Dan Lu, Ph.D.

Senior Staff Scientist
Computational Sciences and Engineering Division
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Professional Experience

2023 – Now	**Senior Staff Scientist** Oak Ridge National Laboratory, Oak Ridge, TN
2016 – 2023	**Staff Scientist** Oak Ridge National Laboratory, Oak Ridge, TN
2013 – 2016	**Postdoctoral Research Associate** Oak Ridge National Laboratory, Oak Ridge, TN
2012 – 2013	**Postdoctoral Research Associate** U.S. Geological Survey, Menlo Park, CA

Education

2007 – 2012	**Ph.D. in Computational Hydrology** Florida State University, Tallahassee, FL, USA
2004 – 2007	**M.S. in Hydrology and Water Resources** China University of Geosciences, Beijing, China
2000 – 2004	**B.S. in Environmental Engineering** Hebei University of Geosciences, Shijiazhuang, China

Research Interests

Computational Hydrology and Earth Sciences
Scientific Machine Learning and Data Analytics
Uncertainty Quantification and Risk Assessment
Bayesian Inferences and Sensitivity Analysis
Multimodel Analysis and Model Averaging
Surrogate Modeling and Model Calibration
Sensor Network Optimization and Experimental Design
Climate Modeling and Subsurface Modeling

Current Grants

DOE - Early Career Award

Integrating Machine Learning Models into E3SM for Understanding Coastal Compound Flooding

$2,500,000 for 10/2023–09/2028, PI

ORNL - Laboratory Directed Research & Development

Assurance of AI Models for Scientific Applications

$700,000 for 10/2021–09/2024, PI

Current Grants (continued)

DOE - Water Power Technologies Office

An Uncertainty-Aware, Machine Learning-Enabled Hydropower Seasonal Forecast Model

$50,000 for 01/2023–12/2023, PI

DOE - Office of Fossil Energy and Carbon Management

Science-informed Machine Learning in Subsurface Applications

$1,100,000 for 10/2020–09/2023, Co-PI

DOE - Advanced Scientific Computing Research

Efficient Machine Learning for Facility Scientific Data Analytics

$3,500,000 for 10/2021–09/2024, Task Lead

ORNL - Laboratory Directed Research & Development

AI for Robust Engineering and Sciences

$1,700,000 per year for 10/2022–09/2025, Task Lead

ORNL - Laboratory Directed Research & Development

Decision-making Framework for Enhanced Weathering

$1,200,000 for 10/2023–09/2025, Senior Investigator

DOE - Advanced Scientific Computing Research

Decision and Control of Complex Systems: a Data-Driven Framework

$4,200,000 for 10/2020–09/2024, Task Lead

DOE - Biological and Environmental Research

Advancing Watershed System Understanding through Machine Learning

$6,200,000 for 10/2020–06/2024, Machine Learning Lead

DOE - Basic Energy Sciences

Machine Learning for Improving Accelerator and Target Performance

$6,900,000 for 10/2020–09/2026, Senior Investigator

DOE - Biological and Environmental Research

Watershed Dynamics and Evolution Scientific Focus Area

$3,500,000 per year for 05/2023–04/2026, Senior Investigator

Awards and Honors

- DOE Early Career Award, 2023
- The Most Exciting Future Direction Project Award, ORNL-LDRD Poster Fair, 2023
- Distinguished Scientific Achievement Award at CSED, ORNL, 2022
- Selected Early Career Scientist to the DOE headquarter, 2018
- Travel Fellowship to the DOE PI meeting, 2012
- Fellowship of Statistical and Applied Mathematical Sciences Institute, 2011
- Scholarship for Excellent Student, China University of Geosciences, 2004–2007
- Excellent Undergraduate Student of Hebei Province, China, 2003
- Scholarship for Excellent Student, Hebei University of Geosciences, China, 2000–2004

Research Publications

Journal Articles (Published)

