Romit Maulik

Argonne Leadership Computing Facility
Building 240, Argonne National Laboratory
9700 Cass Avenue, Lemont, IL 60439

Phone: (405) 982-0161
Email: rmaulik@anl.gov
Homepage: romit-maulik.github.io

Current position

Margaret Butler Postdoctoral Fellow, Argonne National Laboratory, Jun, 2019 - Present.

Research Assistant Professor, Department of Applied Mathematics, Illinois Institute of Technology, Chicago, Oct, 2020 - Present. (Joint appointment)

Prior experience

Predoctoral Appointee - MCS, Argonne National Laboratory, Jan, 2019 - May, 2019.

RA - Computational Fluid Dynamics Laboratory, Oklahoma State University, Jan, 2016 - Jan, 2019.

RA - Computational Biomechanics Laboratory, Oklahoma State University, Aug, 2013 - July, 2015.

TA - Mechanical & Aerospace Engineering, Oklahoma State University, Jan, 2013 - Dec, 2018.

Design Engineer - Tata Technologies Limited, Pune, Aug, 2012 - Aug, 2013.

Academic background

PhD. Mechanical & Aerospace Engineering, Oklahoma State University, 2019.

M.S. Mechanical & Aerospace Engineering, Oklahoma State University, 2015.

B.E. Mechanical Engineering, Birla Institute of Technology, Mesra, 2012.

Research interests

Scientific machine learning, high-performance computing, reduced-order modeling, turbulence modeling, numerical methods.

Projects

1. Margaret-Butler Fellowship project: Scalable machine learning for turbulence closure and reduced-order modeling. (active)
2. RAPIDS2:A SciDAC Institute for Computer Science, Data, and Artificial Intelligence, U.S. Department of Energy. (active)
3. RAPIDS:A SciDAC Institute for Computer Science and Data, and Artificial Intelligence, U.S. Department of Energy.

Mentorship

1. Suraj Pawar (Oklahoma State): Scalable reinforcement learning for computational fluid dynamics, ALCF Summer Internship Project, 2020.

2. Dominic Skinner (MIT): Deep learning reduced-order models for computational physics applications, National Science Foundation, Mathematical Sciences Graduate Fellowship, Summer 2020.

Publications

In preparation

1. **R. Maulik**, R. Egele, B. Lusch, P. Balaprakash: Scalable autoencoder search for advection-dominated PDE reduced-order models.

2. **R. Maulik**, D. Fytanidis, B. Lusch, S. Patel, V. Vishwanath: PythonFoam - Distributed in-situ data analysis with Python bindings to OpenFOAM.

3. S. Renganathan, **R. Maulik**, J. Ahuja: Probabilistic aerodynamic data fusion using deep autoencoders.

4. K. Raghavan, **R. Maulik**, P. Balaprakash: Randomized methods for direct error-driven deep learning.

5. **R. Maulik**, N. Ramachandra: A Bayesian inverse approach for geophysical flow reconstruction under uncertainty.

6. J. Choi, W. Wehde, **R. Maulik**: Comparing Relative Decisiveness for Public Support of Climate Change Mitigation Policies Using Machine Learning.

7. **R. Maulik**, H. Owhadi, B. Hamzi: Easy geophysical emulation with reproducing kernel Hilbert spaces.

Under review

1. K. Fukami, **R. Maulik**, N. Ramachandra, K. Taira, K. Fukagata: Global field reconstruction from sparse sensors with Voronoi tessellation-assisted deep learning, *arXiv:2101.00554*.

2. **R. Maulik**, B. Lusch, P. Balaprakash: Reduced-order modeling of advection-dominated systems with recurrent neural networks and convolutional autoencoders , *arXiv preprint : 2002.00470*.

3. **R. Maulik**, J. Choi, W. Wehde, P. Balaprakash: Determining feature importance for actionable climate change mitigation policies, *arXiv preprint : 2003.10234*.

