Artificial Intelligence for Robust Engineering & Science

AIRES 2: Machine Learning for Robust Digital Twins

January 19 – 21, 2021

Robust engineering is the process of designing, building, and controlling systems to avoid or mitigate failures. The introductory Artificial Intelligence for Robust Engineering and Science (AIRES) workshop in January 2020 explored these foundations. This second AIRES workshop will build on the success of the first workshop to explore and develop the foundations of AI for constructing, deploying, and assuring the robustness of digital twins. The workshop will be comprised of three tracks.

Tuesday, January 19, 2021

11:00–11:05 a.m.	|	**Welcome Remarks: Jeff Nichols, Oak Ridge National Laboratory**
11:05–11:15 a.m.	|	**Agenda Overview: David Womble, Oak Ridge National Laboratory**
11:15–12:00 p.m.	|	**Keynote Speaker: Michael Grieves, Florida Institute of Technology**
		Intelligent Digital Twins: The Role of AI and ML in the Future of Digital Twins
12:00–12:30 p.m.	|	**Break**

Track 1: Construction of Digital Twins

This track will explore the mathematical and computational aspects of using machine learning to construct robust models of physical systems with an emphasis on dynamical and complex systems. Topics of interest include but are not limited to

- Feature engineering and knowledge representation
- Integrating time-series data for anomaly detection and trends predictions
- Incorporating physics-based prior information
- Developing an evolving digital twin through continuous learning
- Data management

Session Chair: Justin Newcomer, Sandia National Laboratories
Session Co-Chair: Malachi Schram, Pacific Northwest National Laboratory

12:30–1:00 p.m.	|	**Invited Speaker 1–1: Nathan Kutz, University of Washington**
		Targeted use of deep learning for physics and engineering
1:00–1:30 p.m.	|	**Invited Speaker 1–2: Farinaz Koushanfar, University of California San Diego**
		Robust and private machine learning

1:30–1:45 p.m.	**Speaker 1–1: Eric Darve, Stanford University**	
	Machine learning for inverse modeling in mechanics	
1:45–2:00 p.m.	**Speaker 1–2: Luke Scime, Oak Ridge National Laboratory**	
	Creating scalable digital twins for advanced manufacturing	
2:00–2:15 p.m.	**Speaker 1–3: Rose Yu, University of California San Diego**	
	Physics-guided AI for learning spatiotemporal dynamics	
2:15–2:30 p.m.	**Speaker 1–4: WaiChing Sun, Columbia University**	
	Microstructure-sensitivity plasticity inferred via graph neural network	
2:30–3:00 p.m.	**Break**	

Session Chair: Pradeep Ramuhalli, Oak Ridge National Laboratory
Session Co-Chair: Iris Bahar, Brown University

3:00–3:30 p.m.	**Invited Speaker 1–3: George Em Karniadakis, Brown University**	
	DeepM&Mnet: A new neural network architecture based on operator regression for digital twins	
3:30–3:45 p.m.	**Speaker 1–5: Piyush Modi, NVIDIA Corporation**	
	Tools to accelerate design, development, and deployment of digital twins	
3:45–4:00 p.m.	**Speaker 1–6: David Schmidt, University of Massachusetts Amherst**	
	Accelerated DL representation of turbulent, reacting flow	
4:00–4:15 p.m.	**Speaker 1–7: Jeph Wang, Los Alamos National Laboratory**	
	Digital twins for x-ray and neutron cameras	
4:15–4:20 p.m.	**Breakout Session Overview**	
4:20–4:55 p.m.	**Breakout Sessions**	

No.	FULL BREAKOUT TITLE	SHORT BREAKOUT TITLE
1	Methods for Physics-Informed DT Construction	Physics-Informed Construction
2	Requirements and Methods for DT Construction	Req'ts and Methods for Construction
3	Time Series Prediction for Dynamical Systems	Time Series Predictions
4	Robustness and Validation of Models and DTs	Robustness/Validation (Model)
5	Robustness and Validation for DT Deployment	Robustness/Validation (Deployment)
6	Use of Digital Twins in Real-Time Control Systems	Real-Time Control Systems
7	Methods for Continual and Online Learning for Digital Twins	Continual and Online Learning
8	Constructing DTs Using High-Dimensional Data	Using High-Dimensional Data
9	Constructing and Using DTs for Anomaly Detection	Anomaly Detection
11	Hardware and Software Issues in Edge Deployment of DTs	HW-SW in Edge Deployment
12	Scaling and Realization of Deep-Learning-Aided DTs on Cloud and HPC Systems	Scaling on Cloud and HPC Systems
13	Earth Systems: Challenges and Application of DTs	Earth Systems Challenges
14	Nuclear Energy: Challenges and Application of DTs	Nuclear Energy Challenges
15	Manufacturing: Challenges and Application of DTs	Manufacturing Challenges

