NSF WORKSHOP ON EXUBERANCE OF MACHINE LEARNING IN TRANSPORT PHENOMENA

FEBRUARY 10 — 11, 2020

DALLAS, TX

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 AM	Technical Session
10:20 AM to 10:40 AM	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 to 6:30 PM	Poster Session & Reception

Tuesday, February 11, 2020

8:45 AM	Welcoming Remarks
9:00 AM to 10:20 AM	Technical Session
10:20 AM to 10:40 AM	Coffee Break
10:40 AM to 12:00 PM	Technical Session
12:00 PM to 1:30 PM	Lunch
1:30 PM to 2:10 PM	Technical Session
2:10 PM to 2:20 PM	Coffee Break
2:20 PM to 3:50 PM	Panel Discussion
3:50 PM to 4:00 PM	Closing Remarks

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	Dr. Weiqi Ji, MIT (on behalf of 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 & Reception

Invited Lectures

Tuesday, February 11, 2020

Session & Chair	Time	Presentation
	8:00-8:45	Registration and Breakfast
	8:45-9:00	Announcements
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
	14:10-14:20	Coffee Break
Moderator: Professor D. Scott Stewart, University of Illinois at Urbana-Champaign	**14:20-15:50**	Panel Discussion
	15:50-16:00	Closing Remarks

List of Posters

No	Title	Authors	Affiliation
1	A soft computing approach for estimating the specific heat capacity of molten salt-based nanofluids	Ahmed Abdelhalim[1], Debjyoti Banerjee[2]	[1]Cairo University. [2]Texas A&M University
2	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
3	Neural network flame closure model for liquid propellant rocket engine	Zeinab Shadram	University of California Irvine
4	Subgrid-scale parametrization of unresolved scales in forced Burgers equation using generative adversarial networks (GAN)	Jeric Alcala, Ilya Timofeyev	University of Houston
5	Oil production analysis by machine learning methods	Darkhan Akhmed-Zaki Timur Imankulov, Yedil Nurakhov, Yerzhan Kenzhebek	Al-Farabi Kazakh National University
6	Multi-fidelity learning with heterogeneous domains	Soumalya Sarkar, Michael Joly, Paris Perdikaris	University of Pennsylvania
7	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
8	Data-driven modeling for fluid dynamics: Turbulence closure model order reduction and super resolution	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
9	PDE discovery using convolutional LSTM	Kazem Meidani, Amir Barati Farimani	Carnegie Mellon University
10	Machine learning potential for phonon transport in perfect Si and Si with vacancies	Ruiqiang Guo, Hasan Babaei, Amirreza Hashemi, Sangyeop Lee	University of Pittsburgh
11	Machine learning enabled study of phonon transport from first principles	Sangyeop Lee, Ruiqiang Guo	University of Pittsburgh
12	Predicting time dependent solutions to the viscous Burger's equation using Gaussian process regression	Francis Ogoke[1], Michael Glinsky[2], Amir Barati Farimani[1]	[1]Carnegie Mellon University [2]Sandia National Laboratories
13	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
14	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
15	KiNet: A deep neural network representation of chemical kinetics	Weiqi Ji, Sili Deng	Massachusetts Institute of Technology
16	Time-dependent POD (tPOD): Real-time reduced order modeling	Michael Donello, Hessam Babaee	University of Pittsburgh

No	Title	Authors	Affiliation
17	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
18	Machine learning for turbulence in supernovae	Platon Karpov Chengkun Huang Ghanshyam Pilania Stan Woosley Chris Fryer	Los Alamos National Laboratory
19	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
20	Neural network potential for lattice dynamics calculations and thermal conductivity prediction	Jie Gong, Hyun-Young Kim, Alan McGaughey	Carnegie Mellon University
21	Prospect of data-driven red blood cell micro mechanical models for computational simulations	Amir Saadat Eric Shaqfeh	Stanford University
22	Real-time reduced order modeling for chemical kinetics	Arash Nouri, Hessam Babaee, Peyman Givi	University of Pittsburgh
23	Predicting droplet traffic in microfluidic networks using machine learning	Masoud Norouzi, Siva Vanapalli, Mark Vaughn	Texas Tech University
24	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
25	Data-driven (super-) parametrization with deep learning: Experimentation with the multi-scale Lorenz' 96 system and transfer learning	Ashesh Chattopadhyay Adam Subel Pedram Hassanzadeh	Rice University
26	Spatio-temporal predictions of IC engine flow field using ResNet and bi-RNN models	David Hung	Univ of Michigan-Shanghai Jiao Tong Univ Joint Institute
27	Embedded tensor basis neural networks for RANS simulation of 3D flows	Andrew J. Banko David S. Ching John K. Eaton	Stanford University Sandia National Laboratories Stanford University
28	Tensor basis neural networks for scalar flux modeling	Pedro M. Milani Julia Ling John K. Eaton	Stanford University Citrine Informatics Stanford University
29	Machine learning for segmentation of echocardiography	Taeouk Kim Mohammadali Hedayat Marek Belohlavek Iman Borazjani	Texas A&M University
30	A phase shift DNN for solving PDEs with oscillatory solutions	Wei Cai Xiaoguang Li Lizuo Liu	Southern Methodist University
31	Optimal sensor location and early detection of lean blowout in a realistic gas turbine combustor using machine learning	Veeraraghava Hasti, Abhishek Navarkar, Jay P. Gore	Purdue University

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1. Locate the **WiFi settings** on your device.
2. Connect to **SMU_Guest.**
3. Launch a **web browser** (Firefox, Safari, Chrome or Internet Explorer).
4. If the portal page does not appear, type in a web address such as **smu.edu** and hit enter. You should then be redirected to the portal page.
5. If you do not have an account on the guest network, click the link next to "***Need an account?***" and follow the instructions below. Otherwise, continue to step 6.
    a. *(Required)* Enter your **name** in the Name Field.
    b. *(Optional)* If you'd like to receive your password via text message, enter your **cellular phone number** in the Phone Number field (ex: 2147682000).
    c. *(Required)* Enter a **valid email address** in the Email Address field.
    d. **Check the box** to accept the terms of use.
    e. Click **Register.**
    f. You will see a confirmation page. Click the link to **Login**
6. **Login** using your temporary credentials.
    a. Enter the **email address** you provided as your username.
    b. Enter the **password** provided in the email or text message confirmation.
    c. **Check** the box to accept the terms of use.
    d. Click **Login.**

SMU guest access is for 24 hours. Hence, you will need to do this procedure each day.

Places to visit on campus

George W. Bush Presidential Library and Museum:
https://www.georgewbushlibrary.smu.edu/

Meadows Museum of Art: https://meadowsmuseumdallas.org/

Venue: 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.