Peer-reviewed articles

1. S. Renganathan, **R. Maulik**, J. Ahuja: Enhanced data efficiency using deep neural networks and Gaussian processes for aerodynamic design optimization, *Aerospace Science and Technology, 2020, Accepted*.

2. S. Pawar, **R. Maulik**: Distributed deep reinforcement learning for simulation control, *Machine Learning: Science and Technology, 2020, Accepted*.

3. J. Burby, Q. Tang, **R. Maulik**: Fast neural Poincaré maps for toroidal magnetic fields, *Plasma Physics and Controlled Fusion*, 63, 024001.

4. **R. Maulik**, T. Botsas, N. Ramachandra, M. Lachlan, I. Pan: Latent-space time evolution of non-intrusive reduced-order models using Gaussian process emulation, *Physica D*, 132797, 2020.

5. **R. Maulik**, H. Sharma, S. Patel, B. Lusch, E. Jennings : A turbulent eddy-viscosity surrogate modeling framework for Reynolds-Averaged Navier-Stokes simulations, *Computers and Fluids*, 104777, 2020.

6. **R. Maulik**, K. Fukami, N. Ramachandra, K. Fukagata, K. Taira : Probabilistic neural networks for fluid flow model-order reduction and data recovery, *Physical Review Fluids*, 5, 104401, 2020.

7. **R. Maulik**, P. Balaprakash, B. Lusch: Non-autoregressive time-series methods for stable parameteric reduced-order models, *Physics of Fluids*, 32, 087115, 2020.

8. **R. Maulik**, N. Garland, X. Tang, P. Balaprakash: Neural network representability of fully ionized plasma fluid model closures, *Physics of Plasmas*, 27, 072106, 2020.

9. J. Choi, S. Robinson, **R. Maulik**, W. Wehde: What Matters the Most for Individual Disaster Preparedness? Understanding Emergency Preparedness Using Machine Learning, *Natural Hazards*, `https://doi.org/10.1007/s11069-020-04029-1`, 2020.

10. S. Renganathan **R. Maulik**, V. Rao : Machine learning for Nonintrusive Model Order Reduction of the Parametric Inviscid Transonic Flow past an airfoil, *Physics of Fluids*, 32, 047110, 2020.

11. **R. Maulik**, O. San: Numerical assessments of a parametric implicit large eddy simulation model, *Journal of Computational and Applied Mathematics*, 112866, 2020.

12. **R. Maulik**, O. San, J. Jacob: Spatiotemporally dynamic implicit large eddy simulation using machine learning classifiers, *Physica D.*, 406, 132409, 2020.

13. **R. Maulik**, A. Mohan, B. Lusch, S. Madireddy, P. Balaprakash, D. Livescu: Time-series learning of latent-space dynamics for reduced-order model closure, *Physica D.*, 405, 132368, 2020.

14. Y. Hossain, **R. Maulik**, H. Park, M. Ahmed, C. Bach, O. San: Improvement of Unitary Equipment and Heat Exchanger Testing Methods, *ASHRAE Transactions*, 125.2, 2019.

15. **R. Maulik**, O. San, J. Jacob, C. Crick: Online turbulence model classification for large eddy simulation using deep learning, *Journal of Fluid Mechanics*, 870, 784-812, 2019.

16. O.San, **R. Maulik**, M. Ahmed: An artificial neural network framework for reduced order modeling of transient flows, *Communications in Nonlinear Science and Numerical Simulation*, 77, 271-287, 2019.

17. **R. Maulik**, O. San, A. Rasheed, P. Vedula: Subgrid modeling for two-dimensional turbulence using artificial neural networks, *Journal of Fluid Mechanics*, 858, 122-144, 2019.

18. **R. Maulik**, O. San, A. Rasheed, P. Vedula: Data-driven deconvolution for large eddy simulation of Kraichnan turbulence, *Physics of Fluids*, 30, 125109, 2018.

19. O.San, **R.Maulik**: Stratified Kelvin-Helmholtz turbulence of compressible shear flows, *Nonlinear Processes in Geophysics*, 25, 457–476, 2018.

