

# Romit Maulik

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## Research interests

Scientific machine learning, dynamical systems, high-performance computing, computational fluid dynamics, reduced-order modeling, numerical methods, stochastic processes.

## Positions held

### **July 2023 - Present**

Assistant Professor & Institute of Computational and Data Sciences Co-Hire, Information Sciences and Technology, Pennsylvania State University  
&  
Joint Appointment, Mathematics and Computer Science Division, Argonne National Laboratory.

### **Jun, 2021 - Jun 2023**

Assistant Computational Scientist, Mathematics and Computer Science, Argonne National Laboratory.

### **Oct, 2020 - Jun 2023**

Research Assistant Professor, Department of Applied Mathematics, IIT-Chicago.

### **Jun, 2019 - May, 2021**

Margaret Butler Postdoctoral Fellow, Leadership Computing Facility, Argonne National Laboratory.

### **Jan, 2019 - May, 2019**

Predocutorial Appointee - Mathematics and Computer Science Division, Argonne National Laboratory.

### **Jan, 2016 - Jan, 2019**

Research Assistant - Computational Fluid Dynamics Laboratory, Oklahoma State University.

### **Aug, 2013 - Jul, 2015**

Research Assistant - Computational Biomechanics Laboratory, Oklahoma State University.

### **Jan, 2013 - Dec, 2018**

Teaching Assistant (Introductory Dynamics, Introductory Fluid Mechanics, Practical CFD) - Mechanical & Aerospace Engineering, Oklahoma State University.

### **Aug, 2012 - Aug, 2013**

Design Engineer - Tata Technologies Limited, India.

## Education

PhD. Mechanical & Aerospace Engineering, Oklahoma State University.	<b>2016-2019</b>
M.S. Mechanical & Aerospace Engineering, Oklahoma State University.	<b>2013-2015</b>
B.E. Mechanical Engineering, Birla Institute of Technology, India.	<b>2008-2012</b>

## Honors & awards

Early Career Award, Army Research Office, 2024-2027.

Best paper award, May 2024, ICLR 2024 Workshop on Climate Change and AI: ‘Scaling transformer neural networks for skillful and reliable medium-range weather forecasting’.

Impact Argonne Award, September 2023: ‘For developing an AI model for climate and creating an innovated data assimilation methodology’.

Best paper award - Machine Learning-Enabled Prediction of Transient Injection Map In Automotive Injectors With Uncertainty Quantification, 2021 ASME Internal Combustion Engine Fall Conference, <https://doi.org/10.1115/ICEF2021-67888>.

Impact Argonne Award, September, 2021: ‘For tackling several climate model challenges and advancing the field of downscaled climate modeling and impact analysis’.

Editor’s pick - Reduced-order modeling of advection-dominated systems with recurrent neural networks and convolutional autoencoders , *Physics of Fluids*, <https://doi.org/10.1063/5.0039986>.

Editor’s pick - Non-autoregressive time-series methods for stable parametric reduced-order models , *Physics of Fluids*, <https://doi.org/10.1063/5.0019884>.

Margaret Butler Fellow, Argonne Leadership Computing Facility, Argonne National Laboratory, 2019-2021.

SIAM Travel Grant: 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, 2018.

SIAM TX-LA Section 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.

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

John Brammer Fellowship, Oklahoma State University, 2016.

Graduate College Top Tier Fellowship, Oklahoma State University, 2016.

## Funding & support

(Active, 2024-2027) EARLY CAREER PROGRAM: RIFLES: Rapid Information Fusion through Learning Effective ClosureS, Army Research Office (Modeling of Complex Systems), Role: PI.

(Active, 2024-2027) Using Machine Learning to Uncover Deep Convective Cloud Processes with TRACER Observations, U.S. Department of Energy (Atmospheric System Research), Role: Co-PI.

(Active, 2021-2025) Inertial neural surrogates for stable dynamical prediction, U.S. Department of Energy (Advanced Scientific Computing Research), Role: Institutional PI.

(Active, 2023-2026) DeepFusion Accelerator for Fusion Energy Sciences in Disruption Mitigations, U.S. Department of Energy (Fusion Energy Sciences), Role: Institutional PI.

(Active, 2020-2025) RAPIDS2: A SciDAC Institute for Computer Science, Data, and Artificial Intelligence, U.S. Department of Energy (Advanced Scientific Computing Research). Role: Institutional PI.

(Active, 2024-2026) Koopman-operator learning for stable and physical dynamical systems forecasting, Los Alamos National Laboratory Subaward. Role: Institutional PI.

(Active, 2024-2025) Foundation models for surface hydrology, Argonne National Laboratory Subaward. Role: Institutional PI.

(Finished, 2021-2023) AI emulator assisted data assimilation, Future computing, LDRD-Prime, Argonne National Laboratory, U.S. Department of Energy. Role: Co-PI (Argonne National Laboratory).

(Finished, 2022-2023) A Scalable, Energy Efficient HPC Environment for AI-Enabled Science, National Science Foundation Collaborative PPOSS funding. Role: Co-PI (IIT-Chicago).

(Finished, 2021) SambaWF: Highly resolved surrogate models for weather forecasting, LDRD-Expedition, Argonne National Laboratory, U.S. Department of Energy. Role: PI (Argonne National Laboratory).

(Finished, 2019-2021) Scalable machine learning for turbulence closure and reduced-order modeling, Margaret Butler Fellowship, Role: PI (Argonne National Laboratory).

## Supervision

Asterisks indicate active supervision.

Dr. Shivam Barwey\*, AETS Named Postdoctoral Fellow, Argonne National Laboratory, 2022-Present.

