"Extracting design rules for materials from atomistic simulations guided by scientific machine learning and causal relations."

Dr. Ayana Ghosh
Computational Sciences and Engineering Division
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Every key facet of physical sciences including design of materials description to estimation of structure-property relationships to process optimizations, have experienced tremendous growth in utilization of data-driven machine learning models in the past decade. There exists plenty of studies to encode complex graphs, symbolic representations, invariances, and positional embeddings in these models for targeted design. However, the intrinsically in-built correlative nature of ML models does not capture the causal hypothesis-driven nature of physical sciences. This presentation will focus on how predictive ML models combined with causal relations and hypotheses-driven active learning can be exploited in combination with material representations to extract governing fundamental atomistic mechanisms with direct ties to experimental observables for a variety of systems such as perovskite oxides, and small organic molecules.

Acknowledgments:

This research is sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U.S. Department of Energy.

Bio: Dr. Ayana Ghosh is a Research Scientist at the Computational Sciences & Engineering Division at Oak Ridge National Laboratory (ORNL). She was a postdoctoral researcher at ORNL from 2020 to early 2023. She received her MS, PhD in Materials Science and Engineering from the University of Connecticut in 2020 and BS in Physics and Abstract Mathematics from the University of Michigan-Flint in 2015.

Her research focuses on scientific machine learning methods combined with state-of-the-art first principles computations to study a wide range of materials ranging from inorganic perovskites, 2D systems to organic crystals and polymers. Bridging the gap between appropriate utilization of data generated by simulations and experiments requires a great deal of understanding of the nuances present in both fields, which remains the central goal of her efforts. She has so far, published ~30 papers in peer-reviewed journals including Chemistry of Materials, npj Computational Materials, and Nature Physics. She was the recipient of the Rising Stars in Computational and Data Sciences 2022 nomination at the Sandia National Laboratories and Extraordinary Performance Awards 2022, 2023 from ORNL.

She enjoys writing poetries, short narratives, listening to music and hiking in her leisure.
"Probing the Protein Dynamics of Profilin-1 and TDP-43: Function and Dysfunction in Two ALS-linked Proteins"

Abstract: Profilin-1 (PFN1) and TDP-43 are two proteins that have been linked to the neurodegenerative disease amyotrophic lateral sclerosis (ALS). We have used a combination of NMR spectroscopy and molecular dynamics (MD) simulation to characterize their structure and dynamics in solution. We observed that two ALS-linked mutations of PFN1, G1118V, and M114T, impact the internal dynamics of the protein, and therefore have the potential to impact the interaction of PFN1 with its binding partners actin and formin. For TDP-43, we have identified a core nucleus of structure for a folding intermediate in its second RNA recognition motif (RRM2). Our studies suggest a role for this RRM2 intermediate in normal TDP-43 function as well as in dysfunction by serving as a template for misfolding, aberrant interactions and aggregation.
“Unstructured Mesh Tools to Support Massively Parallel DOE Simulation Codes”

Dr. Mark Shephard  
Department of Mechanical, Aerospace and Nuclear Engineering  
Rensselaer Polytechnic Institute  

Wednesday, December 6, 2023  
10:30 AM – 11:30 AM  
DCC 324

Abstract: The Department of Energy Office of Science Advance Scientific Computing Research supports the development of massively parallel simulation codes that address key areas of scientific investigation. As the ability to account for additional physics and geometric complexity has increased, a number of the simulation codes have moved to the use of unstructured mesh methods. This presentation will discuss unstructured mesh technologies being developed to support the needs of multiple fusion energy system and ice sheet modeling codes. The tools to be discussed include:

- Geometry clean-up and combination tools to construct analysis geometries of the desired level of fidelity.
- Procedures to generate and adapt meshes meeting specific simulation code requirements.
- An infrastructure for massively parallel particle in cell simulations on unstructured meshes that has been used for fusion plasma and impurity transport simulations, as well as material point methods used in ice sheet modeling.
- An infrastructure for the in-memory coupling of massively parallel simulation codes that employ unstructured and structured mesh methods.