4:55–5:00 p.m. | **Day 1 Wrap Up**

Wednesday, January 20, 2021

11:00–11:15 a.m. | **Day 2 Welcome and Introduction**

Track 2: Application and Deployment of Digital Twins

This track focuses on the practical challenges when using digital twins, such as

- Edge deployment for real-time and power-efficient deployment of digital twins
- Federated learning for privacy or for data reduction
- Integrating HPC and edge systems, including model and data management
- Online and offline continuous learning on edge-based systems
- Human-machine interface design

Session Chair: Kevin Cao, Arizona State University
Session Co-Chair: Dali Wang, Oak Ridge National Laboratory

11:15–11:45 a.m. | **Invited Speaker 2–4: Felipe Viana, University of Central Florida**

Digital twins for prognosis applications with hybrid physics-informed neural networks

11:45–12:00 p.m. | **Speaker 2–8: David Stracuzzi, Sandia National Laboratories**

Preliminary work on a digital twin for cancer patients

12:00–12:15 p.m. | **Speaker 2–9: Chetan Kulkarni, KBR. Inc., NASA Ames Research Center**

Hybrid model-based approaches for systems health management and prognostics

12:15–12:30 p.m. | **Speaker 2–10: Sandra Biedron, University of New Mexico and Element Aero**

Experiences in dynamic systems – how we better model can help us understand and control intelligently

12:30–1:00 p.m. | **Break**

Session Chair: Abhinav Saxena, GE Research
Session Co-Chair: Malachi Schram, Pacific Northwest National Laboratory

1:00–1:30 p.m. | **Invited Speaker 2–5: Draguna Vrabie, Pacific Northwest National Laboratory**

Deep learning digital twins for model predictive control

1:30–2:00 p.m. | **Invited Speaker 2–6: Junshan Zhang, Arizona State University**

Edge intelligence in IoT ecosystems: From continual learning to collaborative learning

2:00–2:15 p.m.	**Speaker 2–11: Hao Huang, GE Research** *Industrial data anomaly detection and diagnosis with variable association change*
2:15–2:30 p.m.	**Speaker 2–12: Jibonanda Sanyal, Oak Ridge National Laboratory** *Transportation/Mobility digital twin for Chattanooga*
2:30–2:45 p.m.	**Speaker 2–13: Jason St. John, FermiLab** *Digital twins for the FermiLab particle accelerator complex*
2:45–3:00 p.m.	**Speaker 2–14: Abha Moitra, GE Research** *Automating construction of formal assurance case fragments*
3:00–3:30 p.m.	**Break**
3:30–4:55 p.m.	**Breakout Sessions** *(same as day one)*
4:55–5:00 p.m.	**Day 2 Wrap Up**

Thursday, January 21, 2021

11:00–11:15 a.m. | **Day 3 Welcome and Introduction**

Track 3: Techniques to Provide Assurance

This track will address issues of assuring that the digital twin is appropriately designed, constructed, and deployed with a level of rigor that is consistent with the intended use, including the level of risk. Assurance should be broadly interpreted to include

- Verification, validation, and calibration
- Security and resilience
- Uncertainty quantification (UQ)
- Causal inference
- Detecting and dealing with bias
- Explainability and interpretability

Session Chair: Dan Lu, Oak Ridge National Laboratory
Session Co-Chair: Sudip Seal, Oak Ridge National Laboratory

11:15–11:45 a.m. | **Invited Speaker 3–7: Nurali Virani, GE Research**

Humble AI for competence-aware digital twins

11:45–12:00 p.m. | **Speaker 3–15: Jaideep Ray, Sandia National Laboratories**

Assembling training datasets for generalizable machine-learned models of physical phenomena

12:00–12:15 p.m. | **Speaker 3–16: Varun Chandola, University at Buffalo**

Anomaly detection and clustering for evolving data streams

12:15–12:30 p.m. | **Speaker 3–17: Bhavya Kailkhura, Lawrence Livermore National Laboratory**

Can we design assured deep learning systems?

12:30–1:00 p.m. | **Break**

Session Chair: Iris Bahar, Brown University
Session Co-Chair: Laura Pullum, Oak Ridge National Laboratory

1:00–1:30 p.m. | **Invited Speaker 3–8: Auralee Edelen, Stanford/SLAC**

Digital twins for particle accelerators at SLAC

1:30–1:45 p.m. | **Speaker 3–18: Xueping Li, University of Tennessee**

Maintenance advanced technology initiative (MATI)

1:45–2:00 p.m. | **Speaker 3–19: Anthony Corso, Stanford Intelligent Systems Lab**

Adaptive stress testing for validating safety-critical autonomous systems

2:00–2:15 p.m.	**Speaker 3–20: Aashwin Mishra, SLAC National Laboratory** *Reliable uncertainty quantification for deep learning applications in particle accelerators*
2:15–3:00 p.m.	**Breakout Session Out-briefs**
3:00–3:30 p.m.	**Break**
3:30–4:30 p.m.	**Breakout Session Out-briefs, continued**
4:30–5:00 p.m.	**Workshop Wrap-up and Next Steps**