Dr. James Henry\*, Postdoctoral Scholar, Pennsylvania State University, 2024-Present.

Dr. Xuyang Li\*, Postdoctoral Scholar, Pennsylvania State University, 2024-Present.

Dibyajyoti Chakraborty\*, PhD Student, Pennsylvania State University, 2023-Present.

Haiwen Guan\*, PhD Student, Pennsylvania State University, 2024-Present.

Hojin Kim\*, PhD Student, Pennsylvania State University, 2024-Present.

Matthew Poska\*, Graduate Student, Pennsylvania State University & Argonne National Laboratory. DOE SCGSR Fellow, 2022-Present (co-advised with Dr. Sharon Huang, IST, Penn State).

Zachariah Malik, Visiting graduate Student, Argonne National Laboratory, NSF MSGI Fellow, Summer 2023, 2024.

Vinamr Jain, Undergraduate Intern, IIT-Delhi, 2023-2024.

Aaryan Bavishi, Undergraduate Student, Pennsylvania State University, 2023-Present.

Abhinab Bhattacharjee, Graduate Student, Argonne National Laboratory, Givens Associate, Summer 2023.

Deepinder Jot Singh Aulakh, Graduate Student, Argonne National Laboratory, ALCF Research Aide, Summer 2023.

Trent Gerew, Undergraduate Student, Argonne National Laboratory, DOE SULI Program, Spring 2023-Present.

Jonah Botvinick-Greenhouse, Visiting Graduate Student, Cornell University & Argonne National Laboratory, NSF MSGI Fellow, Summer 2022.

Sen Lin, Graduate Student, Argonne National Laboratory, Givens Associate, Summer 2022.

Cyril Le Doux, Undergraduate Student, Argonne National Laboratory, DOE SULI Program, Summer 2022.

Gurpreet Singh Hora, Graduate Student, Columbia University, With Laurent White at AMD Research, Summer 2022.

Sahil Bhola, Graduate Student, Argonne National Laboratory, ALCF Research Aide, Summer 2021.

Alec Linot, Graduate Student, Argonne National Laboratory, Givens Associate, Summer 2021.

William McClure, Graduate Student, IIT-Chicago, Masters Thesis, 2021.

Janah Richardson, High-school student, Afro-Academic, Cultural, Technological and Scientific Olympics (ACT-SO) High School Research Program, 2020-2021. Gold medal winner in Computer Science category-Illinois.

Suraj Pawar, Graduate Student, Argonne National Laboratory, ALCF Research Aide, Summer 2020.

Dominic Skinner, Graduate Student, Argonne National Laboratory, NSF MSGI Fellow, Summer 2020.

## Publications

### *Under review*

1. S. Barwey, P. Pal, S. Patel, R. Balin, B. Lusch, V. Vishwanath, **R. Maulik**, R. Balakrishnan: Mesh-based Super-Resolution of Fluid Flows with Multiscale Graph Neural Networks
2. V. Jain, **R. Maulik**: Higher order quantum reservoir computing for non-intrusive reduced-order models, *arXiv:2407.21602*.
3. D. Chakraborty, S. Chung, **R. Maulik**: Divide and conquer: Learning chaotic dynamical systems with multistep penalty neural ordinary differential equations, *arXiv:2407.00568*.
4. D. Chakraborty, S. Barwey, H. Zhang, **R. Maulik**: A note on the error analysis of data-driven closure models for large eddy simulations of turbulence, *arXiv:2405.17612*.
5. T. Chang, A. Gillette, **R. Maulik**: Leveraging Interpolation Models and Error Bounds for Verifiable Scientific Machine Learning, *arXiv:2404.03586*.
6. A. Nair, S. Barwey, P. Pal, J. MacArt, **R. Maulik**: Understanding Latent Timescales in Neural Ordinary Differential Equation Models for Advection-Dominated Dynamical Systems, *arXiv:2403.02224*.
7. S. Barwey, **R. Maulik**: Interpretable Fine-Tuning and Error Indication for Graph Neural Network Surrogate Models, *arXiv:2311.07548*.
8. V. Shankar, **R. Maulik**, V. Vishwanathan: Differentiable turbulence II, *arXiv:2307.13533*.
9. V. Shankar, D. Chakraborty, V. Vishwanathan, **R. Maulik**: Differentiable turbulence: Closure as PDE-constrained optimization, *arXiv:2307.03683*.

10. C. Moss, **R. Maulik**, G. V. Iungo: Modeling Wind Turbine Performance and Wake Interactions with Machine Learning, *arXiv:2212.01483*.
11. V. Shankar, S. Barwey, Z. Kolter, **R. Maulik**, V. Viswanathan: Importance of equivariant and invariant symmetries for fluid flow modeling, , *arxiv:2307.05486*.