Bio: Mark S. Shephard is the Samuel A. and Elisabeth C. Johnson, Jr. Professor of Engineering at Rensselaer Polytechnic Institute. He is the director of Rensselaer’s Scientific Computation Research Center. Dr. Shephard has made contributions to the areas of automatic mesh generation, automated and adaptive analysis methods, and parallel adaptive simulation technologies. He is a fellow and past president of the US Association for Computational Mechanics and was recipient of the 1997 USACM Computational and Applied Sciences Award, and the 2011 John von Neumann medal; a fellow of the International Association for Computational Mechanics; and a fellow of ASME. Dr. Shephard was a co-founder of Simmetrix Inc., a computer-aided engineering company dedicated to producing the technologies and associated software components to enable simulation-based engineering.
Phase Separation in Elastic Networks

Svetlana Morozova
Department of Macromolecular Science and Engineering
Case Western Reserve University

Abstract: Gels are key materials in biological systems such as tissues and may control biocondensate formation and structure. To further understand the effects of elastic environments on biomacromolecular assembly, we have investigated phase behavior and radii of coacervate droplets in polyacrylamide (PAM) networks as a function of the gel modulus. Poly-L-lysine (PLL) and sodium hyaluronate (HA) coacervate phases were prepared in PAM gels with moduli varying from 0.035 – 9.0 kPa. The size of the coacervate droplets is reported from brightfield microscopy and confocal fluorescent microscopy. Overall, the coacervate droplet volume decreases inversely with the modulus. Fluorescence microscopy is used to determine the phase behavior and concentration of fluorescently tagged HA in the coacervate phases as a function of ionic strength (100 - 250 mM). We find the critical ionic strength and coacervate stability is nonmonotonic as a function of the network modulus and that the local gel concentration can be used to control phase behavior and coacervate droplet size scale. By understanding how elastic environments influence simple electrostatic assembly, we can further understand more complicated biomacromolecular assemblies like collagen in the extracellular matrix. We have also observed how collagen assembly is limited in PAM networks using cryogenic electron microscopy and high resolution optical microscopy, and find that even in extremely crosslinked networks, collagen assembles, and the radial size and orientation is determined by the network topology.

Biosketch: Dr. Svetlana Morozova is an Assistant Professor of Macromolecular Science and Engineering at Case Western Reserve University. Dr. Morozova’s lab is broadly focused on studying polymer dynamics in solutions and gels by setting up new scattering and microscopy techniques. A particular interest in the lab is the effect of polymer flexibility on bulk properties such as viscosity and modulus, and polymer dynamics and assembly in complex environments. These processes are relevant to protein dynamics in cells, fluid flows, droplet formation, and filtration devices. Recently, Dr. Morozova has been awarded the ACS PRF Doctoral New Investigator, Lubrizol Innovation Prize, and NSF CAREER awards. Before joining CWRU in July 2019, Dr. Morozova worked as a post-doctoral researcher in the Department of Chemistry at University of Minnesota Twin Cities. She received her Ph. D. in Polymer Science and Engineering from University of Massachusetts at Amherst in 2017.
Efficient Bilevel Optimization and Application in Continual Learning

Kaiyi Ji

University of Buffalo

Wednesday, December 6, 2023

4:00pm

JEC 3117

Abstract: Bilevel optimization (BO) has received increasing attention in modern machine learning (ML), and has become a theoretical foundation for designing efficient computational tools for various ML areas such as meta-learning, autoML, fair ML, continual learning, and etc. In the first part of this talk, I will briefly introduce several recent BO applications in hyperparameter optimization and rehearsal based continual learning. In the second part, I will propose a novel stochastic bilevel optimization algorithm named stocBiO, which features a sample-efficient hypergradient estimation via Hessian-vector computations and automatic differentiation. I will then present the convergence analysis for stocBiO and discuss its application in coreset selection for rehearsal based continual learning by proposing a new bilevel problem formulation. I will finally discuss the opportunities such as application of Hessian-free bilevel algorithms in large-scale continual learning, etc.