20. **R.Maulik**, O.San, C. Bach: A computational investigation of the effect of ground clearance in vertical ducting systems, 2018, Purdue University, Herrick Labs Conferences 2018. `https://docs.lib.purdue.edu/ihpbc/308/`.

21. O.San, **R.Maulik**: Extreme learning machine for reduced order modeling of turbulent geophysical flows, *Physical Review E*, 97, 042322, 2018.

22. O.San, **R.Maulik**: Machine learning closures for model order reduction of thermal fluids, *Applied Mathematical Modelling*, https://doi.org/10.1016/j.apm.2018.03.037, 2018.

23. **R.Maulik**, O.San, R. Behera : An adaptive multilevel wavelet framework for scale-selective WENO reconstruction schemes, *International Journal of Numerical Methods in Fluids*, https://doi.org/10.1002/fld.4489, 2018.

24. O.San, **R.Maulik**: Neural network closure models for nonlinear model order reduction, *Advances in Computational Mathematics*, https://doi.org/10.1007/s1044, 2018.

25. **R.Maulik**, O. San: A dynamic closure modeling framework for large eddy simulation using approximate deconvolution: Burgers equation, *Cogent Physics*, 5, 1464368, 2018.

26. **R.Maulik**, O.San: A neural network approach for the blind deconvolution of turbulent flows, *Journal of Fluid Mechanics*, 831, 151-181, 2017.

27. **R.Maulik**, O.San: A novel dynamic framework for subgrid-scale parametrization of mesoscale eddies in quasigeostrophic turbulent flows, *Computers and Mathematics with Applications*, 74, 420-445, 2017.

28. **R.Maulik**, O.San: Explicit and implicit LES closures for Burgers turbulence, *Journal of Computational and Applied Mathematics*, 327, 12-40, 2017.

29. **R.Maulik**, O.San: Resolution and Energy Dissipation Characteristics of Implicit LES and Explicit Filtering Models for Compressible Turbulence, *Fluids*, 2(2)-14, 2017.

30. **R.Maulik**, O.San: A dynamic subgrid-scale modeling framework for Boussinesq turbulence, *International Journal of Heat and Mass Transfer*, 108, 1656-1675, 2017.

31. **R.Maulik**, O.San: A dynamic framework for scale-aware parameterizations of eddy viscosity coefficient in two-dimensional turbulence, *International Journal of Computational Fluid Dynamics*, 31(2), 69-92, 2017.

32. **R.Maulik**, O.San: A stable and scale-aware dynamic modeling framework for subgrid-scale parameterizations of two-dimensional turbulence, *Computers & Fluids* 158, 11-38, 2016.

33. **R.Maulik**, O.San: Dynamic modeling of the horizontal eddy viscosity coefficient for quasigeostrophic ocean circulation problems, *Journal of Ocean Engineering and Science* 1, 300-324, 2016.

34. H. H. Marbini, **R. Maulik**: A biphasic transversely isotropic poroviscoelastic model for the unconfined compression of hydrated soft tissue, *Journal of Biomechanical Engineering* 138, 031003, 2016.

Peer-reviewed conference proceedings

1. **R. Maulik**, H. Sharma, S. Patel, B. Lusch, E. Jennings: Deploying deep learning in OpenFOAM with TensorFlow: A tutorial, AIAA SciTech Forum 2021, `https://doi.org/10.2514/6.2021-1485`.

2. P. Milan, R. Torelli, B. Lusch, **R. Maulik**, G. Magnotti: Data-Driven Modeling of Large-Eddy Simulations for Fuel Injector Design, AIAA SciTech Forum 2021, `https://doi.org/10.2514/6.2021-1016`.

3. **R. Maulik**, V. Rao, S. Renganathan, S. Letizia, G. Iungo: Cluster analysis of wind turbine wakes measured through a scanning Doppler wind LiDAR, AIAA SciTech Forum 2021, `https://doi.org/10.2514/6.2021-1181`.