### Peer-reviewed journal articles

1. B. Sanderse, P. Stinis, **R. Maulik**, S. Ahmed: Scientific machine learning for closure models in multiscale problems: a review, *Foundations of Data Science*, *Accepted*.
2. C. Moss, **R. Maulik**, V. Iungo: Augmenting Insights from Wind Turbine Data through Data-Driven Approaches, *Applied Energy*, 376, 124116, 2024.
3. D. Aulakh, X. Yang, **R. Maulik**: Robust experimental data assimilation for the Spalart-Allmaras turbulence model, *Physical Review Fluids*, 9, 084608, 2024.
4. S. Yang, H. Kim, Y. Hong, K. Yee, **R. Maulik**, N. Kang: Data-driven Physics-Informed Neural Networks: A Digital Twin Perspective, *Computer Methods in Applied Mechanics and Engineering*, Volume 428, 117075, 2024.
5. M. Rogowski, B. Yeung, O. Schmidt, **R. Maulik**, M. Parsani, L. Dalcin, G. Mengaldo: Unlocking massively parallel spectral proper orthogonal decompositions in the PySPOD package, *Computer Physics Communications*, Volume 302, 109246, 2024.
6. K. Asztalos, R. Steijl, **R. Maulik**: Reduced-order modeling on a near-term quantum computer, *Journal of Computational Physics*, Volume 510, 113070, 2024.
7. C. Moss, **R. Maulik**, G. Iungo: A Call for Enhanced Data-Driven Insights into Wind Energy Flow Physics, *Theoretical and Applied Mechanics Letters*, Volume 14, Issue 1, 2024, 100488.
8. S. Barwey, V. Shankar, V. Vishwanathan, **R. Maulik**: Multiscale graph neural network autoencoders for interpretable scientific machine learning, *Journal of Computational Physics*, Volume 495, 15 December 2023, 112537.
9. C. Moss, M. Puccioni, **R. Maulik**, C. Jacquet, D. Apgar, G. V. Iungo : Predicting Wind Farm Operations with Machine Learning and the P2D-RANS model: A Case Study for an AWAKEN Site, *Wind Energy*, 2023.
10. S. Lin, G. Mengaldo, **R. Maulik**: Online data-driven changepoint detection for high-dimensional dynamical systems, *Chaos: An Interdisciplinary Journal of Nonlinear Science*, 33, 10, 2023.
11. J. Botvinick-Greenhouse, Y. Yang, **R. Maulik**: Generative Modeling of Time-Dependent Densities via Optimal Transport and Projection Pursuit, *Chaos: An Interdisciplinary Journal of Nonlinear Science*, 33, 10, 2023.
12. C. Jang, J. Choi, **R. Maulik**, D. Lim: Determinants of Adult Education and Training Participation in the United States: A Machine Learning Approach, *Adult Education Quarterly*, 2023.
13. **R. Maulik**, R. Egele, K. Raghavan, P. Balaprakash: Quantifying uncertainty for deep learning based forecasting and flow-reconstruction using neural architecture search ensembles, *Physica D.*, 454, 133852, 2023.
14. A. Aygun, **R. Maulik**, A. Karakus: Physics-Informed Neural Networks for Mesh Deformation with Exact Boundary Enforcement, *Engineering Applications of Artificial Intelligence*, 125, 106660, 2023.

15. S. Bhola, S. Pawar, P. Balaprakash, **R. Maulik**: Multi-fidelity reinforcement learning framework for shape optimization, *Journal of Computational Physics*, 482, 112018, 2023.
16. V. Shankar, V. Puri, R. Balakrishnan, **R. Maulik**, V. Vishwanathan: Differentiable physics-enabled closure modeling for Burgers' turbulence, *Machine Learning Science and Technology*, 4, 015017, 2023.
17. J. Choi, W. Wehde, **R. Maulik**: Politics of Problem Definition: Comparing Public Support of Climate Change Mitigation Policies using Machine Learning, *Review of Policy Research*, 2022.
18. S. Mondal, G. Magnotti, B. Lusch, **R. Maulik**, R. Torelli: Machine Learning-Enabled Prediction of Transient Injection Map in Automotive Injectors With Uncertainty Quantification, *Journal of Engineering for Gas Turbines and Power*, 145(4), 041015, 2023
19. A. Linot, J. Burby, Q. Tang, P. Balaprakash, M. Graham, **R. Maulik**: Stabilized Neural Ordinary Differential Equations for Long-Time Forecasting of Dynamical Systems, *Journal of Computational Physics*, 474, 111838, 2022.
20. N. Garland, **R. Maulik**, Q. Tang, X. Tang, P. Balaprakash, Efficient training of artificial neural network surrogates for a collisional-radiative model through adaptive parameter space sampling, *Machine Learning Science and Technology*, 3 (4), 045003, 2022.
21. M. Morimoto, K. Fukami, **R. Maulik**, R. Vinuesa, K. Fukagata: Assessments of model-form uncertainty using Gaussian stochastic weight averaging for fluid-flow regression, *Physica D: Nonlinear Phenomena*, 133454, 2022.
22. A. Lario, **R. Maulik**, G. Rozza, G. Mengaldo: Neural-network learning of SPOD dynamics, *Journal of Computational Physics*, 111475, 2022.
23. G. Iungo, **R. Maulik**, S. Renganathan, S. Letizia: Machine-learning identification of the variability of mean velocity and turbulence intensity for wakes generated by onshore wind turbines: Cluster analysis of wind LiDAR measurements, *Journal of Renewable and Sustainable Energy*, 14 (Cover article), 023307, 2022.
24. **R. Maulik**, V. Rao, J. Wang, G. Mengaldo, E. Constantinescu, B. Lusch, P. Balaprakash, I. Foster, R. Kotamarthi, Efficient high-dimensional variational data assimilation with machine-learned reduced-order models, *Geoscientific Model Development*, 15, 3433–3445, 2022..
25. Y. Lu, **R. Maulik**, T. Gao, F. Dietrich, I. Kevrekidis, J. Duan: Learning the temporal evolution of multivariate densities via normalizing flows, *Chaos: An Interdisciplinary Journal of Nonlinear Science*, 32 (3), 033121, 2022.
26. **R. Maulik**, D. Fytanidis, B. Lusch, S. Patel, V. Vishwanath: PythonFOAM: In-situ data analyses with OpenFOAM and Python, *Journal of Computational Science*, 62, 101750, 2022.
27. S. Renganathan, **R. Maulik**, G. Iungo, S. Letizia: Data-driven wind turbine wake modeling using probabilistic machine learning, *Neural Computing and Applications*, 34, 6171–618, 2022.
28. K. Lyras, **R. Maulik**, D. Schmidt: Machine-learning accelerated turbulence modelling of transient flashing jets, *Physics of Fluids*, 33, 127104 (2021).
29. K. Fukami, **R. Maulik**, N. Ramachandra, K. Taira, K. Fukagata: Global field reconstruction from sparse sensors with Voronoi tessellation-assisted deep learning, *Nature Machine Intelligence*, 2021.
30. B. Hamzi, **R. Maulik**, H. Owhadi: Simple, low-cost, and accurate, data-driven geophysical forecasting with learned kernels, *Proceedings of the Royal Society A*, 477: 20210326, 2021.