Bio: Kaiyi Ji is currently an assistant professor at the Department of Computer Science and Engineering of the University at Buffalo (UB), and is also an affiliated faculty with the Institute for Artificial Intelligence and Data Science (IAD). Dr. Ji was a postdoctoral research fellow at the Electrical Engineering and Computer Science Department of the University of Michigan, Ann Arbor, in 2022. Dr. Ji received the Ph.D. degree from the Electrical and Computer Engineering Department of The Ohio State University in December, 2021. Dr. Ji was a visiting student research collaborator at the department of Electrical Engineering, Princeton University. Previously Dr. Ji obtained the B.S. degree from the University of Science and Technology of China in 2016. Dr. Ji has worked at the intersection of optimization, machine learning and communication networks, on both the theory and application sides. His current major interest lies in bilevel optimization and its application to various machine learning areas including meta-learning, continual learning, hyperparameter optimization, etc. He received the prestigious Presidential Fellowship at OSU in 2020, and two NSF awards in 2023.
ABSTRACT: Thin film synthesis methods of complex transition metal oxides had their wake-up call when superconductivity was discovered in cuprates in 1986. Advancements in sputter deposition, pulsed laser deposition, and most notably in molecular beam epitaxy followed and culminated in customized layering growth methods that allowed for artificially designed complex transition metal oxides. Besides, rich magnetic ordering phenomena in manganates, ferrites, cobaltates, and nickelates triggered a burst into thin film synthesis methods of complex transition metal oxides. Yet, such materials of interest are all centered around 3d complex transition metal oxides. Regarding thin film synthesis methods like pulsed laser deposition, complex transition metal oxides based on 4d or 5d systems are accessible, yet at the cost of crystalline quality. On the other hand, the synthesis of 4d or 5d complex transition metal oxides from bare metals is not feasible owing to the typically low vapor pressures of these elements. We overcame this problem by developing a molecular beam epitaxy system that is empowered exclusively by electron guns. These electron guns are controlled by electron impact emission spectrometry (EIES), where individual elemental fluxes are tuned to meet desired stoichiometries in real time. For 4d and 5d complex transition metal oxides a true rate control system is indispensable as the oxidation process is commonly accompanied by the formation of volatile oxides. For example, for the synthesis of superconducting Sr2RuO4 thin films with ozone as an oxidizing agent, the Ru flux is 13–14% higher than stoichiometrically required. The excess ruthenium will be converted to RuO3 and RuO4 during the synthesis process and eventually condense at the vacuum chamber walls. Furthermore, we discuss the synthesis of Nd2−xCexPdO4 thin films by molecular beam epitaxy. Finally, we will stroll through the synthesis procedures of complex osmates. In there, extremely high temperatures coincide with the formation of extremely volatile species, e.g., OsO3 and OsO4. Nonetheless, this materials synthesis exploration approach is an enabler for hitherto unknown and unexplored materials with intriguing physical properties.
I will tell two stories from my lab. The first story is how biophysical cues dictate the formation and maintenance of dense connective tissues. This work includes how muscle loading during embryogenesis dictates the growth of tissues in the knee joint and how cell contractility regulates cell fate and tissue homeostasis. The second story, which started with a serendipitous discovery during my graduate studies, is focused on how the hedgehog signaling pathway is a master regulator of fibrocartilage formation during enthesis development and tendon-to-bone repair in adults.

I obtained my undergraduate degree in Materials Science and Engineering with a specialization in Biomaterials from the University of Illinois at Urbana-Champaign in 2005. I completed my PhD in the Functional Tissue Engineering laboratory under the direction of Dr. David Butler at the University of Cincinnati in 2011. After postdoctoral training in musculoskeletal biology with Dr. David Rowe at UConn Health, I moved to the University of Pennsylvania where I developed an independent research program in the McKay Orthopaedic Research Laboratory. My lab’s primary research goals are directed towards understanding the genetic, cellular, and mechanical mechanisms that regulate normal development, disease, and repair of joint tissues. I am particularly interested in identifying markers that define resident progenitors vs. mature cell types and the environmental cues (e.g., molecular and mechanical) that regulate their differentiation. I was awarded a K99/R00 grant (AR067283) in 2015 to define the tendon cell lineage and pathways that regulate tenogenesis, which led to my first independent R01 (AR076381) to investigate the role of hedgehog in tendon-to-bone repair and an R21 (AR078429) to develop novel drug delivery systems to target the hedgehog pathway to improve repair outcomes. My lab also investigates how mechanical forces impact the formation and maintenance of dense connective tissues (e.g., R01AR075418 and P50AR080581), which have resulted in a recent publication in PNAS (PMC10235980) defining the mechanotransductive signaling that regulate tensional homeostasis. The long-term goals of my lab are directed towards translating these mechanistic studies to novel therapeutic strategies.