. We identified two *Salix purpurea* receptors in this protein family that were able to trigger defense signaling upon overexpression in *Arabidopsis* and tobacco. These receptors accumulated mutations in conserved amino acid residues of the Plasminogen-Apple-Nematode domain. Restoration of these mutations to their conserved state impaired defense signaling. Further, we demonstrated that the domain was required for receptor oligomerization, ubiquitination and proteolytic degradation of both receptors. Collectively, our results suggest that proteolytic degradation plays a role in sequestering receptors to impair downstream defense signaling cascades.

PAN domain of proteins regulates immunosuppression

Debjani Pal

ORNL

The Plasminogen-Apple-Nematode (PAN) domain, with a core of four to six conserved cysteine residues, is found in > 28,000 proteins across 959 genera but its role in protein function is not fully understood. The PAN domain was initially characterized to be present in numerous proteins including Hepatocyte Growth Factor (HGF) and Novel COVID-19 receptor. Dysregulation of HGFmediated signaling results in numerous deadly cancers. All biological impacts of HGF in cell proliferation are triggered by docking of HGF on its cell surface receptor, cellular Mesenchymalepidermal transition (c-MET). Here, we show that four PAN domain cysteine residues are essential for HGF/c-MET signaling. Mutating these residues, either singly or together, resulted in retardation of perinuclear localization, cellular internalization or degradation of HGF and its receptor c-MET. Our observations indicate that the PAN domain is necessary for the subsequent c-MET autophosphorylation and phosphorylation of its downstream targets Protein kinase B (AKT), Extracellular signal-regulated kinase (ERK) and Signal transducer and activator of transcription 3 (STAT3). Our analysis on COVID-19 receptor showed the presence of four conserved cysteines on the PAN domain of receptor provide the novel binding site for SARS-CoV19 receptor, and point mutation on those cysteines not only inhibits the binding of viral spike protein and the overall density, expression of the infectious spike protein also downregulates. We propose that the PAN domain and its conserved cysteine residues offers a novel target for therapeutic intervention in disease management including cancer and COVID-19.

Investigating the ability of SERCA2b activation to mitigate hepatic lipotoxicity

Tomasz Krzysztof Bednarski

Vanderbilt University

Non-alcoholic fatty liver disease (NAFLD) is the most common form of liver disease that, when progressed, leads to nonalcoholic steatohepatitis (NASH) and later to cirrhosis. There is currently no established therapy to treat the progression of NAFLD to NASH. Moreover, the acute effect of saturated fatty acid overload on liver metabolism is not well investigated, even though, it has been previously shown to trigger endoplasmic reticulum (ER) stress and lead to apoptosis, by impairing the function of ER proteins such as sarco/endoplasmic reticulum Ca^{2+}-ATPase (SERCA2). Conscious, unrestrained, overnight fasted 12-wks old male C57Bl/6J mice were given continuous, intravenous infusion of either saline or 20% lard oil emulsions for 5 hrs. One group of animals was given lard oil in combination with single IP injection of CDN1163, a potent SERCA2 activator, one week prior to study. Our studies showed that SERCA2 activation was able to decrease expression of genes involved in ER stress and unfolded protein response such as: Hypoxia Inducible Factor 1 Alpha (HIF1a), Erythropoietin (EPO), Heat Shock Protein Family A Member 5 (HSPA5), BCL2 Interacting Protein 3 (BNIP3) and Activating Transcription Factor 4 (ATF4) compared to lard oil infused animals. This study suggest that SERCA2 activation may have potential to mitigate hepatic lipotoxicity.
This research was supported by NIH grant R01 DK106348.

Role of nSMase-2 in the onset of glucocorticoid hypersensitivity in hepatocytes

Leobarda Robles-Martinez

University of Kentucky

Glucocorticoids (GC) are steroid hormones, and synthetic GC are the most prescribed drugs worldwide due to their anti-inflammatory actions. The prolonged use of GC is associated with the onset of GC hypersensitivity in different organs and tissues; in the case of liver, it manifests with dysregulation of glucose and fat metabolism, hepatosteatosis and insulin resistance. Previous data have suggested that sustained, low-grade inflammation is associated with up-regulated basal levels of glucocorticoid receptor (GR) and transient activation of nSMase-2 (a sphingomyelinase) that might be linked to GC hypersensitivity. To delineate a new role of nSMase-2 in the regulation of GC hypersensitivity in hepatocytes, Hep-G2 cells were treated with IL-1b (a proinflammatory cytokine) in the presence or absence of dexamethasone (a GC agonist), and nSMase-2 was silencing using shRNAi or inhibition with pharmacological inhibitor GW4869. GR protein levels of the cytosol and nuclear fractions combined with immunofluorescent, expression of 11bHSD1 (an enzyme that catalyzes re-activation of inactive cellular GC), and the transcription of Glucocorticoid Response Elements dependent mRNAs were quantified. IL-1 b and nSMase-2 are chronically upregulated in aged rats and mice, and to test the role of nSMase-2 in regulation of GR levels and sensitivity to chronic inflammation, young and aged animals will be used.

Wednesday

Oral Session 4

Discovery and Characterization of Pyridoxal-5'-Phosphate-Dependent Alkyl Transferase in Nucleoside Antibiotic Muraymycin Biosynthesis

Zheng Cui

University of Kentucky

Nucleoside antibiotics muraymycins are structurally characterized by a 5"-amino-5"-deoxyribose (ADR) appended via a glycosidic bond to a high-carbon sugar nucleoside (5' S, 6' S)-5'-Cglycyluridine (GlyU). By using a combination of feeding experiments with isotopically labeled precursors and functional assignment and characterization of recombinant proteins, the biosynthetic mechanism for N-alkylamine installation for ADR-GlyU-containing nucleoside antibiotics has been uncovered. The data reveal S-adenosylmethionine (AdoMet) as the direct precursor of the Nalkylamine, but unlike conventional AdoMet- or decarboxylated AdoMet-dependent alkyltransferases, the reaction is catalyzed by a pyridoxal-5'-phophosate (PLP)-dependent aminobutyryltransferase (ABTase) using a stepwise γ-replacement mechanism that couples -elimination of AdoMet with azaγ-addition onto the disaccharide alkyl acceptor. In addition to catalyzing a PLP-dependent alkyl group transfer from the donor AdoMet, the newly discovered ABTase requires a phosphorylated disaccharide alkyl acceptor, revealing a cryptic intermediate in the biosynthetic pathway.

Leveraging Transfer Learning to Analyze Behavioral Intentions Toward COVID-19 Vaccines

Siru Liu

Vanderbilt University

The COVID-19 vaccine is considered to be the most promising approach to alleviate the pandemic. However, in recent surveys, acceptance of the COVID-19 vaccine has been low. Our objective is to analyze the potential of leveraging transfer learning to detect tweets containing opinions, attitudes, and behavioral intentions toward COVID-19 vaccines, and to explore temporal trends as well as automatically extract topics across a large number of tweets on Twitter. We developed transfer learning models to classify tweets, followed by temporal analysis and topic modeling on a dataset of COVID-19 vaccine-related tweets posted from November 01, 2020 to January 31, 2021. We used F1 values as the primary outcome. We collected 2,678,372 tweets related to COVID-19 vaccines with 841,978 unique users and annotated 5,000 tweets. The F1 values of transfer learning models were 0.792 [0.789, 0.795], 0.578 [0.572, 0.0.584], and 0.614 [0.606, 0.622] for these three tasks, which significantly outperformed the machine learning models (logistic regression, random forest, and support vector machine). Overall, we provided a method to automatically analyze public reception of COVID-19 vaccines from realtime data in social media, which can be used to tailor educational programs and other interventions to effectively promote public acceptance.

A trans-eQTL, PtrXBAT35, regulates root architecture and shoot stature in Populus

Tao Yao

ORNL

Plant architecture comprises of root and shoot systems which are determined by genetic factors and environmental conditions. By analyzing 444 developing xylem and 390 leaf RNAseq datasets, we performed expression quantitative trait loci (eQTL) mapping to uncover genome-wide distribution of transcriptional regulatory elements in *Populus trichocarpa*. Here, we report a trans-eQTL, whose expression varied significantly across genotypes among the mapping population and was associated with altered expression of 492 and 81 genes in xylem and leaf transcriptomes, respectively. This locus is predicted to encode a C3HC4 RING-type E3 ligase, PtrXBAT35. Heterologous expression of *PtrXBAT35* in the *Populus tremula x Populus alba* 717-1B4 hybrid genotype led to pleiotropic effects including enhanced adventitious root formation and compact shoot architecture. Transcriptomics and proteomics studies revealed that several transcription factor families, such as AP2/ERF, WOX and IDD, were involved in *PtrXBAT35*-induced adventitious root formation and shoot development. In addition, plant hormone signals including auxin, ethylene and auxin, also participate in *PtrXBAT35*-mediated shoot growth and root development. These results demonstrate that a pleiotropic eQTL modulates adventitious root formation and tree architecture, entitling a candidate gene to be used in tree improvement prog

Chemical Imaging of Microbial and Plant Systems via Liquid-Extraction Mass Spectrometry

Courtney Walton

ORNL

One of the current challenges in the analysis of plant and microbial systems is the ability to garner both spatial and temporal chemical information from living samples. These living biological systems and the interface between them rely on chemical communication, but there is limited knowledge on the types of molecules used, the concentrations of the molecules, and the timescales at which they exude these molecules. Herein, we describe the use of a liquid-extraction mass spectrometry technique paired with novel soil-mimic microfluidic devices to analyze plant and microbial systems *in situ*. The biological systems, *Populus trichocarpa* cuttings and *Pantoea sp. YR343*, were separately grown in microfluidic devices that have a porous membrane attached to them. A liquid-microjunction surface sampling probe was utilized to extract small, nanoliter amounts of liquid containing exudates from the biological systems through the porous membrane on the microfluidic device. Chemical imaging of amino acid exudates was observed from the microbial *Pantoea sp. YR343*, indicating that the technique can be used for in situ spatial chemical imaging. Further, we show that the technique could also be utilized to garner chemical information from the exudates from the roots of *Populus trichocarpa* plants at various time points in root growth.