31. G. Mengaldo, **R. Maulik**, PySPOD: A Python package for Spectral Proper Orthogonal Decomposition (SPOD), *Journal of Open Source Software*, 6 (60), 2862, 2021.
32. **R. Maulik**, B. Lusch, P. Balaprakash: Reduced-order modeling of advection-dominated systems with recurrent neural networks and convolutional autoencoders, *Physics of Fluids*, 33, 037106, 2021.
33. S. Pawar, **R. Maulik**: Distributed deep reinforcement learning for simulation control, *Machine Learning: Science and Technology*, 2, 025029, 2021.
34. S. Renganathan, **R. Maulik**, J. Ahuja: Enhanced data efficiency using deep neural networks and Gaussian processes for aerodynamic design optimization, *Aerospace Science and Technology*, 111, 106522, 2021.
35. J. Burby, Q. Tang, **R. Maulik**: Fast neural Poincaré maps for toroidal magnetic fields, *Plasma Physics and Controlled Fusion*, 63, 024001, 2021.
36. **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: Nonlinear Phenomena*, 132797, 2021.
37. **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.
38. **R. Maulik**, K. Fukami, N. Ramachandra, K. Fukagata, K. Taira : Probabilistic neural networks for fluid flow surrogate modeling and data recovery, *Physical Review Fluids*, 5, 104401, 2020.
39. **R. Maulik**, P. Balaprakash, B. Lusch: Non-autoregressive time-series methods for stable parametric reduced-order models, *Physics of Fluids*, 32, 087115, 2020.
40. **R. Maulik**, N. Garland, X. Tang, P. Balaprakash: Neural network representability of fully ionized plasma fluid model closures, *Physics of Plasmas*, 27, 072106, 2020.
41. J. Choi, S. Robinson, **R. Maulik**, W. Wehde: What Matters the Most for Individual Disaster Preparedness? Understanding Emergency Preparedness Using Machine Learning, *Natural Hazards*, 103, 1183-1200, 2020.
42. 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.
43. **R. Maulik**, O. San: Numerical assessments of a parametric implicit large eddy simulation model, *Journal of Computational and Applied Mathematics*, 112866, 2020.
44. **R. Maulik**, O. San, J. Jacob: Spatiotemporally dynamic implicit large eddy simulation using machine learning classifiers, *Physica D: Nonlinear Phenomena*, 406, 132409, 2020.
45. **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: Nonlinear Phenomena*, 405, 132368, 2020.
46. 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.
47. **R. Maulik**, O. San, J. Jacob, C. Crick: Sub-grid scale model classification and blending through deep learning, *Journal of Fluid Mechanics*, 870, 784-812, 2019.

48. 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.
49. **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.
50. **R. Maulik**, O. San, A. Rasheed, P. Vedula: Data-driven deconvolution for large eddy simulation of Kraichnan turbulence, *Physics of Fluids*, 30, 125109, 2018.
51. O. San, **R. Maulik**: Stratified Kelvin-Helmholtz turbulence of compressible shear flows, *Nonlinear Processes in Geophysics*, 25, 457-476, 2018.
52. O. San, **R. Maulik**: Extreme learning machine for reduced order modeling of turbulent geophysical flows, *Physical Review E*, 97, 042322, 2018.
53. O. San, **R. Maulik**: Machine learning closures for model order reduction of thermal fluids, *Applied Mathematical Modelling*, 60, 681-710, 2018.
54. **R. Maulik**, O. San, R. Behera : An adaptive multilevel wavelet framework for scale-selective WENO reconstruction schemes, *International Journal of Numerical Methods in Fluids*, 87 (5), 239-269, 2018.
55. O. San, **R. Maulik**: Neural network closure models for nonlinear model order reduction, *Advances in Computational Mathematics*, 44, 1717-1750, 2018.
56. **R. Maulik**, O. San: A dynamic closure modeling framework for large eddy simulation using approximate deconvolution: Burgers equation, *Cogent Physics*, 5, 1464368, 2018.
57. **R. Maulik**, O. San: A neural network approach for the blind deconvolution of turbulent flows, *Journal of Fluid Mechanics*, 831, 151-181, 2017.
58. **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.
59. **R. Maulik**, O. San: Explicit and implicit LES closures for Burgers turbulence, *Journal of Computational and Applied Mathematics*, 327, 12-40, 2017.
60. **R. Maulik**, O. San: Resolution and energy dissipation characteristics of implicit LES and explicit filtering models for compressible turbulence, *Fluids*, 2(2)-14, 2017.
61. **R. Maulik**, O. San: A dynamic subgrid-scale modeling framework for Boussinesq turbulence, *International Journal of Heat and Mass Transfer*, 108, 1656-1675, 2017.
62. **R. Maulik**, O. San: A dynamic framework for functional parameterisations of the eddy viscosity coefficient in two-dimensional turbulence, *International Journal of Computational Fluid Dynamics*, 31(2), 69-92, 2017.
63. **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.
64. **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.
65. 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 publications*

