NSF WORKSHOP ON EXUBERANCE OF MACHINE LEARNING IN TRANSPORT PHENOMENA
FEBRUARY 10 — 11, 2020
DALLAS, TX

MLTP2020.COM

Organizers

Amir Barati Farimani	Carnegie Mellon University
Ali Beskok	Southern Methodist University
Peyman Givi	University of Pittsburgh

Machine Learning in Transport Phenomena

The objective of this workshop is to assess the state of progress in development, implementation and application of Machine Learning (ML) in transport phenomena. Of particular interest are applications in fluid dynamics, including turbulence, heat & mass transfer, multi-phase flows, biological transport, combustion and other reactive flows. Considering the complexity of such phenomena, the question is to what to expect from ML and to what extend such learnings can assist in modeling and inference of transport phenomena. Distinguished scholars with expertise in both machine learning and transport phenomena are invited to discuss their recent results, and to identify the paths to be taken in future to merge ML into transport modeling.

Agenda

Monday, February 10, 2020.

	8:30 AM	Welcoming Remarks
9:00 AM to	10:20 PM	Technical Session
10:20 AM to	10:40 PM	Coffee Break
10:40 AM to	12:00 PM	Technical Session
12:00 PM to	1:30 PM	Lunch
1:30 PM to	2:50 PM	Technical Session
2:50 PM to	3:30 PM	Coffee Break
3:30 PM to	5:00 PM	Panel Discussion
	5:00 PM	Poster Session

Tuesday, February 11, 2020.

	8:30 AM	Welcoming Remarks
9:00 AM to	10:20 PM	Technical Session
10:20 AM to	10:40 PM	Coffee Break
10:40 AM to	12:00 PM	Technical Session
12:00 PM to	1:30 PM	Lunch
1:30 PM to	2:50 PM	Technical Session
2:50 PM to	3:30 PM	Coffee Break
3:30 PM to	5:00 PM	Panel Discussion
	5:00 PM	Adjourn

Invited Lectures

Monday, February 10, 2020:

Session & Chair	Time	Presentation
	8:00-8:30	Registration and Breakfast.
	8:30-9:00	NSF Program Managers and Organizers Welcome.
Session I. Chair: Professor Hessam Babaee, University of Pittsburgh	**9:00-9:40**	Professor Steven Brunton, University of Washington: Introduction to data driven modeling and machine learning
	9:40-10:20	Professor George Karniadakis, Brown University: Physics-informed neural networks (PINNs) in fluid mechanics and heat transfer
	10:20-10:40	Coffee Break.
Session II. Chair: Professor Tony Rosato, New Jersey Institute of Technology	**10:40-11:20**	Professor Michael Mahoney, University of California, Berkeley: Machine learning and science?
	11:20-12:00	Professor Sharath Girimaji, Texas A&M University: Machine learning for turbulence modeling: A perspective
	12:00-13:30	Lunch.
Session III Chair: Dr. Ramakanth Munipalli, AFRL/RQRC	**13:30-14:10**	Professor Karen Willcox, University of Texas at Austin: Challenges and progress in learning physics-based reduced models for combustion processes
	14:10-14:50	Professor Linau Ren, Tsinghua University: Machine learning in turbulent reactive flow simulations
	14:50-15:30	Coffee Break.
Moderator: Professor Dimitrios Papavassiliou, University of Oklahoma	**15:30-17:00**	Panel Discussion.
	17:00-18:30	Poster Session.

Invited Lectures

Monday, February 10, 2020:

Session & Chair	Time	Presentation
	8:00-8:45	Registration and Breakfast.
	8:45-9:00	Introduction and Overview.
Session IV. Chair: Dr. Cosmin Safta, Sandia National Laboratories	**9:00-9:40**	Professor Michael Brenner, Harvard University: Machine learning for PDE's
	9:40-10:20	Dr. Kevin Carlberg, University of Washington: Nonlinear model reduction: Using machine learning to enable rapid simulation of extreme-scale physics models
	10:20-10:40	Coffee Break
Session V. Chair: Professor Alan McGaughey, Carnegie Mellon University	**10:40-11:20**	Dr. Mujeeb Malik, NASA Langley Research Center: CFD vision 2030 and potential for machine learning
	11:20-12:00	Professor Justin Sirignano, University of Illinois at Urbana-Champaign: Deep learning closure models for large-eddy simulation
	12:00-13:30	Lunch
Session VI. Chair: Professor Sangyeop Lee, University of Pittsburgh	**13:30-14:10**	Professor Gianluca Iaccarino, Stanford University: (Machine) Learning to differentiate
	14:10-14:50	Professor Weinan E, Princeton University: Machine learning for fluid dynmics
	14:50-15:30	Coffee Break.
Moderator: Professor D. Scott Stewart, University of Illinois at Urbana-Champaign	**15:30-17:00**	Panel Discussion.
	17:00	Adjourn.