Understanding the Effects of Nutrient Concentration on Mercury Cycling within Fluvial Periphyton

Spencer J. Washburn

ORNL

Periphyton biofilms play an important role in the biogeochemical cycling of mercury (Hg) within watersheds, but relatively little is known about the impact of nutrient concentrations on the methylation and demethylation potentials of the complex consortia of microbiota within these biofilms. To address this knowledge gap, we are conducting experiments to better quantify the effects of nutrient concentrations on the net Hg methylation and methylmercury (MeHg) demethylation potentials of periphyton, periphyton microbial community structure, and the production of specific low molecular weight thiol compounds by organisms within biofilms. A translocation experiment utilizing a natural gradient of nutrient concentrations between locations within the Hg-impacted East Fork Poplar Creek (EFPC, located in Oak Ridge, Tennessee, USA) is being conducted. This experiment is designed to assess what changes in periphyton community and Hg methylation potential are associated both with biofilms colonized under relatively low and high nutrient concentrations across multiple seasons, as well as the impacts of altering the nutrient regime to which an established periphyton community is exposed via physical translocation between locations. This work aims to improve our understanding of how future anthropogenic activity, including land use change and runoff management practices, will impact the production of MeHg within stream ecosystems.

Wednesday

Oral Session 5

A Comparison of OpenACC and OpenMP Target Offload for NVIDIA and AMD GPUs: Application to Computational Fluid Dynamics

Nicholson Konrad Koukpaizan

ORNL

Graphical Processing Units (GPUs) have emerged as the accelerators of choice for current petascale and upcoming exascale supercomputers. Applications that can leverage the GPUs demonstrate significant performance improvements compared to implementations relying solely on Central Processing Units (CPUs). Several programming models can target the GPUs, including vendor-supported languages (e.g., CUDA, HIP, DPC++), directive-based models (e.g., OpenMP, OpenACC) and portability frameworks(e.g., Kokkos, RAJA). Directive-based programming models have the advantages that they require fewer code modifications and facilitate a gradual porting of the codes. Though they may not provide as much control for performance optimization on specific architectures (in contrast with vendor-supported languages), they offer some portability and support Fortran (important in many domains).

We present two directive-based porting strategies to target NVIDIA and AMD GPUs with a Computational Fluid Dynamics (CFD) flow solver. The CFD code is written in free format Fortran 90 and solves the three-dimensional, time-dependent, Navier-Stokes equations on blockstructured grids using a finite-volume formulation. Earlier work described the relevant OpenACC directives and reported performance results on the Summit supercomputer at the Oak Ridge Leadership Computing Facility (OLCF). Recent developments have focused on the OpenMP Target Offload model in preparation for the upcoming Frontier supercomputer at OLCF, and the talk will compare the OpenMP and OpenACC implementations.

Topological Interpretation of Deep-Learning Models

Adam Spannaus

ORNL

With the adoption of AI-based systems across everyday life, the need to look inside these black-box systems has steadily increased. Developing trust in the predictions made from an AI-based algorithm is of tantamount concern in systems such as threat detection or medical diagnosis where outcomes may have tragic consequences. Furthermore, determining whether to trust a model or not, can be strengthened by understanding why a model made a specific prediction. Gaining an insight into the decision process can yield actionable insights on why a model is correct, or how to improve an incorrect one. In this work, we present a topologically informed methodology for inferring prominent features in a deep-learning classification model. We create a graph of the model's prediction space, clustering the inputs into the vertices, and extract subgraphs demonstrating highpredictive accuracy for a given label. These nodes contain a wealth of information about features the deep-learning model has recognized as important. We use these features to create a model correction layer, to improve predictive accuracy in subsequent models and to demonstrate qualitatively that subsequent predictions are made with an understanding between the input and the model's prediction.

Parallel Accelerated 1-bit Dense Matrix Multiplies for Large-scale Correlation Analysis

Paul Eller

ORNL

Large-scale correlation analysis provides data-driven techniques to help identify and understand the relationships between entries in large datasets. A number of vector similarity algorithms are implemented in CoMet, the Combinatorial Metrics tool, to help perform largescale correlation analyses for a wide variety of domains including genomics and climate. These algorithms primarily rely on dense matrix-matrix multiplies (GEMMs), which perform well on GPUs due to their high operational intensity and ability to use tensor core operations to perform fast matrix multiply accumulate operations on small matrix blocks. This work focuses on the DUO method, which can use 1-bit matrices and 1-bit tensor core operations due to binning data into high or low values. The DUO method is implemented by transforming input data to use native GEMM kernels or developing adapted GEMM kernels. This work investigates a variety of 1-bit GEMM approaches for CoMet to better understand how CoMet and other applications can most effectively use the ultralow precision operations provided by many new architectures to achieve high performance at large-scales. This approach allows us to obtain over four PetaOps on a single Nvidia Ampere GPU and provides potential to obtain exascaleclass performance on Ampere GPU accelerated supercomputers.

Analyzing Machine Learning Workloads on Leadership Scale HPC Storage Systems

Arnab Kumar Paul

ORNL

Historically, high performance computing (HPC) workloads have been dominated by simulation jobs which are write-intensive. However, with the increase in popularity of machine learning (ML), we are observing an increasing number of HPC users are incorporating ML methods into their workflow and scientific discovery process, across a wide spectrum of domain sciences such as biology, geosciences, and astrophysics. This gives rise to a different set of data-hungry I/O patterns which are speculatively read-intensive. The details of such ML I/O workloads on leadership-scale supercomputers have not been studied extensively. My work aims to provide an in-depth analysis to gain understanding of such access patterns using Darshan - an I/O characterization tool designed for lightweight tracing and profiling. We study the Darshan logs of more than 25,000 HPC ML jobs over a time period of one year running on Summit - the second fastest supercomputer in the world. The work provides a systematic I/O characterization of ML jobs to understand how it differs across science domains, scale of the workloads, and the usage of burst buffer in ML workloads.

High performance computing and modern data analytics to develop accurate ReaxFF interatomic potentials

N. S. Harsha Gunda

ORNL

Models in material science are typically high-dimensional in nature. To develop a model that can predict accurate material properties, multiple model parameters must be optimized at the same time. Interatomic potentials, which are used in atomistic simulations such as molecular dynamics (MD), also have multiple parameters that must be simultaneously optimized. Manual model optimization takes significant amount of time and effort. We developed an integrated workflow employing supercomputing and advanced data analytics approaches such as neural networks and simulated annealing to generate accurate interatomic potentials. Using the example of bcc-Cr, we demonstrate the development of reactive force field (ReaxFF) interatomic potentials that contain 18 model parameters. Supercomputers were used to perform high-throughput MD calculations for parametrization study in the context of machine learning (ML). We used the large MD data to train multiple high-dimensional ML neural network models capable of replicating ReaxFF predictions of several material properties. Then, using simulated annealing, we optimize individual ReaxFF model parameters in order to reproduce the temperature-based trend observed in experiments. The resulting ReaxFF interatomic potential models were highly accurate in predicting lattice parameters and elastic constants of bcc-Cr. This research was sponsored by the Department of Energy, Vehicle Technologies Office, Propulsion Materials Program.

Coupled multi-physics simulations using preCICE

Arpan Sircar

ORNL

Coupled multi-physics simulations are of great relevance today as they can capture the complexity of physical processes and model the highly interconnected nature of systems, especially, in fusion reactor blanket designs. Fusion reactors serve as an appropriate test case for such coupled physics phenomena with fluid-dynamics, conjugate heat transfer, fluid-structure interactions, radiation shielding and tritium breeding. The major challenge is to couple a suite of codes in a single multi-physics simulation environment. Some of the know codes for fusion reactor physics are: MCNP (Monte-Carlo N-Particle) for neutron transport, OpenFOAM for fluid flow and heat transfer of the coolant and Diablo for structural mechanics simulation of the various components. The preCICE coupling library provides a framework to couple these codes using a peer-to-peer approach which is adopted to leverage the expertise of certain codes in simulating specific physical processes. This approach allows coupling codes in a minimally invasive manner so that they need only make a few function calls to the preCICE libraries for exchange of relevant information while performing their respective simulation tasks. The aim of the current work is to extend the surface coupling feature of preCICE to volumetric coupling between the above codes and test their scalability for parallel computations.