1. R. Egele, **R. Maulik**, K. Raghavan, P. Balaprakash, B. Lusch: AutoDEUQ: Automated Deep Ensemble with Uncertainty Quantification, *26th International Conference on Pattern Recognition*, 1908–1914, 2022.
2. Sudeepa Mondal, Gina M. Magnotti, Bethany Lusch, **Romit Maulik**, Roberto Torelli: Machine Learning-Enabled Prediction of Transient Injection Map in Automotive Injectors With Uncertainty Quantification, *ASME Internal Combustion Engine Fall Conference*, 2021.
3. H. Shan, Y. Sun, **R. Maulik**, T. Xu: Application of Artificial Neural Network in the APS LINAC Bunch Charge Transmission Efficiency, *12th International Particle Accelerator Conference (IPAC)*, 2021., <https://accelconf.web.cern.ch/ipac2021/papers/tupab287.pdf>.
4. V. Sastry, **R. Maulik**, V. Rao, B. Lusch, S. Renganathan, R. Kotamarthi: Data-driven deep learning emulators for geophysical forecasting, *International Conference on Computational Science*, 433-446, 2021, [https://doi.org/10.1007/978-3-030-77977-1\\_35](https://doi.org/10.1007/978-3-030-77977-1_35). Acceptance rate: 30.7%.
5. **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. Acceptance rate: 20%.
6. V. Rao, **R. Maulik**, E. Constantinescu, M. Anitescu: A machine learning method for computing rare event probabilities, *International Conference on Computational Science*, 169-182, 2020, [https://link.springer.com/chapter/10.1007/978-3-030-50433-5\\_14](https://link.springer.com/chapter/10.1007/978-3-030-50433-5_14). Acceptance rate: 30.7%.
7. **R. Maulik**, O. San, C. Bach: A computational investigation of the effect of ground clearance in vertical ducting systems, *International High Performance Buildings Conference*, Herrick Laboratories, Purdue University, 2018. <https://docs.lib.purdue.edu/ihpbc/308/>.

### *Conference publications*

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>.

### *Peer-reviewed workshop proceedings*

1. S. Barwey, R. Balin, B. Lusch, S. Patel, R. Balakrishnan, P. Pal, **R. Maulik**, V. Vishwanath: Scalable and Consistent Graph Neural Networks for Distributed Mesh-based Data-driven Modeling, (Workshop on Machine Learning with Graphs in High Performance Computing Environments), Supercomputing 2024.
2. H. Guan, T. Arcomano, A. Chattopadhyay, **R. Maulik**: LUCIE: A Lightweight Uncoupled Climate Emulator with long-term stability and physical consistency for O(1000)-member ensembles, (Machine Learning for Earth System Modeling Workshop, ICML 2024).

3. T. Nguyen, R. Shah, H. Bansal, T. Arcomano, S. Madireddy, **R. Maulik**, V. Kotamarthi, I. Foster, A. Grover: Scaling transformers for skillful and reliable medium-range weather forecasting, ICLR AI4DiffEqtnsInSci Workshop 2024 (Accepted as spotlight presentation and awarded best paper).
4. A. Nair, S. Barwey, P. Pal, **R. Maulik**: Investigation of Latent Time-Scales in Neural ODE Surrogate Models, ICLR AI4DiffEqtnsInSci Workshop 2024 (Accepted as poster).
5. H. Zhang, Y. Liu, **R. Maulik** Semi-Implicit Neural Ordinary Differential Equations for Learning Chaotic Systems, NeurIPS 2023 Workshop Heavy Tails in Machine Learning, NeurIPS 2023.
6. V. Shankar, S. Barwey, **R. Maulik**, V. Vishwanathan: Practical implications of equivariant and invariant graph neural networks for fluid flow modeling, Physics4ML Workshop, ICLR 2023, <https://openreview.net/forum?id=3Y6XRCIUT5>.
7. **R. Maulik**, G. Mengaldo: PyParSVD: A streaming, distributed and randomized singular-value-decomposition library, (7th International Workshop on Data Analysis and Reduction for Big Scientific Data (DRBSD-7), Supercomputing 2021).
8. D. Skinner, **R. Maulik**: Meta-modeling strategy for data-driven forecasting, *Tackling Climate Change with Machine Learning Workshop, NeurIPS*, 2020. <https://www.climatechange.ai/papers/neurips2020/13.html>.
9. 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. [https://ml4physicalsciences.github.io/2020/files/NeurIPS\\_ML4PS\\_2020\\_79.pdf](https://ml4physicalsciences.github.io/2020/files/NeurIPS_ML4PS_2020_79.pdf).
10. 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. [https://ml4physicalsciences.github.io/2020/files/NeurIPS\\_ML4PS\\_2020\\_7.pdf](https://ml4physicalsciences.github.io/2020/files/NeurIPS_ML4PS_2020_7.pdf)
11. **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. [https://ml4physicalsciences.github.io/2019/files/NeurIPS\\_ML4PS\\_2019\\_134.pdf](https://ml4physicalsciences.github.io/2019/files/NeurIPS_ML4PS_2019_134.pdf)
12. **R. Maulik**, V. Rao, S. Madireddy, B. Lusch, P. Balaprakash: Using recurrent neural networks for non-linear component computation in advection-dominated reduced-order models, *Machine Learning for Physical Sciences Workshop, NeurIPS*, 2019. [https://ml4physicalsciences.github.io/2019/files/NeurIPS\\_ML4PS\\_2019\\_99.pdf](https://ml4physicalsciences.github.io/2019/files/NeurIPS_ML4PS_2019_99.pdf).