List of Posters

Title	Authors	Affiliation
A soft computing approach for estimating the specific heat capacity ofmolten salt-based nanofluids	Ahmed Abdelhalim[1], Debjyoti Banerjee[2]	[1]Cairo University. [2]Texas A&M University
A framework for reduced-order modeling of turbulent reacting flows	Opeoluwa Owoyele[1], Tarek Echekki[2], Pinaki Pal[2]	[1]Argonne National Laboratory, [2]North Carolina State University
Neural network flame closure model for liquid propellant rocket engine	Zeinab Shadram	University of California Irvine
Subgrid-scale parametrization of unresolved scales in forced Burgers equation using Generative Adversarial Networks (GAN)	Jeric Alcala, Ilya Timofeyev	University of Houston
Oil production analysis by machine learning methods	Darkhan Akhmed-Zaki Timur Imankulov, Yedil Nurakhov, Yerzhan Kenzhebek	al-Farabi Kazakh National University
Multi-fidelity learning with heterogeneous domains	Soumalya Sarkar, Michael Joly, Paris Perdikaris	University of Pennsylvania
In-situ coupled OpenFOAM and TensorFlow: Generic data science for CFD	Romit Maulik[1], Himanshu Sharma[1], Saumil Patel[2], Bethany Lusch[1], Elise Jennings[1]	[1]Argonne Leadership Computing Facility Argonne National Laboratory [2]Computational Physics Division Argonne National Laboratory
Data-driven modeling for fluid dynamics: Turbulence closure model order reduction and superresolution	Suraj Pawar[1], Shady Ahmed[1], Harsha Vaddireddy[1], Romit Maulik[2], Omer San[1], Adil Rasheed[3]	[1]Oklahoma State University [2]Argonne National Laboratory [3]Norwegian University of Science and Technology
PDE discovery using convolutional LSTM	Kazem Meidani, Amir Barati	Carnegie Mellon University
Machine learning potential for phonon transport in perfect Si and Si with vacancies	Ruiqiang Guo, Hasan Babaei, Amirreza Hashemi, Sangyeop Lee	University of Pittsburgh

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Title	Authors	Affiliation
Machine learning enabled study of phonon transport from first principles	Sangyeop Lee, Ruiqiang Guo	University of Pittsburgh
Predicting time dependent solutions to the viscous Burger's equation using Gaussian Process Regression	Francis Ogoke[1], Michael Glinsky[2], Amir Barati[1]	[1]Carnegie Mellon University [2]Sandia National Laboratories
Data-driven prediction of a multi-scale Lorenz 96 chaotic system using deep learning methods: Reservoir computing ANN and RNN-LSTM	Pedram Hassanzadeh Ashesh Chattopadhyay Devika Subramanian	Rice University
Learn a low-rank arbitrary Lagrangian Eulerian frame to reduce the dimensionality of convection dominated nonlinear flows	Rambod Mojgani Maciej Balajewicz	University of Illinois at Urbana-Champaign
KiNet: A deep neural network representation of chemical kinetics	Weiqi Ji, Sili Deng	Massachusetts Institute of Technology
Physics embedded neural networks for spatio-temporal turbulence	Arvind Mohan[1], Nicholas Lubbers[1], Daniel Livescu[1], Misha Chertkov[2]	[1]Los Alamos National Laboratory [2]University of Arizona
Machine Learning for Turbulence in Supernovae	Platon Karpov Chengkun Huang Ghanshyam Pilania Stan Woosley Chris Fryer	Los Alamos National Laboratory
Deep learning for transport in heterogeneous media: forward and inverse problems	Haiyi Wu, Wen-Zhen Fang, Hongwei Zhang, Qinjun Kang, Guoqing Hu, Wen-Quan Tao, Rui Qiao	Virginia Polytechnic Institute and State University
Neural Network potential for lattice dynamics calculations and thermal conductivity prediction	Jie Gong, Hyun-Young Kim, Alan McGaughey	Carnegie Mellon University
Prospect of data-driven red blood cell micro mechanical models for computational simulations	Amir Saadat Eric Shaqfeh	Stanford University

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Title	Authors	Affiliation
Real-time reduced order modeling for chemical kinetics	Arash Nouri, Hessam Babaee, Peyman Givi	University of Pittsburgh
Predicting droplet traffic in microfluidic networks using machine learning	Masoud Norouzi Darabad, Siva Vanapalli, Mark Vaughn	Texas Tech University
Time-dependent POD (tPOD): real-time reduced order modeling	Michael Donello, Hessam Babaee	University of Pittsburgh
Data-driven classification and modeling of combustion regimes in a detonation wave	Supraj Prakash[1], Shivam Barwey[1], Malik Hassanaly[2], Venkat Raman[1]	[1]University of Michigan [2]National Renewable Energy Laboratory

Notes

Venues

The workshop will be held at Martha Proctor Mack Ballroom, located on the third floor of the Umphrey Lee Center at 3300 Dyer Street, Dallas, TX in Southern Methodist University.