Wednesday

Oral Session 6

Optimization of Water Systems through Model Free Controllers

Dhrubajit Chowdhury

ORNL

Due to the increase in water demand worldwide, the paradigm to produce potable water is shifting from conventional water sources to less traditional water sources such as wastewater effluent and fracking water. The use of non-conventional water sources makes the energy consumption to produce potable water from these technologies demanding. The current optimization algorithms are specific for the optimized processes, regional context, and individual production plant configuration. In contrast, we employ model-free optimization algorithms, namely the extremum seeking control (ESC) and Bayesian Optimization (BO), to optimize the energy consumption of water systems. The main advantages of using these algorithms are (a) No requirement of highfidelity models, (b) Robustness to disturbances like change in influent water concentration (c) Transferability to other water systems using different desalination technologies. These algorithms move the process to an operating point where specific objectives like minimizing energy or maximizing the volume of potable water are satisfied. At this time, the algorithm's performance has been demonstrated on a proxy model of the closed-circuit desalination reverse osmosis (CCDRO) system.

Towards generalizable, scalable & explainable AI methods for satellite imagery analysis

Philipe Ambrozio Dias

ORNL

The ever-increasing availability of high-quality satellite imagery presents great potential for applications such as urban dynamics planning, environment monitoring and disaster response. A crucial requirement to harness such potentials is the ability to generate accurate, reliable estimates of structures of interest from the available data. While models based on deep neural networks have significantly advanced the state of the art of image analysis, their application for Earth observation is still hampered by three major challenges characteristic of current AI-models. First, models often fail to *generalize* across different areas of interest, image acquisition conditions and data distributions. Second, image analysis at larger- scales (e.g. country-level) imposes *scalability* challenges, both from a computational as well as model- design perspective. And third, many of these methods are not interpretable nor explainable, leaving users without an answer for questions like "how did you reach this decision? Why should I trust you?". At the GeoAI group, we are conducting research on domain adaptation techniques, model- and data- distributed frameworks, as well as uncertainty estimation and visualization techniques towards frameworks for analysis of satellite imagery that are generalizable, scalable and explainable. In this way, humans will be provided with reliable, trustworthy and fair estimates to assist better decision making.

Comprehensive Evaluation of Semi-Conductor Technology for Solid-State Circuit Breaker Application

Satarupa Bal

ORNL

The paper attempts to comprehensively compare the technologies (Si and Wide band gap) in terms of not just their steady-state performance but also transient characteristics which is critical for Solid-State Breaker Application. Even though steady-state characteristics is an important parameter given it will determine the efficiency and heat sink size; a solid-state breaker also spends considerable amount of time in the saturation region during start-up or shut-down. This necessitates a closer look into those transient features as well. 5 critical parameters are identified for comparison and those parameters are averaged over different manufacturers of the same technology for Si IGBT, SiC MOSFET and SiC cascode JFET. From the comparison, SiC JFETs offer the lowest steady-state loss and require the smallest heatsink for the same power dissipation. However, in SiC technology the drain current increases with drain voltage even in the saturation region making it difficult to operate in that region for longer time. Also, due to higher dependence on threshold voltage (Vth) over electron mobility when gate voltage (Vgs) is closer to Vth, SiC technology suffers from thermal instability in saturation region and requires caution. Even though the comparison made in this paper is for DC breaker application, similar conclusion can be drawn even for AC breaker, motor starter application.

Continuous Variable Quantum Imaginary-Time Evolution Algorithm for Quantum Field Theories

Kubra Yeter-Aydeniz

ORNL

Quantum fields are fundamental constituents of the physical world, describing quantum many-body systems of matter at all energy scales, as well as electromagnetic and gravitational radiation. Simulating quantum field theories (QFTs) using quantum computers would be one of the most significant contributions of quantum computers since QFTs help us understand how the Nature works. Although QFTs have been studied on quantum computers with discrete variables, the use of continuous variables (CVs) for studying the QFTs is a natural platform because the fields are also CVs. Quantum imaginary time evolution (QITE) algorithm is used to find the ground state energy when the initial state has non-zero overlap with the ground state. In this work, we use Xanadu's Strawberry Fields photonic quantum simulator to calculate the ground and excited state energies of a quartic self-interacting scalar QFT using QITE algorithm. We use also explore methods and sources needed for implementing this algorithm on a photonic continuous variable quantum hardware.

Nucleosynthesis with Modern Supernova Simulations

Andre Sieverding

ORNL

Supernova explosions of massive stars pose a very complicated multi-physics problem but they are key to understand the chemical composition of the solar system and the universe as a whole. Self-consistent, numerical simulations of supernova explosions have made great progress in the last decade and the mechanism that turns the collapse of a star many times more massive than our sun into one of the most energetic astrophysical explosions is increasingly well understood. I am going to show results from nucleosynthesis calculations based on self-consistent, three-dimensional supernova simulations and highlight the challenges that need to be addressed in order to obtain accurate nucleosynthesis predictions from state-of-the art supernova simulations.

Symmetry consequences on phonons and thermal transport

Rinkle Juneja

ORNL

Structural symmetries determine the underlying physical properties of materials and thereby govern their potential functionalities. Here, I will discuss the role of twist structural symmetry in determining vibrational and thermal transport properties of one dimensional and bulk materials. The developed twist dynamics dictate symmetry-enforced band degeneracies, non-trivial topologies, phonon interactions, and unique scattering observables. This will be demonstrated by first-principles calculations supported by inelastic neutron scattering measurements.

Thursday

Oral Session 7

Overview of the DELFIC atmospheric transport model for nuclear fallout modeling

Matthew J. Krupcale

ORNL

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. Here we present an overview of the atmospheric transport and dispersion models of DELFIC. The objective of the atmospheric transport model (ATM) is to simulate the trajectory, dispersion, and deposition of the cloud particulates in the atmosphere after the cloud rise module initializes the cloud mass, geometry, and particulate size distribution. Fundamentally, the DELFIC ATM is a hybrid Eulerian–Lagrangian deterministic transport model that discretizes the fallout cloud into independent parcels of a given particle size. Given specified meteorological conditions, the parcels are transported using the Lagrangian advection plus settling model until the parcels deposit on the ground. Simultaneously, each parcel independently undergoes atmospheric dispersion in the horizontal dimension according to a bivariate Gaussian distribution with the variance determined according to a four-thirds scaling law and Fickian diffusion. Using a simple test case, we discuss the DELFIC ATM and present the results of the DELFIC model.

Reactor modeling and simulation to underpin the science of safeguarding thorium fuel cycles

Richard Reed

ORNL

Some new breeder reactor designs under evaluation convert thorium into fissile uranium-233 by neutron irradiation. Notably, the conversion of thorium to uranium proceeds through an intermediary (i.e., pre-cursor) called protactinium. Presently, protactinium is not considered an accountable nuclear material despite decaying into direct-use material (uranium-233) with a half-life of 27 days. Breeder reactor designs using thorium range from familiar concepts such as pressurized water reactors to advanced reactors such as molten salt reactors. To safeguard a new breeder reactor design requires knowledge of the proposed facility's inventory and production rate of protactinium. In this work, we simulated a wide range of theoretical breeder reactor designs to predict the expected quantities of protactinium and uranium isotopes during standard operation. Somewhat surprisingly, all of the reactors in the study produced approximately the rate of protactinium (and resulting uranium) after normalizing for initial mass and system burnup. International safeguards and nuclear material accounting and control approaches, measures, and technologies rely on detailed knowledge of the nuclear inventory and resulting signatures for detection. Stakeholders such as the US Department of Energy and the International Atomic Energy Agency can use this study to inform policy decisions regarding new reactor designs.

Role of lattice dynamics in the structural stability of uranium Laves phases

Erik Nykwest

ORNL

Uranium Laves phases, have received only minor attention despite their unusual functional properties. Laves phases are binary intermetallic compounds possessing AB_2 stoichiometry, where B atoms form tetrahedra around the A atoms, typically with a size ratio between 1.05 and 1.67, and exhibit novel thermoelectric properties due to their interconnected network of tetrahedra. Three distinct structural phases exist, denoted C14, C15, and C36. The factors governing the formation of a Laves phase into one structure over another remain an open question. In particular, the role of phonons, which may provide information on phase transition mechanisms, transition temperatures, and vibrational contributions to entropy, has been widely overlooked. We present a density functional theory study on the vibrational properties of the UCo_xNi_{2-x} ternary system. This system is an ideal test case because it presents all three Laves phase structure types. The UCo_2 and UNi_2 binary Laves phases form in C15 and C14 structure types, respectively, with the C36 phase present at half mixing. Thus, this system enables an investigation into the factors governing phase transformation and provides insights about the structural stability of the three crystal types, thermal behaviors, and the influence of alloying on the phonon properties.