## Talks presented

1. Scalable, adaptive, and explainable geometric deep learning with applications to computational physics, **Invited talk**, University of Illinois at Chicago, September 20, 2024.
2. PDE-constrained machine learning of data-driven closure models, **Invited talk**, Argonne National Laboratory, September 19, 2024.
3. PDE-constrained machine learning of data-driven closure models, **Invited talk**, Society of Petroleum Engineering CFD Seminar, August 22, 2024.
4. Differentiable physics for closure modeling from data, **Invited talk**, ONR Erosion Workshop, Johns Hopkins University, August 14, 2024.

5. Interpretable Fine-Tuning and Error Indication for Graph Neural Network Surrogate Models, US-ACM UQ-MLIP, Washington DC, August 13, 2024.
6. Interpretable SciML for fluid flows using multiscale graph neural networks, **Invited talk**, Healthy People and Healthy Planet Workshop, Imperial College, July 25, 2024.
7. Scalable, adaptive, and explainable scientific machine learning with applications to computational fluid dynamics, **Invited talk**, Hong Kong University of Science and Technology Mechanical Engineering Seminar Series, April 17, 2024.
8. Differentiable physics for turbulence closure modeling from data, **Invited talk**, Unravel project meeting, University of Eindhoven, April 17, 2024.
9. Scalable, adaptive, and explainable scientific machine learning with applications to computational fluid dynamics, **Guest lecture**, NUEN 689 “Deep Learning for Engineering Applications”, Texas A & M University, April 9, 2024.
10. Differentiable physics for turbulence closure modeling from data, **Invited talk**, University of Maryland Numerical Analysis Seminar Series, April 2, 2024.
11. Scalable, adaptive, and explainable scientific machine learning with applications to computational fluid dynamics, **Invited talk**, Fluid Dynamics Research Consortium Seminar Series, Pennsylvania State University, March 28, 2024.
12. Turbulence modeling for large-eddy simulations using neural differential equations, **Invited talk**, International Conference on Differential Equations for Data Science 2024 (DEDS2024), Feb 19-21, 2024.
13. Scalable, adaptive, and explainable scientific machine learning with applications to computational fluid dynamics, **Invited talk**, Advanced Modeling and Simulations Seminar Series, University of Texas, El Paso, Feb 9, 2024.
14. On the construction of data-driven closures for large eddy simulations of turbulence, **Invited talk**, ERCOFTAC Workshop on Machine Learning for Fluid Dynamics, Sorbonne University, Paris, France, 6-8 March 2024.
15. Data assimilation with scientific machine learning, **Invited talk**, Indian Institute of Science, Education, and Research, Pune, December, 2023.
16. Anomaly detection for dynamical systems using Bayesian online changepoint detection, **Invited talk**, Brij Disa Center for Data Science and AI, Indian Institute of Management, Ahmedabad, December 2023.
17. Multiscale Graph Neural Network Architectures for Interpretable Scientific Machine Learning, **Invited talk**, CMAI Seminar Series, George Mason University, October, 2023.
18. The research program of the Interdisciplinary Scientific Computing Laboratory, **Invited talk**, AI/ML Technical Group, Department of Aerospace Engineering, Pennsylvania State University, October, 2023.
19. Differentiable turbulence modeling, **Invited talk**, Aerospace Seminar Series, TU Delft, October, 2023.
20. Differentiable turbulence modeling, **Invited talk**, Autumn school on Scientific Machine Learning, CWI Amsterdam, October, 2023.

21. PythonFoam: In-situ data analyses with OpenFOAM and Python, **Invited talk**, MS 421.1, "Software Tools for Uncertainty Quantification and Machine Learning with Applications to Computational Science", 17th U.S. National Congress on Computational Mechanics, Albuquerque, 2023.
22. Multiscale Graph Neural Network Autoencoders for Interpretable Scientific Machine Learning, **Invited talk**, BIRS Scientific Machine Learning workshop, Banff International Research Station, June, 2023.
23. Neural architecture search for scientific machine learning, **Invited talk**, ICERM topical workshop on Mathematical and Scientific Machine Learning, Brown University, June, 2023.
24. Multiscale graph neural networks for scalable surrogate modeling of fluid dynamical systems, **Invited talk**, International Workshop on Reduced Order Methods, National University of Singapore, May, 2023.
25. Breaking boundaries: Why interdisciplinary research is key for tackling grand challenges, **Plenary talk**, Oklahoma State University, Mechanical and Aerospace Engineering Graduate Search Symposium, March 24, 2023.
26. A stabilized neural ordinary differential equation for scientific machine learning, **Invited talk**, SIAM Conference on Computational Science and Engineering, Amsterdam, 2023.
27. Neural architecture search for scientific machine learning, **Invited talk**, Rutgers Efficient AI Seminar Series, February, 2023.
28. Accelerating scientific discovery using physics-informed machine learning, **Invited talk**, Machine Learning for e-Science, Swedish e-Science Research Centre, November 30, 2022.
29. Efficient high-dimensional variational data assimilation with machine-learned reduced-order models, Bulletin of the American Physical Society, Division of Fluid Dynamics, November, 2022.
30. A stabilized neural ordinary differential equation for scientific machine learning, **Invited talk**, SIAM Mathematics of Data Science, San Diego, September 28, 2022.
31. Neural forecasting of high-dimensional dynamical systems, **Invited talk**, University of Pittsburgh Computational Mathematics Seminar, September 20, 2022.
32. Quantifying Uncertainty in Deep Learning for Fluid Flow Reconstruction, **Invited talk**, USACM Thematic Conference on Uncertainty Quantification for Machine Learning Integrated Physics Modeling (MLIP), Crystal City, Virginia, August 18-19, 2022.
33. A stabilized neural ordinary differential equation for scientific machine learning, **Invited talk**, Argonne Training Program on Exascale Computing (ATPESC), August 12, 2022.
34. Learning nonlinear dynamical systems from data using scientific machine learning, **Invited talk**, 2022 AI + Science Summer School, University of Chicago, Data Sciences Institute, August 9, 2022.
35. Learning Nonlinear Dynamical Systems from Data Using Scientific Machine Learning, **Invited talk**, Accurate ROMs for Industrial Applications, Virginia Tech, July 7, 2022.
36. Non-intrusive reduced-order modeling using scientific machine learning, **Invited talk**, Summer School on Reduced Order Methods in CFD, SISSA Trieste, July 13, 2022.
37. Learning nonlinear dynamical systems from data using scientific machine learning, **Invited talk**, Brown University CRUNCH Seminar series, May 27, 2022.