4. **R. Maulik**, R. Egele, B. Lusch, P. Balaprakash: Recurrent neural network architecture search for geophysical emulation, *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC), 2020, 10.5555/3433701.3433711*

5. V. Rao, **R. Maulik**, E. Constantinescu, M. Anitescu: A Machine Learning Method for Computing Rare Event Probabilities, *International Conference on Computational Science, 2020*, `https://link.springer.com/chapter/10.1007%2F978-3-030-50433-5_14`.

Peer-reviewed workshop proceedings

1. D. Skinner, **R. Maulik**: Meta-modeling strategy for data-driven forecasting, *Tackling Climate Change with Machine Learning workshop, NeurIPS*, 2020.

2. N. Garland, **R. Maulik**, Q. Tang, X. Tang, P. Balaprakash: Progress towards high fidelity collisional-radiative model surrogates for rapid in-situ evaluation, *Machine learning for Physical Sciences workshop, NeurIPS*, 2020.

3. K. Fukami, **R. Maulik**, N. Ramachandra, K. Fukagata, K. Taira: Probabilistic neural network-based reduced-order surrogate for fluid flows, *Machine learning for Physical Sciences workshop, NeurIPS*, 2020.

4. **R. Maulik**, R. S. Assary, P. Balaprakash: Site-specific graph neural network for predicting protonation energy of oxygenate molecules, *Machine learning for Physical Sciences workshop, NeurIPS*, 2019.

5. **R. Maulik**, V.Rao, S. Madireddy, B. Lusch, P. Balaprakash: Using recurrent neural networks for nonlinear component computation in advection-dominated reduced-order models, *Machine learning for Physical Sciences workshop, NeurIPS*, 2019.

Workshop participation

1. Invited participant, Vistas in the Applied Mathematical Sciences, Institute for Mathematical Statistical Innovation (IMSI), The University of Chicago, IL, 2020.

2. Invited participant, NSF workshop on Machine Learning for Transport Phenomena, Southern Methodist University, TX, 2020.

3. Invited participant, Mathematics of Reduced Order Models, ICERM, Brown University, RI, 2020.

4. Invited participant, Algorithms for Dimension and Complexity Reduction, ICERM, Brown University, RI, 2020.

5. Invited participant, IPAM Workshop III: Validation and Guarantees in Learning Physical Models: from Patterns to Governing Equations to Laws of Nature, UC Los Angeles, October 2019.

6. Invited participant, Department of Energy - AI for Science Townhall, Argonne National Laboratory, June 2019.

7. Invited participant, Advances in PDEs: Theory, Computation and Application to CFD, ICERM, Brown University, RI, 2018.

8. Invited participant, SDSC Summer program in HPC and Data Science, UC San Diego, 2017.

Talks

1. K. Fukami, **R. Maulik**, N. Ramachandra, K. Fukagata, K. Taira: MUnstructured fluid flow data recovery using machine learning and Voronoi diagrams, Bulletin of the American Physical Society 73, 2020.

2. **R. Maulik**: Scalable scientific machine learning for computational fluid dynamics, **Invited talk**, Department of Mechanical Engineering, The City College of New York, October 1, 2020.

3. **R. Maulik**: Data-driven model order reduction for geophysical emulation. **Invited talk** at the Second Symposium on Machine Learning and Dynamical Systems, Fields Institute, Toronto, Sept. 21-25, 2020.

4. **R. Maulik**: Scalable scientific machine learning for computational fluid dynamics, **Invited talk**, Department of Mechanical Engineering, Rice University, September 9, 2020.

5. **R. Maulik**: Machine Learning Enablers for System Optimization and Design, MCS-LANS seminar, Argonne National Laboratory, August 2020.

6. **R. Maulik** : Surrogate-based machine-learning for system optimization and design, **Invited talk** at Los Alamos National Laboratory for Tokamak Disruption Simulation (TDS) working group.

7. **R. Maulik** : Non-intrusive reduced-order model search for geophysical emulation, **Guest lecture**, MAE259a: data science for fluid dynamics (offered by Kunihiko Taira), University of California Los Angeles.