Effects of Ink Concentration and Mixing on Fuel Cell Catalyst Layers

Erin Creel

ORNL

Roll-to-roll slot die coating of polymer electrolyte membrane fuel cell (PEMFC) cathode catalyst layers is a scalable, continuous, and highly automated deposition method that could help to make PEMFCs economically viable. Before a catalyst can be deposited, it must first be dispersed in a liquid ink, typically with a high shear mixer. Here, we will explore the effects of ink mixing conditions and ink concentration on coatability. The mixer type and geometry, mixing time, and mixing speed all impact the catalyst particle agglomerate distribution and the viscosity of the ink. Catalyst particle agglomerates decrease the availability of catalyst active sites and may even puncture the thin membrane adjacent to the catalyst layer. Increasing the concentration of the ink further lowers manufacturing costs by reducing the thermal energy budget for drying but also increases ink viscosity, which limits the coating parameter space ("coating window"). A 2D simulation and an equation-based model successfully predict the boundaries of the coating windows for a dilute and a concentrated PEMFC ink. This allows coating machine operators to easily deposit a defect-free catalyst coating without the need to find a suitable set of parameters by trial and error.

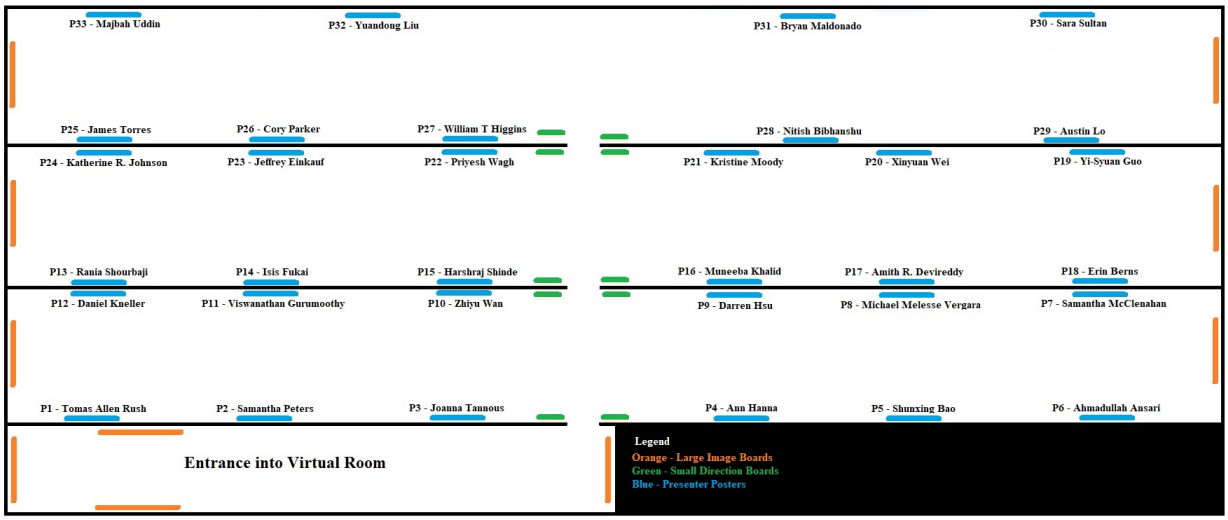
Impact of fuel chemistry and distillation temperature on emissions from a single-cylinder multimode engine

Yeonshil Park

ORNL

Increased societal concerns about global warming and pollution generated by light-duty vehicles has spurred the development of technologies to improve fuel economy and reduce emissions. The DOE's CoOptimization of Fuels and Engines initiative aims to co-develop advanced engine designs and fuel technologies to improve fuel efficiency, reduce emissions, and increase utilization of renewable fuels. These advanced engines are capable of "multimode" operation, which combines conventional sparkignition (SI) operation with advanced compression ignition (ACI) modes. Multimode engines combine the full-load power density of SI operation with the higher-efficiency unthrottled operation of ACI operation at part load. One challenge with multimode is the different fuel properties required for each mode. ACI combustion modes require fuel autoignition to operate, while autoignition is actively avoided for SI. Lean and stratified operation of ACI mode combined with its lower combustion efficiency leads to higher levels of particulate matter (PM) and gaseous hydrocarbon emissions. As a result, fuel chemistry and distillation temperature may influence the emissions from multimode engines. In this set of experiments, the effects of fuel distillation temperature and aromatic content using 6 different fuels across three combustion modes: conventional SI operation, Partial Fuel Stratification Gasoline Compression Ignition (PFS-GCI), and Spark-Assisted Compression Ignition (SACI).

Poster Presentation Layout



Layout inside iSeeVC platform. **Zoom-in for details**

Important: Please see Notes for installing, troubleshooting and navigating iSeeVC.

List of Abstracts – Posters

Poster Session

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P3	Joanna Tannous	Understanding the establishment of Sphaerulina musiva and development of genetic approaches to enhance poplar disease control
P4	Ann Hanna	Modeling the clinical presentation of breast cancer in vivo to identify efficacious therapeutic combinations and improve response to immunotherapy
P5	Shunxing Bao	Random Multi-Channel Image Synthesis for Multiplexed Immunofluorescence Imaging
P6	Ahmadullah Ansari	SNASE enzyme structure as an electrostatic model system to calculate exact pKa value of inner cavity charged residues, and H-bonding network crucial for proper folding and stability of the protein
P7	Samantha McClenahan	VU_20_6: a novel small-molecule potentiator of Kir4.1/5.1 channels
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P13	Rania Shourbaji	Molecular Diagnostic Testing for SARS-CoV-2 and mRNA Immunogenicity Post-Vaccination in a Large Workforce
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P15	Harshraj Shinde	Co-expression network-based analysis of genes associated with leaf temperature and stomatal conductance in grapevine
P16	Muneeba Khalid	Engineered habitats enable in situ chemical monitoring and visualization of Populus root development and cross-kingdom interactions
P17	Amith R. Devireddy	Role of Cation/H^+ exchanger CHX20 in mediating drought stress responses in *Populus*

P18	Erin Berns	Linking groundwater table fluctuations to oxygen availability and CO_2 and CH_4 release from soil
P19	Yi-Syuan Guo	An engineered approach to fungal growth in soil
P20	Xinyuan Wei	Climate and atmospheric deposition drive the variability and trend of a large flux of dissolved organic carbon from US watersheds
P21	Kristine Moody	Environmental DNA (eDNA) applications for hydropower aquatic community monitoring and environmental impact studies
P22	Priyesh Wagh	Recovery of Critical Materials from End-of-Life Lithium-Ion Batteries using Supported Membrane Solvent Extraction
P23	Jeffrey Einkauf	Sulfate Recognition by a Pyridine-Functionalized Diiminoguanidinium Photoswitch: Structural and Kinetic Studies
P24	Katherine R. Johnson	Influences of DGA functionalization on the liquid-liquid extraction of lanthanides
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P27	William T. Higgins	Optimization of GP-SANS Guide Upgrade
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Poster Session

Bioprospecting Trichoderma: A systematic roadmap to screen genomes and natural products for biocontrol applications

Tomás A. Rush

ORNL

Natural products derived from microbes are crucial innovations that would help in reaching sustainability development goals worldwide while achieving bioeconomic growth. *Trichoderma* species are well-studied model fungal organisms used for their biocontrol properties with great potential to alleviate the use of agrochemicals in agriculture. However, identifying and characterizing effective natural products in novel species or strains as biological control products remains a meticulous process with many known challenges to be navigated. Integration of recent advancements in various "omics" technologies, next generation biodesign, machine learning, and artificial intelligence approaches could greatly advance bioprospecting goals. Herein, we propose a roadmap for assessing the potential impact of already known or newly discovered *Trichoderma* species for biocontrol applications. By screening publicly available *Trichoderma* genome sequences, we first highlight the prevalence of putative biosynthetic gene clusters and antimicrobial peptides among genomes as an initial step toward predicting which organisms could increase the diversity of natural products. Next, we discuss high-throughput methods for screening organisms to discover and characterize natural products and how these findings impact both fundamental and applied research fields.

Characterization of time-dependent signatures of microbial modulation of human immune proteins linked to intestinal homeostasis and inflammation

Samantha L. Peters

ORNL and University of Tennessee, Knoxville

The gut microbiome plays an essential role in host health by producing metabolic resources andtraining the immune system. Due to the time-driven expansion of microbial complexity in early life, metaproteomics tracks details about colonization, community functional dynamics, and host responses. This study examines differences in temporal relationships between microbial activities and the host proteome during the normal and dysbiotic establishment of the gut. The preterm human infant microbiome is a tractable model to look at microbial colonization and development -compared to a fully established adult gut microbiome. Using necrotizing enterocolitis (NEC) as a representative dysbiotic condition, 91 metaproteomic measurements were taken from seventeen preterm infants over the first 90 days of life. Six infants developed NEC. On average, 3000 human and9000 microbial proteins were identified per infant. Preliminary results show functional partitioning among infants based on antibiotic administration. Maternal antibiotic administration drives the separation of immune proteins between infants, while infant antibiotic administration drives normal and dysbiotic microbial establishment. Metaproteomics provides a unique approach to studying the developing gut environment as it allows simultaneous examination of host and microbial metabolic activities. Understanding this interplay may elucidate the microbiome's potential immunomodulatory roles relevant to dysbiotic conditions.

