AIRES

Artificial Intelligence for
Robust Engineering and Science Workshop

DAILY AGENDA

Tuesday, May 21

Start Time	Session Information	Speaker	Title
7:30 - 8:15 AM	**Registration**		
8:15 - 8:25 AM	**Welcome**	Dr. Wendy J. Shaw, Chief Science and Technology Officer (Physical and Computational Sciences Directorate, PNNL)	
8:25 - 8:30 AM	**Agenda Overview**	Mahantesh Halappanavar	
8:30 - 9:30 AM	**Keynote #1 (National Academies)**	Derek Bingham & Ruby Leung	Foundational Research Gaps and Future Directions for Digital Twins
9:30 - 9:45 AM	*BREAK*		
9:45 - 10:45 AM	**Trustworthy Digital Twins**	Prasanna Balaprakash	Advancing Secure, Trustworthy, and Energy-Efficient AI for Science
Day 1, Session 1 (Chair: Sudip Seal)			
10:45 - 11:10 AM	**Robust Multi-Model AI and Data**	Alexandre Cortiella	Generative AI approaches for the design and transition of modern energy systems
11:10 - 11:35 AM		Sai Munikoti	Generative AI to Solve Real-World Challenges: A Case Study on Streamlining Environmental Review and Permitting Processes
11:35 - 12:00 PM		Tadbhagya Kumar	Physics-Constrained Neural Ordinary Differential Equations for Robust Learning of Stiff Chemical Kinetics
12:00 - 12:15 PM	**Group Photo**		
12:15 - 1:15 PM	**Working Lunch**	Ananth Kalyaraman	Making AI Work for Agricultural Decision Support: Farm and Water Intelligence at the AgAID Institute
Day 1, Session 2 (Chair: Lekha Patel)			
1:15 - 1:40 PM	**Robust Multi-Model AI and Data**	Thomas Beckers	A Physics-Informed Composable Learning Framework
1:40 - 2:05 PM		Panos Stinis	When big networks are not enough: physics, multifidelity and kernels
2:05 - 2:30 PM		Sandeep Madireddy	Probabilistic Neural Architecture Search for Uncertainty Quantification in Neural Networks
2:30 - 2:55 PM		Ruby Leung	A non-intrusive and an online machine learning framework for bias correcting climate simulations of extreme weather events
2:55 - 3:10 PM	*BREAK*		
3:10 - 5:30 PM	**Flash Talks followed by Poster Session (Chair: Jan Strube)**		
		Kim DeSousa	Empowering Discovery: AI's Potential in Automated Laboratory Platforms
		Maruthi Kumar Mudunuru	AI for SoilChip: Lab-on-a-chip designs to accelerate model-data-experiment workflows informed by soil datasets
		Aowabin Rahman	Mitigating Adversarial Interference in Multi-agent Reinforcement Learning
		Charles Koll	Decentralized Runtime Verification for Safety of Distributed Cyber-Physical Systems
		Dewei Wang	Reinforcement learning for automated conceptual design of energy and chemical systems
		Grant Hutchings	Fast Emulation and Modular Calibration for Simulators with Functional Response
		Ashfiqur Rahman	Enhancing Primary Biological Aerosol Particle Identification by Supervised Machine Learning from High-Resolution Scanning Electron Microscopy Data
		Maruthi Kumar Mudunurun	ML-based NMF analysis for MONet data synthesis and scaling

Wednesday, May 22

Start Time	Session Information	Speaker	Title
7:30 - 8:15 AM	**Registration**		
8:15 - 8:30 AM	**Agenda Overview**	James Ang	
8:30 - 9:30 AM	**Keynote #2**	Manish Parashar	Democratizing Access to Science Data
9:30 - 9:45 AM	*BREAK*		
Day 2, Session 1 (Chair: Chitra Sivaraman)			
9:45 - 10:10 AM	**Robust Multi-Model AI and Data**	Lekha Patel	Heterogenous Data Fusion with Variational Autoencoders
10:10 - 10:35 AM		Eric Crop	Toward Particle Accelerator Digital Twins: Time-Dependent Multi-Modal Model Calibration with Uncertainty Quantification
10:35 - 11:00 AM		Chetan Kumar	Multi-modal machine learning based surrogate model for flood prediction
11:00 - 12:00 PM	**Tutorial**	Michael Chertkov	Mixing Artificial and Natural Intelligence
12:00 - 1:00 PM	**Working Lunch**	Samantha Koretsky	The National Academies of Sciences, Engineering, and Medicine and its AIRES-Related Activities
Day 2, Session 2 (Chair: Malachi Schram)			
1:00 - 1:25 PM	**Robust Multi-Model AI and Data**	Sutanay Choudhury	ChemReasoner: Bridging Generative AI and Computational Chemistry
1:25 - 1:50 PM	**Trustworthy Digital Twins**	Laura Fierce	Combining advanced modeling with AI/ML to improve aerosol effects on climate
1:50 - 2:15 PM		Shivam Barwey	Towards Explainable Mesh-based Surrogate Models for Energy Conversion Systems
1:50 - 2:15 PM		Kevin Griffin	Adaptive Computing: uncertainty-guided real-time training with distributed computing
2:40 - 2:55 PM	*BREAK*		
Day 2, Session 3 (Chair: Jan Drgona)			
2:55 - 3:55 PM	**Tutorial**	Antonino Tumeo	Bridging Python to Silicon: The SODA Toolchain
3:55 - 4:55 PM		Nicholas Wimer	Comparison of Uncertainty Quantification Methods for Scientific Machine Learning

Thursday, May 23

Start Time	Session Information	Speaker	Title
8:00 - 8:30 AM	**Registration**		
8:30 - 8:35 AM	**Welcome & Agenda Overview**		
Day 3, Session 1 (Chair: Malachi Schram)			
8:35 - 9:00 AM	**Deployment**	Jan Strube	The L-CAPE project at Fermilab
9:00 - 9:25 AM		Auralee Edelen	Progress on Combining Digital Twins and Machine Learning Based Control for Accelerators at SLAC
9:25 - 9:50 AM		Nathan Tallent	Advanced co-design for Distributed AI Systems
9:50 - 10:05 AM	*BREAK*		
Day 3, Session 2 (Chair: Auralee Edelen)			
10:05 - 10:30 AM	**Deployment**	Chitra Sivaraman	Digital Twins for hydropower
10:30 - 10:55 AM		Oceane Bel/Kim Desousa	Guiding the Future: Ensuring Reliable AI Predictions for Instruments
10:55 - 11:20 AM		Aowabin Rahman	Adversarial Search and Rescue via Multi-Agent Reinforcement Learning
11:20 - 11:45 AM	**Workshop Summary**	Pradeep Ramuhalli & Mahantesh Halappanavar	Workshop Summary and Outlook
11:45 - 12:00 PM	**Closeout**		Closeout
12:00 - 1:00 PM	*Lunch On Your Own*		
1:00 - 5:00 PM	**Optional Tours**		
	PNNL Campus Tour (Preregistered attendees only) I Meet outside Discovery Hall at 1 PM)		
	LIGO Hanford I Ride-share or drive on your own to LIGO Hanford; meet at LIGO Visitor Center at 1:00 PM		