8. **R. Maulik** : Machine learning for computational fluid dynamics, **Invited talk** at PyData Meetup Chicago, May 2020.

9. **R. Maulik**, R. Egele, B. Lusch, P. Balaprakash : Recurrent neural architecture search for geophysical emulation using DeepHyper, **Invited talk** at AI-HPC seminar, Argonne National Laboratory, 2020.

10. **R. Maulik**, B. Lusch, P. Balaprakash: Machine Learned Reduced-Order Models for Advective Partial Differential Equations, MCS-LANS seminar, Argonne National Laboratory, Feb 2020.

11. **R. Maulik**, B. Lusch, P. Balaprakash : Machine Learned Reduced-Order Models for Advective Partial Differential Equations, 2020 Spring Multiscale Seminar, Illinois Institute of Technology, Chicago, IL, Feb 2020.

12. **R. Maulik**, O. San, J. D. Jacob : Spatiotemporally dynamic implicit large eddy simulation using machine learning classifiers, **Invited talk** at Session on Domain-Aware, Interpretable and Robust Scientific Machine Learning Methods Applied to Computational Mechanics, AIAA Aviation Forum 2020, Reno NV.

13. **R. Maulik**, H. Sharma, S. Patel, B. Lusch, E. Jennings, P. Balaprakash: General purpose data science for general purpose CFD: Integrating Tensorflow into OpenFOAM at scale, **Invited poster** at the workshop for Machine Learning for Transport Phenomena 2020, Dallas, TX.

14. **R. Maulik**, S. Madireddy, B. Lusch, P. Balaprakash: Closures for Parameteric Reduced-Order Models Using Convolutional Autoencoders, SIAM Conference on Mathematics of Data Science 2020, Cincinnati, Ohio.

15. J. Choi, S. Robinson, **R. Maulik**, W. Wehde: What Matters the Most for Individual Disaster Preparedness? Understanding Emergency Preparedness Using Machine Learning, SPSA Conference on Politics of Disasters, Resilience, and Recovery, San Juan, Puerto Rico, 2020.

16. **R. Maulik**, A. Mohan, S. Madireddy, B. Lusch, P. Balaprakash, D. Livescu: Machine learning of sequential data for non-intrusive reduced-order models, Bulletin of the American Physical Society 72, 2019.
17. **R. Maulik**, B. Lusch, P. Balaprakash: Tackling the limitations of conventional ROMs for advection-dominated nonlinear dynamical systems using machine learning, **Invited talk** at the Advanced Statistics meets Machine Learning-III workshop, Argonne National Laboratory, November 2019.
18. **R. Maulik**, B. Lusch, O. San, P. Balaprakash: Data-driven sub-grid models for the large-eddy simulation of turbulence, **Invited talk** at John Zink Hamworthy Combustion, Tulsa, 2019.
19. **R. Maulik**, H. Sharma, S. Patel, E. Jennings, B. Lusch, P. Balaprakash, V. Vishwanath: Novel turbulence closures using physics-informed machine learning, **Invited talk** at the Argonne Physical Sciences and Engineering Division AI Townhall 2019.
20. **R.Maulik**, O.San, A. Rasheed, P. Vedula: Data-driven deconvolution for the sub-grid modeling of large eddy simulations of two-dimensional turbulence, SIAM-CSE, 2019.
21. **R.Maulik**, O.San, A. Rasheed, P. Vedula: Data-driven deconvolution for the large eddy simulation of Kraichnan turbulence, Bulletin of the American Physical Society 71, 2018.
22. **R.Maulik**, O.San, C. Bach: A computational investigation of the effect of ground clearance in vertical ducting systems, 2018, Purdue University, Herrick Labs Conferences 2018.
23. **R.Maulik**, O.San: A neural network approach for the blind deconvolution of turbulent flows, Bulletin of the American Physical Society 70, 2017.
24. **R.Maulik**, Ratikanta Behera, O.San: A generalized wavelet based grid-adaptive and scale-selective implementation of WENO schemes for conservation laws, Texas Applied Mathematics and Engineering Symposium 2017, The University of Texas, Austin.
25. **R.Maulik**, O.San: An explicit filtering framework based on Perona-Malik anisotropic diffusion for shock capturing and subgrid scale modeling of Burgers' turbulence, Bulletin of the American Physical Society 69, 2016.
26. **R.Maulik**, O.San: A dynamic hybrid subgrid-scale modeling framework for large eddy simulations, Bulletin of the American Physical Society 69, 2016.
27. O.San, **R.Maulik**: A dynamic framework for subgrid-scale parametrization of mesoscale eddies in geophysical flows, Bulletin of the American Physical Society 69, 2016.