Understanding the establishment of Sphaerulina musiva and development of genetic approaches to enhance poplar disease control

Joanna Tannous

ORNL

Sphaerulina musiva is the causal agent of one of the most detrimental diseases affecting hybrid poplar and other hosts in North America. Breeding and cultivation of resistant plant species have been the main approaches to control the damage caused by this pathogen. The limited amount of information about genetic functional markers involved in *S. musiva*'s establishment and pathogenicity combined with the lack of genetic tools have greatly hampered the development of disease mitigation strategies at the pathogen level. We aim to quantify the genetic determinants influencing the establishment of *S. musiva* within native *Populus* and *Salix* microbial communities. We have selected two *S. musiva* strains that represent the extremes of the virulence spectrum *P. trichocarpa*, with a long-term goal of validating this work on the large collection of 122 *S. musiva* isolates. Transcriptomic and proteomic data will be leveraged to identify functional markers associated with successful establishment to interrogate the persistence of *S. musiva* in *Populus* and its associated microbiome. The collected omic datasets will be used to implement CRISPR RNA-guided gene drive systems to eradicate host-recognition mechanisms between *Sphaerulina* and *Populus* and attenuate its pathogenicity which has adverse outcomes on the production of the ecologically and commercially significant DOE biofeedstock *Populus*.

Modeling the clinical presentation of breast cancer in vivo to identify efficacious therapeutic combinations and improve response to immunotherapy

Ann Hanna

ORNL

Immune checkpoint blockade (ICB), an immunotherapy that activates cytotoxic immune cells to mount anti-tumorigenic responses, has yielded limited success in treating breast cancer. Clinical trials demonstrate that combining ICB with standard-of-care chemotherapy increases survival and pathologic complete response in patients. Despite promising evidence for immunotherapy success, clinical trials lacked an experimental ICB-only arm, and thus cannot address the therapeutic benefit of ICB alone, or which chemotherapy combination would maximize this benefit. We sought to model ICB response *in vivo* to elucidate the mechanisms responsible for immunotherapy efficacy in breast cancer and explore the synergistic effects of ICB with chemotherapies. In this study, we investigated the efficacy of anti-PD-L1 as single-agent or in combination with chemotherapy in an immunocompetent orthotopic mammary tumor model. We discovered that single-agent immunotherapy was sufficiently efficacious in: 1) blunting primary tumor growth, 2) extending survival, and 3) significantly enhancing the infiltration and activation of immune cells into primary mammary tumors compared to combination treatments. We report the immunogenic efficacy of single-agent ICB that upregulates tumoricidal immune cell infiltration into the primary tumor, thereby controlling tumor growth. This study has potentially significant clinical implications for re-evaluating the contributions of chemotherapy in combination with ICB in TNBC patients.

Random Multi-Channel Image Synthesis for Multiplexed Immunofluorescence Imaging

Shunxing Bao

Vanderbilt University

Multiplex immunofluorescence (MxIF) is an emerging imaging technique that produces the high sensitivity and specificity of single-cell mapping. With a tenet of "seeing is believing", MxIF enables iterative staining and imaging extensive antibodies, which provides comprehensive biomarkers to segment and group different cells on a single tissue section. However, considerable depletion of the scarce tissue is inevitable from extensive rounds of staining and bleaching. Moreover, the immunofluorescence imaging can occasionallyfail for particular rounds ("missing stain"). It would be appealing to develop digital image synthesis approaches to restore missing stain images. Herein, we aim to develop image synthesis approaches for 11 MxIF structural molecular markers. We propose a novel multi-channel high-resolution image synthesis approach, called pixN2N-HD, to tackle possible missing stain scenarios via a high-resolution generative adversarial network (GAN). Our contribution is three-fold:(1) a deep network framework is proposed to tackle missing stainin MxIF; (2) the proposed "N-to-N" strategy reduces theoretical 4 years of computational time to 20 hours when covering up to five random missing stains and (3) this work is the first comprehensive experimental study of investigating cross-stain synthesis in MxIF. Our results elucidate a promising direction of advancing MxIF imaging with deep image synthesis.

SNASE enzyme structure as an electrostatic model system to calculate exact pKa value of inner cavity charged residues, and H-bonding network crucial for proper folding and stability of the protein

Ahmadullah Ansari

ORNL

Staphylococcal nuclease (SNASE) is a well-studied model system used to expand the fundamental understanding of processes central to protein folding, stability, and dynamics, as well as the ionization state of charged residues. It is a ∼16 kDa globular protein that functions as a “bioscissor" in cells. Hundreds of variants have been experimentally and computationally characterized. However, the position of hydrogen atoms and the orientation of associated water molecules have been predicted or inferred using chemical and geometrical knowledge, as hydrogen atoms cannot be directly visualized in the available X-ray crystal structures. To address this problem, we have determined the neutron structure of SNASE with a substrate-bound analogue at 2.5 Å resolution, which has enabled the position of exchangeable hydrogen atoms and the orientation of buried water molecules to be determined proton level of detail. In addition to directly observing the protonation states of key charged residues, we also identify crucial H-bonding networks that have been demonstrated to be central to this protein archetype’s folding & stability. Further, we have designed and produced three (two single and one double) mutants in which key hydrophobic core residues are replaced with charged amino acids. The perdeuterated variant proteins were purified and crystallized, producing ∼0.6-1 mm^3 crystals. A 2.3 Å neutron dataset has been collected for the V99E variant, and preliminary structure analysis will be presented and discussed.

VU206: a novel small-molecule potentiator of Kir4.1/5.1 channels

Samantha McClenahan

Vanderbilt University

Heteromeric inward rectifier potassium (Kir) channels containing Kir4.1 and Kir5.1 subunits play key roles in brain electrophysiology and kidney salt transport, suggesting they represent new molecular targets for anti-epileptic and anti-hypertensive/edema drugs, respectively. Because the pharmacology of Kir4.1/5.1 has been limited to non-specific inhibitors, we performed a highthroughput screen of 87,475 compounds from the Vanderbilt Institute of Chemical Biology library for novel channel modulators. 427 inhibitors and 107 activators were identified in the primary screen, including one activator, termed VU0493206, which we describe here. In whole-cell patch clamp experiments, VU0493206 potentiates Kir4.1/5.1 by approximately 600% with an EC50 of 11 μM and is selective for Kir4.1/5.1 over Kir4.1, Kir1.1, Kir7.1, and Kir4.2/5.1 channels. In cellattached single-channel recordings, VU0493206 increases the number and single-channel current amplitude of Kir4.1/5.1. The membrane phospholipid, PIP2, is essential to maintain the active conformation of all Kir channels, raising the possibility that VU0493206 simply acts as a PIP2 surrogate to activate Kir4.1/5.1. However, depletion of membrane PIP2 or mutation of a PIP2-binding site in Kir4.1 prevented Kir4.1/5.1 activation by VU0493206. Thus, VU0493206 activates PIP2-bound Kir4.1/5.1 channels through a novel mechanism of action.

Counteracting CRISPR/Cas9 activity via RNA-based tool

Michael Vergara

ORNL

As advances in CRIPSR based genomic engineering technologies become ubiquitous, their application frontiers continue to expand. In the rush to make these advances, there have been minimal efforts that investigate the unintended effects of Cas9 introduction into a host cell. 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 prevent undesirable genomic engineering efforts. These gRNAs are designed to redirect Cas9 specificity towards its own locus are effective in reducing Cas9 transcripts and protecting the genome. The principal of adapting the naturally occurring molecular machines for other applications provides another avenue of research. One such tool under development is use of the CRIPR adaptation machinery for recording transcripts into DNA arrays, called Record-seq. 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.

High-throughput pose refinement for potential SARS-CoV-2 main protease inhibitors

Darren Hsu

ORNL

Virtual ligand screening has become a fundamental step in the drug candidate discovery process. As the ligand libraries grow to billions of compounds, and with generative artificial intelligence models that provide arbitrary numbers of ligand structures, a workflow tailored for such a data-rich regime is required. We present the development of a high-throughput ligand pose refinement workflow for the SARS-CoV-2 main protease active site. The physics-based workflow takes in coarsely-docked ligand poses and parametrizes them for atomistic simulation with a fixed protein core. We evaluate different strategies to assemble the protein core and improve numerical stability. Finally, we discuss the workflow in the context of a drug discovery pipeline that includes automatic generation of molecules, and quantum mechanical refinement.

