

Workshop on AI for Physical Sciences

March 13-14, 2023

Discovery Hall and Hybrid



March 13th

9:00am – 4:00pm

9:00-9:15 Introduction: Sotiris Xantheas

9:15-11:45 Session 1: Needs

Lightning talks on science drivers for each of the areas.

What are the driving applications?

What are the challenges they need help with?

- Simulation and Multi-scale Modeling of Complex Atomistic Systems
 - *Chris Mundy, Jay Xu*
- Applications of Predictive Models
 - *Eric Bylaska, Arun Devaraj*
- Optimal Design of Chemical Structures/Mechanisms
 - *Tiffany Kaspar, Yulan Li*

11:45-1:30 Break

1:30-4:00 Session 2: Solutions

Lightning talks on AI-centered research for each of the following ideas. Who from Session 1 can benefit from a partnership?

- Simulation and Multi-scale Modeling of Complex Atomistic Systems
 - *Gokcen Kestor, Erdal Mutlu*
- Optimal Design of Chemical Structures/Mechanisms
 - *Tegan Emerson, Jan Drgona*
- Applications of Predictive Models
 - *Steven Spurgeon, Dragana Vrabie*

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March 14th

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9:15-12:00 Session 3: Deep Dives

Now that we have had a chance to hear each other, let's deep dive into a long-term vision that can range from both technical to computational capability development.

- Quantum Computing
 - *Karol Kowalski, Ang Li*
- Catalysis
 - *Nancy Washton, Rachit Khare, Libor Kovarik, Eric Wiedner & Benjamin Helfrecht*
- Infrastructure for AI-Enabled science
 - *Sutanay Choudhury, Erin Barker*

12:00-1:30 Break

1:30-3:15 Flash Talks

We will have flash talks to promote crosstalk between the AI and Physical Sciences research communities.

- **Sameera Horawalavithana:** Scaling AI for Science and Security
- **Amanda Howard:** Continual Learning for Physical Systems
- **Tianzhixi Yin:** Evaluating Uncertainty-Based Active Learning for Accelerating the Generalization of Molecular Property Prediction
- **Andrew Engel:** Preliminary Results of Adding Domain Informed Constraints to Deep Neural Networks to Advance Understanding the Nature of Dark Energy *and* Deep Nets Realized as Linear Models (on behalf of Tony Chiang)
- **Jeremy Zucker:** Digital Twins for Synthetic Biology
- **Himanshu Sharma:** Surrogate Modeling Framework of Atmospheric Secondary Organic Aerosols (SOA) for Amazon Rainforest.
- **Nick Nelson:** Structural Dynamics of Metals on Oxides
- **Mariefel Olarte:** Modification of Molecular Transformer for Hydrotreating Reaction Prediction
- **Joonhoon Kim:** Predictive Modeling of Biological Systems for Bioprocess Development

10 Minute Break

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- **Bill Cannon:** Learning Control of Chemical Reaction Networks in Biology and Predicting their Emergent Properties
- **Margaret Cheung:** Graph Identification of Proteins in Tomograms
- **David Brown:** Research Data Management: Standards, Processes, and Workflows! Oh My!
- **Yu-Hong Yeung:** Scalable Physics-Informed Machine Learning Methods for Data Assimilation in Inverse Problems
- **Aowabin Rahman:** Machine Learning for Predicting Interfacial Strength of Carbon Nanotube (CNT) Composites
- **Shivam Sharma:** Training Foundational Models for SELFIE Representations of Chemical Molecules
- **Henry Sprueill:** Active Learning to Improve Simulation Accuracy of Atomistic Neural Network Potentials Trained on Biased Datasets
- **Jingshan Du:** Monitoring the Ice Nanostructures and Melting Dynamics at Atomic Resolution: Opportunities of AI in Image/Movie Data Analysis
- **Ram Devanathan:** Materials selection and optimization using machine learning
- **Carlos Ortiz Marrero:** Explorations in Quantum Machine Learning

3:15 Closing remarks – Sotiris Xantheas and Sutanay Choudhury