Honors & awards

3rd Margaret Butler Fellow, Argonne Leadership Computing Facility, Argonne National Laboratory.

Best oral presentation, 2nd MAE Graduate Research Symposium, Oklahoma State University, 2018

SIAM Student Travel Award: 2019 SIAM Conference on Computational Science and Engineering, Spokane, WA, 2019.

Outstanding Graduate Student, College of Engineering Architecture and Technology, Oklahoma State University, 2018

Graduate College Robberson Summer Research Fellowship, Oklahoma State University, 2017

FGSA Travel Award for Excellence in Graduate Research, American Physical Society, 2017

SIAM TX-LA Travel Grant, Texas Applied Mathematics and Engineering Symposium, 2017

Graduate Student Travel Grant, American Physical Society - Division of Fluid Dynamics, 2017

Graduate Student Travel Grant, Graduate Program Student Government Authority, Oklahoma State University, 2017

John Brammer Fellowship, Oklahoma State University, 2016

Graduate College Top Tier Fellowship, Oklahoma State University, 2016

7^{th} place in Worldsteel-SteelChallenge 8 - North American University Category, 2014.

Professional service & outreach

Reviewer: AIAA Journal, Applied Mathematical Modeling, Computer Methods in Applied Mathematics and Engineering, Computer Physics Communications, International Journal of Computational Fluid Dynamics, Journal of Fluid Mechanics, Physics of Fluids, Physica D, International Journal of Numerical Methods in Fluids, Nature Communications, Nature Scientific Reports, Theoretical and Computational Fluid Dynamics, Atmospheric Science Letters, New Journal of Physics.

Program Committee - Argonne Data Science Project and INCITE allocations : Reviewed allocation requests for 24 million core hours and 1600 TB storage.

Organizer - Acceleration and Enhancement of High-fidelity PDE Solvers through Machine Learning, 16th U.S. National Congress on Computational Mechanics, IL, 2021.

Co-organizer - Argonne National Laboratory - AI, Statistics and Machine Learning Journal Club.

Tutorial lead - Autoencoders for PDE surrogate models, ATPESC 2020.

Tutorial lead - Statistical methods for machine learning, ALCF AI4Science tutorial 2019, Argonne National Laboratory.

Tutorial lead - DeepHyper for scalable hyperparameter and neural architecture search on ALCF machines, ALCF Simulation Data and Learning workshop 2019, Argonne National Laboratory.

Session chair - Domain-Aware, Interpretable and Robust Scientific Machine Learning Methods Applied to Computational Mechanics, AIAA Aviation Forum, Reno, NV, 2020.

MS Organizer & Session chair - Domain-Aware, Interpretable and Robust Machine Learning for Computational Science, SIAM Virtual Conference on Computational Science and Engineering, 2021.

Session chair - SIAM Conference on Mathematics of Data Science, Cincinnati, OH, 2020.

MS Organizer & Session chair - Machine Learning methods in Computational Fluid Dynamics, SIAM Conference on Computational Science and Engineering, Spokane, WA, 2019.

Session chair - MAE Graduate Research Symposium, Oklahoma State University, 2018.

Organizer & Lecturer - 2-day TensorFlow workshop, Mechanical & Aerospace Engineering, Oklahoma State University, 2018

Organizer - National Lab Day outreach, Computational Fluid Dynamics Laboratory, Oklahoma State University 2017, 2018.