A Game Theoretic Model for Privacy-Preserving Genomic Data Sharing

Zhiyu Wan

Vanderbilt University

Emerging scientific endeavors are creating big data repositories from millions of individuals. Sharing data in a privacy-respecting manner could lead to important discoveries, but high-profile demonstrations show that links between de-identified genomic data and named persons can sometimes be reestablished. Such re-identification attacks have focused on worst-case scenarios and spurred the adoption of data sharing practices that unnecessarily impede research. To mitigate concerns, organizations have traditionally relied upon legal deterrents, like data use agreements, and are considering suppressing or adding noise to genomic variants. In this report, we use a game theoretic lens to develop more effective, quantifiable protections for genomic data sharing. This is a fundamentally different approach because it accounts for adversarial behavior and capabilities and tailors protections to anticipated recipients with reasonable resources. We demonstrate this approach with a public resource with genomic summary data from over 8000 individuals and show risks can be balanced against utility more effectively than traditional approaches. We further show the generalizability of this framework by applying it to other genomic data collection and sharing endeavors. Recognizing that such models are dependent on a variety of parameters, we perform extensive sensitivity analyses to show that our findings are robust to their fluctuations.

Sortase-mediated segmental labeling allows studying conformations of individual domains of c-Src kinase by SANS

Viswanathan Gurumoorthy

ORNL

c-Src kinase is a non-receptor tyrosine kinase that aberrantly phosphorylates several signaling proteins in different cancers. The regulatory domains, SH3 and SH2, are known to weakly interact with the N-terminal disordered SH4 domain during c-Src activity and upregulation. However, studying the conformations of individual domains, especially disordered regions, during such interactions remains a technical challenge. Here we show how segmental labeling of c-Src domains helps resolving the conformations of individual domains during such interactions by using small angle neutron scattering (SANS). We used an enhanced variant of bacterial transpeptidase, sortase 5M, to conjugate the protiated SH4 domain with deuterated SH3-SH2 domains. Our SANS results show that SH3-SH2 domains assume extended conformations during SH4 interactions and compact conformations in its absence. Based on our computational simulations, we further postulate that the extended conformations of SH3-SH2 domains are caused by flexible regions, nSrc and RT loops, of the SH3 domain that are known to interact with the SH4 domain. Therefore, our studies find interesting observations of therapeutic significance that among other regulatory domains, it is the SH3 domain that assumes multiple conformations during c-Src regulation.

Neutron Crystallography in the fight against COVID-19

Daniel Kneller

ORNL

SARS-CoV-2, the viruses that causes COVID-19, introduced a worldwide economic and public health calamity in 2020. SARS-CoV-2 possesses an essential cysteine protease enzyme (Mpro) which serves as the 'heart' of viral replication and thus is a major target for small-molecule inhibitors. Structural biology strategies historically achieved atomic scale understanding of enzymes from cryogenically preserved samples using X-ray diffraction but are hindered by cryoartifacts and the inability to determine protonation states. Neutrons provide an ideal probe to directly visualize protonation states of ionizable residues at near-physiological temperatures. ONRL's unique contributions to the pandemic response are presented here through room temperature neutron crystallography of Mpro. Details about Mpro function and inhibition by covalent and non-covalent inhibitors are revealed by three joint X-ray/neutron crystal structures of Mpro. Direct observation of protonation states observes the active site electrostatics where the non-canonical catalytic dyad of Cys145-His41 exists in the reactive zwitterionic state at rest. Follow-up neutron crystal structures of deuterated Mpro in complex with inhibitors witnesses the net positive charge of active site residues are maintained through rearrangements of protonation states and remodeling of the active site electrostatics. Neutron crystallography of Mpro exemplifies how accurate experimental models enable atomic level understanding of pathogens.

Molecular Diagnostic Testing for SARS-CoV-2 and mRNA Immunogenicity Post-Vaccination in a Large Workforce

Rania Shourbaji

ORNL

As part of its occupational health mission and layered Coronavirus Disease 2019 (COVID-19) defense strategy, Health Services Division (HSD) of ORNL conducts a comprehensive surveillance program using Reverse Transcription-Polymerase Chain Reaction (RT-PCR) and/or Nucleic Acid Amplification Test (NAAT) technology for identification of SARS-CoV-2 on samples collected from random, targeted, and symptomatic persons. Data from these measurements have been providing guidance for the health and safety of ORNL. To date, HSD has completed 55,466 molecular diagnostic tests in our in-house laboratory. HSD also conducts several quality studies of SARS-CoV-2 antibody status for Immunoglobulin G (IgG) on persons previously diagnosed with COVID-19 and of post-vaccination immunogenicity. These include longitudinal studies. Descriptive data are presented on RT-PCR / NAAT testing volume, positivity rates, and viral load (defined by RT-PCR Cycle threshold [Ct] value) over time. These data are analyzed and compared with other relevant populations. Initial data on variants of concern (VOC) in positive SARS-CoV-2 samples also are presented.

Evaluating Microbial Biosensors for Nuclear Arms Nonproliferation

Isis Fukai

University of Tennessee, Knoxville

Development of robust environmental biosensors for monitoring nuclear fuel cycle activities is needed to strengthen global nonproliferation safeguards and support development of peaceful nuclear technologies. Prior research has shown that correlations between microbial genomes and geochemical parameters can be used to monitor and predict concentrations of uranium, strontium and other associated nuclear materials at radionuclide-contaminated sites.The sensitivity of potential microbial biosensors to proliferation-related activities of the nuclear fuel cycle and the spatial-temporal limitations of their application have not been constrained. It's hypothesized that characteristic microbiomes maybe associated with current and historical uranium enrichment activities, nuclear reactor operations, and spent fuel storage/reprocessing .These characteristic microbiomes could inform development of sensor technologies for rapid detection and screening of special nuclear materials, source materials and their origins. To test these hypotheses, environmental samples are being collected from lateral and vertical contamination gradients associated with specific fuel cycle activities at Oak Ridge National Laboratory, the Y12 National Security Complex, and the Savannah River Site. Data from each site will be integrated to determine how long potential biosensors retain fuel cycle signatures, the lateral and vertical extent of their application, and their ability to differentiate between peaceful and arms-related fuel cycle activities.

Co-expression network-based analysis of genes associated with leaf temperature and stomatal conductance in grapevine

Harshraj Shinde

University of Kentucky

Grapevine (*Vitis vinifera* L. cv. Cabernet Sauvignon) is widely used for winemaking all over the world. Quality and yield of grapevine is increasingly challenged by environmental stresses. Plants' survival under stress depends on the ability to perceive the stress stimulus and initiate appropriate physiological changes. Leaf temperature, stomatal conductance and stem water potential change rapidly in response to abiotic stress. Our study aimed to screen genes regulating these physiological changes in grapevine. We applied weighted correlation network analysis and clust to associate changes in physiological parameters with gene expression data. Four significant modules containing 3521 genes and six clusters containing 14143 genes were identified from transcriptome data. Dakmagenta module showed a strong positive correlation with leaf temperature and significant negative correlation with stem water potential and stomatal conductance. Five hub genes were identified from darkmagenta module, these genes are involved in reactive oxygen species scavenging, histone methylation and so on. Gene ontology analyses of modules and clusters highlighted the key biological processes as biological regulation, response to stimulus and response to stress. Pathway analyses highlighted key pathways as thermogenesis, plant hormone signal transduction and protein processing in endoplasmic reticulum. The candidate genes and metabolic pathways identified in this study are valuable genetic resources or targets for future breeding programs.

Engineered habitats enable in situ chemical monitoring and visualization of Populus root development and cross-kingdom interactions

Muneeba Khalid

ORNL

A deeper understanding of dynamic biological systems requires comprehensive spatial and temporal monitoring of the physical structure and local chemical environment that drives organization and function. Conventional chemical imaging can be destructive, preventing any tracking of biological systems over the course of their development. Here, we describe efforts to develop a platform for nondestructive chemical imaging of plant roots through space and time in environments that mimic the physical architecture of natural soil. A microfluidic device featuring a microchannel design that integrates physical barriers of deterministic shape and size distributions is sealed with a microporous membrane to provide access for online chemical imaging of biological systems. We hypothesize that chemical interactions between *Populus* and the soil microbiome play an essential role in shaping the rhizosphere microbial community and ultimately influence plant colonizatiton. Currently, we are mapping the distribution and growth of *Populus trichocarpa* roots from cuttings grown in our unique membrane-based engineered habitats. Simultaneously, we are observing the growth and motility of select soil and rhizosphere microbial isolates in these systems. Future work will trace microbial distributions along the root and correlate these with the chemical environment to better understand the role of the plant host in shaping its microbiome and local rhizosphere communities.

Role of Cation/H^+ exchanger CHX20 in mediating drought stress responses in Populus

Amith R. Devireddy

ORNL

Drought stress is one of the major abiotic stresses affecting agricultural productivity worldwide. Water deficit conditions beyond a plant's physiological optimum can trigger significant physiological perturbations, reduce the rate of photosynthesis, and accelerate leaf senescence leading to a decrease in canopy size. One of the possible ways to enhance plants drought tolerance in plants is by delaying drought-induced leaf senescence and maintaining leaf water potential. On the basis of Genome-wide association studies (GWAS) in *Populus*, we identified genetic loci highly associated with drought-induced leaf senescence and subsequently validated the function of these genetic loci by generating and analyzing transgenic poplar plants (*Populus tremula x P. alba*) with altered expression (i.e., knocking out or overexpression). We report here the functional characterization of a member of putative Na^+/H^+ antiporter family CATION/H^+ EXCHANGER (CHX20) known to be involved in the osmoregulation through K^+ fluxes in guard cells. The CHX20 transgenic overexpression (OE) plants retained high leaf water potential and photosynthetic activities compared to wildtype (WT) or knockout (KO) lines throughout the duration of the drought treatment. Moreover, the survival rate of transgenic OE lines was at least 2-fold higher compared to the WT plants highlighting the role of the cation/H^+ exchanger in plants. Genetic engineering of drought-tolerant crops that cope with limited water regimes without diminution of yield would ensure plant production in water-limited lands by minimizing drought-related losses.