38. Simple, low-cost and accurate data-driven geophysical forecasting with learned kernels, **Invited talk**, SIAM UQ, Atlanta, Georgia, April 12, 2022.
39. Reduced-order modeling of high-dimensional dynamical systems using scientific machine learning, **Invited talk**, IBiM Seminar Series, March 2022.
40. Emulating nonlinear dynamical systems from data using scientific machine learning, **Invited talk**, APS March Meetings, March 14, 2022.
41. Reduced-order modeling of high-dimensional dynamical systems using scientific machine learning, **Invited talk**, National University of Singapore, Department of Mechanical Engineering, Distinguished Seminar Series, February 10, 2022.
42. Emulating complex systems from data using scientific machine learning, **Invited talk**, North Carolina State University, Department of Mathematics, February 1, 2022.
43. Research at the intersection of mathematics, computation, and data, **Invited webinar**, BIT Mesra Alumni Association North America Faculty Webinar, January 29, 2022.
44. Reduced-order modeling of high-dimensional systems using scientific machine learning, **Invited talk**, IIT-Chicago MMAE Seminar Series, January 27, 2022.
45. Reduced-order modeling of high-dimensional systems using scientific machine learning, **Invited talk**, University of Waterloo, Department of Applied Mathematics, January 18, 2022.
46. Reduced-order modeling of high-dimensional systems using scientific machine learning, **Invited talk**, Florida State university, Department of Scientific Computing, November 19, 2021.
47. Research at the intersection of mathematics, computation, and data, **Invited talk**, Physics & Engineering speaker series, North Park University, November 17, 2021.
48. Reduced-order modeling of high-dimensional systems using machine learning, **Invited talk**, Civil and Environmental Engineering Seminar Series, Duke University, November 12, 2021.
49. Reduced-order modeling of high-dimensional systems using scientific machine learning, **Invited talk**, 2021 CBE Computing Seminar Series, University of Wisconsin-Madison, October 22, 2021.
50. Parallelized emulator discovery and uncertainty quantification using DeepHyper, Mechanistic Machine Learning and Digital Twins for Computational Science, Engineering & Technology, September 26-29, 2021.
51. Modified neural ordinary differential equations for stable learning of chaotic dynamics, **Invited talk**, Applied Mathematics Seminar Series, Texas Tech University, September 1, 2021.
52. Neural architecture search for surrogate modeling, **Invited talk**, ML4I Forum, Lawrence Livermore National Laboratory, August 10-12, 2021.
53. Scalable scientific machine learning for computational fluid dynamics, **Plenary talk**, Computational Sciences and AI in Industry, June 7-9, 2021.
54. Neural architecture search for surrogate modeling, **Invited talk**, DDPS Seminar Series, Lawrence Livermore National Laboratory, May 27, 2021.
55. Incorporating inductive biases for the surrogate modeling of dynamical systems, **Invited talk** at Machine Learning for Dynamical Systems Special Interest Group, Alan Turing Institute, Imperial College London, April 14, 2021.

56. Surrogate modeling with learned kernels (Kernel Flows), **Invited talk**, Uncertainty Quantification in Climate Science, NASA JPL Climate Center Virtual Workshop, March 24, 2021.
57. Scalable recurrent neural architecture search for geophysical emulation, **Invited talk** at SIAM-CSE Minisymposium on Physics-Guided Machine Learning and Data-Driven Methods in Computational Geoscience.
58. Incorporating Inductive Biases as Hard Constraints for Scientific Machine Learning, MCS-LANS seminar, Argonne National Laboratory, February 2021.
59. Scalable scientific machine learning for computational fluid dynamics, **Invited talk**, Department of Mechanical Engineering, The City College of New York, October, 2020.
60. Data-driven model order reduction for geophysical emulation. **Invited talk** at the Second Symposium on Machine Learning and Dynamical Systems, Fields Institute, Toronto, September, 2020.
61. Scalable scientific machine learning for computational fluid dynamics, **Invited talk**, Department of Mechanical Engineering, Rice University, September, 2020.
62. Machine Learning Enablers for System Optimization and Design, MCS-LANS seminar, Argonne National Laboratory, August 2020.
63. Surrogate-based machine-learning for system optimization and design, **Invited talk** at Los Alamos National Laboratory for Tokamak Disruption Simulation (TDS) working group, August, 2020.
64. 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, June 2020.
65. Spatiotemporally dynamic implicit large eddy simulation using machine learning classifiers, Session on Domain-Aware, Interpretable and Robust Scientific Machine Learning Methods Applied to Computational Mechanics, AIAA Aviation Forum, June, 2020, Reno.
66. Machine learning for computational fluid dynamics, **Invited talk** at PyData Meetup Chicago, May 2020.
67. Recurrent neural architecture search for geophysical emulation using DeepHyper, **Invited talk** at AI-HPC seminar, Argonne National Laboratory, April, 2020.
68. Machine Learned Reduced-Order Models for Advective Partial Differential Equations, MCS-LANS seminar, Argonne National Laboratory, February, 2020.
69. Machine Learned Reduced-Order Models for Advective Partial Differential Equations, **Invited talk**, 2020 Spring Multiscale Seminar, Illinois Institute of Technology, Chicago, February, 2020.
70. General purpose data science for general purpose CFD: Integrating Tensorflow into OpenFOAM at scale, **Invited poster**, Workshop for Machine Learning for Transport Phenomena, February, 2020, Dallas.
71. Machine learning of sequential data for non-intrusive reduced-order models, Bulletin of the American Physical Society, Division of Fluid Dynamics, November, 2019.
72. Tackling the limitations of conventional ROMs for advection-dominated nonlinear dynamical systems using machine learning, **Invited talk**, Advanced Statistics meets Machine Learning-III workshop, Argonne National Laboratory, November, 2019.