Linking groundwater table fluctuations to oxygen availability and CO_2 and CH_4 release from soil

Erin Berns

ORNL

Explicit representation of soil redox processes in Earth system models could constrain model uncertainty and enhance simulations. Accurate depiction of hydrobiogeochemical redox controls may be especially important in Arctic soils, as the Arctic is warming more rapidly than the global average and is projected to experience dynamic hydrological change. Aerobic and anaerobic incubations have been used to evaluate CO_2 and CH_4 release from Arctic soils, but there are limited studies that explore dynamic trends across a vertical soil gradient. This project aims to (1) quantify changes in oxygen availability and CO_2 and CH_4 release under saturation and drainage cycles in a soil profile, and (2) develop datasets that support a vertically-resolved redox model that can be coupled to Earth system models. A column instrumented with optical oxygen sensors, thermocouples, and sampling ports was tested in a prototype experiment with model soil materials. Results indicate that pulses of CO_2 and CH_4 are associated with rapid drawdown, and that longer saturation times lead to larger releases of CH_4 during subsequent drawdown. These trends will be discussed relative to preliminary results from Arctic thermokarst soil experiments. Reactive transport and redox parameters determined in column experiments could support future Earth system model simulations.

An engineered approach to fungal growth in soil

Yi-Syuan Guo

ORNL

Fungi play a dominant role in soil network. With its tip-growing mycelium network, fungi can facilitate bacterial or nutrient transport and shape its local environment physically and chemically under plant roots. However, it remains largely unidentified and challenging to study its behavior in natural habitats due to its opacity and complex porosity. In this study, we propose the development and use of an engineered microhabitat to visualize the fungal growth in response to spatial variances. Generally, the microfluidics were fabricated using photolithography and conventional soft lithography and assembled to glass slides for fungal cultures. Selected fungal strains (*Linnemannia elongate, Podila minutissima, Fusarium falciforme and Laccaria bicolor*) were applied to this system and demonstrated their various morphology at hyphal level. Single hypha of each strain was directed to grow through micro-channels with well-defined pore dimensions. The response of individual hypha was monitored using time-lapse microscopy and hyphal elongation rates were determined via image analysis. Our results provide a microfluidics approach to visualize the hyphal growth and serve as a systematic platform to qualitatively investigate fungal behaviors in well-defined geometry.

Climate and atmospheric deposition drive the variability and trend of a large flux of dissolved organic carbon from US watersheds

Xinyuan Wei

ORNL

The lateral flux of dissolved organic carbon (DOC) from soils to inland waters and ultimately to the ocean represents a fundamental component of the global carbon cycle. To estimate the DOC flux, I developed an empirical terrestrial-aquatic DOC fluxes model (TAF-DOC). TAF-DOC incorporates various environmental factors (e.g., meteorology, sulfur and nitrogen deposition) that to-date have not been comprehensively considered or well-represented in existing modeling frameworks. TAF-DOC was applied to estimate spatial-temporal dynamics of DOC flux and potential fates across the conterminous United States during the 1985 to 2018 time period. Our results suggest that the interannual pattern of DOC flux was strongly regulated by precipitation, but the long-term trend was significantly influenced by the rate of atmospheric wet sulfur deposition. From 1985 to 2018, TAF-DOC estimated DOC loading from terrestrial to aquatic ecosystems in the conterminous United States to be 33.5 ± 2.2 TgC per year, which was roughly 0.39-0.49% of total soil organic carbon stock estimates. The dominant fate of terrestrially-derived DOC was delivery to the coastal ocean in riverine export (41%), with another 21% buried in sediment and the remaining 12.8 ± 0.4 TgC per year (38%) returned to the atmosphere through outgassing from inland waters.

Environmental DNA (eDNA) applications for hydropower aquatic community monitoring and environmental impact studies

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Hydropower regulation frequently requires fish biodiversity assessments to better understand and mitigate environmental impacts, yet, are derived most often from conventional fisheries methods (e.g., electrofishing, gill netting, seining). These methods are time-consuming, costly, and present risks for personnel, as well as introduce bias with respect to fish size and species resulting in misrepresentation of the true biotic community. Using environmental DNA (eDNA)— DNA that percolates into the environment from sloughed skin cells, gametes, etc., that can be amplified and sequenced to identify how many and which species are present in an area —has the potential to transform environmental conservation and management. Our research focuses on tailoring eDNA methods in hydropower-impacted systems to quantify spatial, temporal, and organismal variation of eDNA in Melton Hill Dam by sampling tailwater and reservoir sites throughout the year. We anticipate that our work will demonstrate that eDNA can comprehensively characterize species and community dynamics at the local, tributary, and watershed scales. Further, our research will contribute to the growing confidence in eDNA and help overcome inherent uncertainties in its utility so that eDNA can serve as a vital tool for biodiversity and ecosystem assessments of hydropower impacts.

Recovery of Critical Materials from End-of-Life Lithium-Ion Batteries using Supported Membrane Solvent Extraction

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In the recent years, lithium-ion batteries (LIBs) have drawn a huge attention worldwide due to their wide use in portable electronics and hybrid/electric vehicles. As we look to the opportunity of domestic LIB manufacturing, one of the main challenges for the U.S. is lack of production capacity for pure battery materials such as cobalt, lithium, nickel, and manganese. As a result, the U.S. relies heavily on imports of these key materials. On the other hand, there are no established technologies for the recycling of spent LIBs to meet the growing market demands of the critical materials. Hence, the recycling of critical materials from LIBs is important to secure a domestic source of these materials for reuse in new LIB formulations. To achieve this goal, a highly efficient, cost-effective, and environmentally friendly supported membrane solvent extraction (MSX) process is developed at ORNL for the recovery of high purity (>99.9 wt.%) and high yield (>90%) critical elements from a wide range of mixed LIB scrap, where individual constituent elements of a spent LIB cathode are separated and recovered. MSX has the potential to address the challenges to secure a domestic source of critical materials from LIBs for reuse in new LIB formulations.

Sulfate Recognition by a Pyridine-Functionalized Diiminoguanidinium Photoswitch: Structural and Kinetic Studies

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The concept of molecular recognition has found a multitude of uses, from sensing a few molecules of analytes to separating radionuclides from nuclear waste. In the preponderance of these applications, the need to produce a recognition agent that can be cycled between bound and unbound states with a target guest species is of significant interest. Generally, such a reversal is accomplished with chemical swings such as pH; while effective, this requires chemical inputs and produces waste. Building upon the precedents already established with imine photoisomerization, the imine bond in iminoguanidinium groups may undergo *E*–*Z* photoisomerization that can be exploited for switched binding and release of oxoanions. The pair of N–H groups available for directed oxoanion binding in the *E,E* isomer may be deactivated by appending 2-pyridyl groups that can act to close off the binding site by intramolecular hydrogen binding. Following this logic, photoswitching between open *E,E* and closed *Z,Z* photoisomers provides a binding-release mechanism for efficient oxoanion separations. Herein, we report the first example of photoswitching of anion binding by a bis-2-pyridyldiiminoguanidinium salt as specifically demonstrated with sulfate. Photoisomerization in DMSO with UV-visible light was monitored through ^{1}H NMR spectroscopy and crystal structures of the binding *E,E* form with sulfate and the nonbinding *Z,Z* photoisomer. Strong binding of sulfate by the *Z,Z* form vanishes, illustrating an unprecedented efficient light-stimulated release of the sulfate ion.

Influences of DGA functionalization on the liquid-liquid extraction of lanthanides

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Lanthanides are vital elements used for a wide variety of energy technologies and national security applications, including use as high-performance magnets, as catalysts, and in electronics, among others. The U.S. Department of Energy has deemed many lanthanides as “critical" owing to the market’s increasing demand and limited supply chain. Moreover, the isolation and purification of lanthanides remains elusive due to their similar physical and chemical properties. Widely studied for the separations of lanthanides and actinides, diglycolamide (DGA) ligands have shown interesting extraction behavior. The structure activity relationships of several DGAs with various functionalizations at the amide group was recently discussed. Herein, new DGA chelators and their extraction properties will be discussed.

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In-situ ultrasound spectroscopy for neutron scattering

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Resonant ultrasound spectroscopy (RUS) quickly and nondestructively measures the elastic tensor of small, mm-to-cm sized solid materials such as metals, ceramics, and semiconductors with high accuracy and in extreme environments. Moreover, this technique lends itself well to characterize novel materials synthesized in small quantities or irreversible phenomena like glass transitions, precipitation, or re-crystallization where reproducibility is challenging. Through the laboratory directed research and development project “In situ ultrasound spectroscopy for neutron scattering," we are developing sample probes that interface with neutron scattering beamlines at the SNS and HFIR sources to provide users with an intrinsic diagnostic variable to monitor changes in sample conditions in real time as well as to measure elastic properties in the exact same conditions as atomic-scale information gathered from neutron scattering measurements. We will share our progress in RUS-probe assembly, testing, and deployment at the SNS beamlines. Several case studies of a variety of materials are discussed, including those for austenitic steels, yttrium hydride, bismuth-antimony, and bulk metallic glass. Future capabilities such high-temperature RUS and new RUS analysis software are also discussed.

Comparison of Oxidation Behavior of Zircaloy-4 Fabricated Using Ultrasonic Additive Manufacturing and Conventional Methods

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Ultrasonic additive manufacturing (UAM) is a solid-state joining technique for producing planar geometries with cavities or other internal heterogeneous features. The use of UAM for Zr alloys in nuclear reactor applications is in its early stages. Corrosion behavior of Zr alloys (e.g. Zircaloy-4) during exposure to water coolants during normal operation and high temperature steam oxidation during accident scenarios are critical performance metrics. Residual voids formed between layers and other heterogeneities from the UAM process are not present in conventional Zry-4 processing. The oxidation behavior of UAM Zry-4 was studied alongside cast Zry-4 using steam exposures at 700 and 900°C for 1 h and at 1100°C for 10 min. Steam exposures at 1100°C showed mass gain 100% higher for UAM Zry-4 compared to cast Zry-4. Mass change differences decreased with temperature. Interlayer oxidation was observed in all UAM samples. Hydrothermal corrosion was compared using a continuously refreshing autoclave exposure for 500 h at 330°C and 15.2 MPa. Little difference was found in mass change or median oxide scale thickness; interlayer oxidation was observed in UAM samples.
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Optimization of GP-SANS Guide Upgrade

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To determine the effect of altering guide specifications in the GPSANS design, we used Monte Carlo simulation of the GPSANS instrument to determine the flux at the sample position in response to guide sections with varied *m*-values. McStas is a tool for the Monte Carlo simulation of neutron instruments, allowing the modeling of an instrument accurately in terms of of physical components (e.g., source, guide, sample), and providing other variables to define a measurement, (e.g., sample distance, chopper frequency). To optimize some property, such as the *m*, it is possible to iterate the *m*-value of the guide and assess the resultant change in flux. We model the current GPSANS layout and the proposed upgrade and examine the impact of the *m*-value of guide surfaces on the flux following these changes. The layout of the GPSANS includes an optical filter, and by increasing the *m*-value of this optical filter there is a marked increase in the overall flux at the sample position as well as extending the population of low-wavelength neutrons. This change would allow experiments requiring low wavelengths.

Characterization of strain induced martensitic formation in neutron and proton irradiated 316L via in-situ EBSD tensile testing

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Strain-induced martensitic formation is a known phenomenon, but the processes and features in the microstructure that govern their formation are not well established for irradiated 316L austenitic stainless steel. The experiments presented here were performed on irradiated 316L samples from the Spallation Neutron Source (SNS) target vessels after service. Tensile testing and microstructure characterizations were performed with proton and neutron irradiated 316L SNS target samples using in-situ tensile testing and electron backscattered diffraction (EBSD). A detailed investigation was performed throughout the gauge section of the tensile specimens, and the three most interesting locations were selected based on crystallographic orientation, grain boundary characteristics and morphology of grains to characterize the details of strain-induced martensitic formation during deformation. The microstructure features associated with the formation of martensitic include grain boundaries, slip bands, intersection points of the slip bands, and interfaces between deformation twins and parent grains. At these different locations, the martensite phases formed with different shapes and orientations. Along with the location of martensitic formation, their shape and crystallographic orientation were also investigated and quantified. This work shows that martensite formation during plastic deformation in irradiated 316L occurs at several different microstructural features, which evolve and change as deformation progresses.

Advection-Reaction Modeling in Molten Salt Reactors

Austin Lo

ORNL

We develop a theoretical and computationally inexpensive basis for modeling the spatialtemporal advection-reaction effects for delayed neutron precursor (DNP) drift in molten saltfueled reactors (MSRs). Using the Laplace Transform Method, the governing second order PDE is reduced to a first order ODE whose solution is readily obtainable – both analytically and numerically. Here, we present the results from applying the model to two simple scenarios, namely: (1) the equilibrium DNP core and loop distribution at constant power and (2) the spatial-temporal DNP core and loop distribution after a reactivity insertion. Future work will implement this methodology into the SCALE nuclear safety analysis and design suite, developed at Oak Ridge National Laboratory, then tested against the Molten Salt Reactor Experiment (MSRE) model results in VERA and other high fidelity simulation packages.

Optimization of GP-SANS Guide Upgrade

Sara Sultan

University of Tennessee

Phase Change Material (PCM) based thermal energy storage is an increasingly popular tool to level out electrical grid demand and add stability to the grid. PCMs can be used for space heating and cooling applications by embedding into the heat pump equipment or building materials. We have summarized the state of art of heat pump-integrated thermal energy storage for grid-interactive buildings, reporting various active and passive storage configurations to analyze the demand impact, and energy and cost-savings. We concluded that heat pump integrated active PCM storage has demonstrated significant load shifting benefits and offers additional economic benefits when combined with real-time utility demand response. To validate our argument, a building model and HVAC model are evaluated with the simplest heat pump integrated PCM configuration, implying direct use of PCM for the building conditioning during the discharge. A residential TOU utility rate from utility provider in Fresno, California for ASHRAE climate zone 3B is used to determine the economic value and 20% consumer cost savings are reported. The energy analysis showed a 14.5% total energy reduction for space cooling, with 87.5% reduced on-peak energy usage.

Next-Cycle Dilute Combustion Control Using Online Machine Learning

Bryan Maldonado

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Dilute combustion using exhaust gas recirculation (EGR) presents a cost-effective method for increasing the efficiency of spark-ignition engines. However, the maximum amount of EGR that can be used at a given condition is limited by a rapid increment of cycle-to-cycle variability (CCV). This phenomenon is caused by the reduction in the flame propagation speed, which can be counteracted by enriching the cycles where low energy events are prone to occur. This study describes a methodology to design a model-based stochastic optimal controller to adjust the cycle-to-cycle fuel injection quantity in order to reduce CCV and further extend the dilute limit. The controller was enhanced with a machine learning algorithm for online estimation of the statistical properties of combustion efficiency, which are needed to generate predictions for next-cycle events. The experimental results suggested that the dilute limit can be extended from 18.5% to 21% EGR fraction at an operating condition relevant for highway cruising. Moreover, the proposed method was compared with a state-of-the-art artificial intelligence-based controller attempting the same CCV reduction goal. Results indicated that the proposed controller can achieve a larger CCV reduction with less fuel enrichment compared to previous methods

Compilation of the U.S. Pipeline Intermodal Terminal Dataset

Yuandong Liu

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Pipeline is a major mode of transportation for moving petroleum and petroleum products across the nation. Due to considerations of costs and other reasons, pipeline can commonly be connected to rail/truck/water, depending on its location, to transport shipments between their origins and destinations. The facilities that enable such a connection are pipeline intermodal terminals. This study identified and fused various data sources, from both public and private sectors, to establish the pipeline intermodal terminal dataset. The final dataset contains 1,401 terminals and provides attributes on the characteristics of each terminal, including exact location, mode connection, terminal storage capacity, and commodities being handled at the terminal. The location of each terminal was validated using satellite imagery. In addition, available modes that are connected to the terminal were validated using several freight network systems and data, including National Pipeline Mapping System, North American Rail Network, and National Commercially Navigable Waterway Data. Furthermore, online information from websites of companies that own/operate the terminals were examined to confirm the information being gathered. This resulting dataset can be used by freight researchers and planners to better understand the storage and movement of petroleum and petroleum products and to make strategic plans.

Visualizing Travel Patterns in New York State Regional Economic Development Council Regions

Majbah Uddin

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Understanding travel patterns of households and their household members are necessary for assessing the reliability, efficiency, capacity and flexibility of regional transportation system to meet current, and accommodate future, travel demand. Additionally, it helps to determine the feasibility and effectiveness of congestion alleviating and emerging technologies. This study uses 2017 National Household Travel Survey data, the authoritative source on the travel behavior of the American public, to estimate and visualize travel patterns of residents in New York State Regional Economic Development Council (REDC) regions. REDC regions are made up of several adjacent counties and are established to develop long-term strategic plans for economic growth of their regions. The estimates considered for trip patterns include average hourly total person trips by time of day and trip purpose, number of daily person trips by trip length and trip mode, average commute travel time by trip mode, and average vehicle occupancy by vehicle type. These estimates are obtained for all REDC regions and compared against state-level estimates. It is found, based on the visual analytics conducted under this study, that the residents of different REDC regions have different daily travel patterns. The findings could be used in regional transportation planning as well as inputs to travel demand models.

Meeting Notes


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