73. Data-driven sub-grid models for the large-eddy simulation of turbulence, **Invited talk**, John Zink Hamworthy Combustion, Tulsa, August, 2019.
74. Novel turbulence closures using physics-informed machine learning, Argonne Physical Sciences and Engineering Division AI Townhall, July, 2019.
75. Data-driven deconvolution for the sub-grid modeling of large eddy simulations of two-dimensional turbulence, SIAM-CSE, March, 2019.
76. Data-driven deconvolution for the large eddy simulation of Kraichnan turbulence, Bulletin of the American Physical Society, Division of Fluid Dynamics, November, 2018.
77. A computational investigation of the effect of ground clearance in vertical ducting systems, 2018, Purdue University, Herrick Labs Conferences, July, 2018.
78. A neural network approach for the blind deconvolution of turbulent flows, Bulletin of the American Physical Society, Division of Fluid Dynamics, November, 2017.
79. A generalized wavelet based grid-adaptive and scale-selective implementation of WENO schemes for conservation laws, Texas Applied Mathematics and Engineering Symposium, The University of Texas, Austin, September 2017.
80. 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, Division of Fluid Dynamics, November, 2016.
81. A dynamic hybrid subgrid-scale modeling framework for large eddy simulations, Bulletin of the American Physical Society, Division of Fluid Dynamics, November, 2016.

## Professional service

### *Committee membership*

PythonFOAM Workshop Lead Organizer (<https://www.alcf.anl.gov/events/alcf-pythonfoam-workshop>).

DOE INCITE program (2020) - Reviewed 2 proposals every year

ADSP program (2020) - Reviewed 2 proposals every year

International Conference on Parallel Processing, Chicago, 2021 (Reviewed 6 articles).

Wilkinson Postdoctoral Fellowship Committee, MCS Division, Argonne National Laboratory, 2022.

DOE AI for Earth System Predictability workshop session chair for neural networks.

### *Tutorials organized*

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.

TensorFlow workshop, Mechanical & Aerospace Engineering, Oklahoma State University, 2018.

An introduction to high performance computing for middle school kids, National Lab Day, Oklahoma State University 2017, 2018.

## *Minisymposia*

MS Organizer & Session chair, 16th, 17th USNCCM, SIAM-CSE 2019, 2021, 2023, AIAA Aviation 2020, 2024.

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

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

## *Journal Review*

Editor - Results in Engineering, Elsevier.

Journal reviewer for - AIAA Journal, Applied Mathematical Modeling, Chaos, Computer Methods in Applied Mathematics and Engineering, Communications in Computational Physics, Computers and Fluids, Computer Physics Communications, International Journal of Computational Fluid Dynamics, IEEE Transactions on Plasma Science, Journal of Fluid Mechanics, Journal of Scientific Computing, Physics of Fluids, Physica D, International Journal of Numerical Methods in Fluids, Journal of Computational Physics, Journal of Nonlinear Science, Nature Communications, Nature Machine Intelligence, Nature Scientific Reports, Theoretical and Computational Fluid Dynamics, Atmospheric Science Letters, New Journal of Physics, Transactions of Machine Learning Research, Machine Learning Science and Technology, Neurips, ICLR.

## Software developed

1. R. Maulik, D. Fytanidis, S. Patel, B. Lusch, V. Vishwanath, PythonFoam: In-situ data analyses with OpenFOAM and Python. <https://github.com/argonne-lcf/PythonFOAM>.
2. R. Maulik, H. Sharma, S. Patel, B. Lusch, E. Jennings, TensorFlowFoam: A framework that enables the deployment of deep learning (in Python) and partial differential equation solutions concurrently in OpenFOAM - a C++-based open-source finite-volume based computational physics package. <https://github.com/argonne-lcf/TensorFlowFoam>.
3. R. Maulik, S. Pawar, PAR-RL: A framework that leverages the Ray library to deploy scalable deep reinforcement learning for arbitrary scientific environments on leadership class machines. Tested on ALCF supercomputer Theta for controlling simulations of dynamical systems. <https://github.com/Romit-Maulik/PAR-RL>.
4. R. Maulik, G. Mengaldo, PyParSVD: A Parallelized, streaming, and randomized implementation of the SVD for Python using mpi4py. <https://github.com/Romit-Maulik/PyParSVD>. DOI: 10.5281/zenodo.4562889.
5. G. Mengaldo, R. Maulik, PySPOD: Python Spectral Proper Orthogonal Decomposition. <https://github.com/mengaldo/PySPOD>. DOI: <https://doi.org/10.21105/joss.02862>.