1. Fan, M., Wang, H., Zhang, J., Hosseini, S., and **Lu, D.**, *Advancing spatiotemporal forecasts of CO2 plume migration using deep learning networks with transfer learning and interpretation analysis. International J. Of Greenhouse Gas Control*, https://doi.org/10.1016/j.ijggc.2024.104061, 2024.
2. Fan, M., Liu, S., and **Lu, D.**, *Advancing subseasonal reservoir inflow forecasts using an explainable machine learning method*, Journal of Hydrology, V50, https://doi.org/10.1016/j.ejrh.2023.101584, 2023.
3. Fan, M., Liu, S., **Lu, D.**, Gangrade, S., and Kao S., *Explainable machine learning model for multi-step forecasting of reservoir inflow with uncertainty quantification*, Environmental Modeling and Software, V170, https://doi.org/10.1016/j.envsoft.2023.105849, 2023.
4. **Lu, D.**, Yang, T., and Liu, X., *Editorial: Data-driven machine learning for advancing hydrological and hydraulic predictability*, Frontier in Water, V5, https://doi.org/10.3389/frwa.2023.1215966, 2023.
5. Liu, S., Fan, M., and **Lu, D.** *Uncertainty quantification of the convolutional neural networks on permeability estimation from micro-CT scanned sandstone and carbonate rock images*, Geoenergy Science and Engineering, 212160, http://dx.doi.org/10.2139/ssrn.4279760, 2023.
6. Alanazi, Y., Schram, M., Rajput, K., Goldenberg, S., T.,Vidyaratne, Pappas, C., Radaideh, M., **Lu, D.**, Ramuhalli P., Cousineau, S., *Multi-module based CVAE to predict HVCM faults in the SNS accelerator*. Machine Learning with Applications, V13, https://doi.org/10.1016/j.mlwa.2023.100484, 2023.
7. Wilson, A. J., Tran, H., and **Lu, D.** *Uncertainty quantification of capacitor switching transient location using machine learning*. IEEE Transactions on Power Systems, doi: 10.1109/TPWRS.2023.3286173, 2023.
8. Topp, S., Barclay, J., Diaz, J., Sun, A., Jia, X., **Lu, D.**, Sadler, J., and Appling A., *Stream temperature prediction in a shifting environment: The influence of deep learning architecture*, Water Res. Research. V59(4), https://doi.org/10.1029/2022WR033880, 2023.
9. Chen, A., Ricciuto, D., Mao, J., Wang J., **Lu, D.**, and Meng F., *Improving E3SM land model photosynthesis parameterization via satellite SIF, machine learning, and surrogate modeling*, Journal of Advances in Modeling Earth Systems, https://doi.org/10.1029/2022MS003135, 2023.
10. Liu, S., **Lu, D.**, Painter, S.L., Griffiths, N.A., and Pierce, E.M., *Uncertainty quantification of machine learning models to improve streamflow prediction in changing climate and environmental conditions*. Frontiers in Water, V5, https://doi.org/10.3389/frwa.2023.1150126, 2023
11. Fan, M., Zhang, L., Liu, S., Yang, T., and **Lu, D.**, *Investigation of hydrometeorological influences on reservoir releases using explainable machine learning methods*. Frontiers in Water, V5, 2023.
12. Chen, X., Serrano, M., Hernandez, R., **Lu, D.**, Sokolov, M. A., Gonzalez De Vicente S. M., and Katoh, Y., *Influence of fatigue precracking and specimen size on the master curve fracture toughness measurements of EUROFER97 and F82H steels*. Nuclear Materials and Energy, V34, 2023.
13. Hao, Y., Feng, E., **Lu, D.**, Zimmer, L., Morgan, Z., Chakoumakos, B. C., Zhang, G., and Cao, H., *Machine learning assisted automation of single crystal neutron diffraction*. Journal of Applied Crystallography, V56, 519-525, 2023.
14. Bhanja, S. N., Coon, E. T., **Lu, D.**, and Painter S. L., *Evaluation of distributed process-based hydrologic model performance in diverse catchments using only a priori information*, Journal of Hydrology, V618, 2023.
15. Fan, M., **Lu, D.**, and Liu, S., *A deep learning-based direct forecasting of CO2 plume migration*. Geoenergy Science and Engineering, V221, 2023.
16. Fan, M., **Lu, D.**, Rastogi, D., and Pierce, E. M., *A spatiotemporal-aware climate model ensembling method for improving precipitation predictability*. Journal of Machine Learning in Modeling and Simulation, V3 (4), 29-55, doi: 10.1615/JMachLearnModelComput.2022046715, 2022.

17. **Lu, D.**, Painter, S. L., Azzolina, N. A., Burton-Kelly, M., Jiang T., and Williamson C., *Accurate and rapid forecasts for geologic carbon storage via learning-based inversion-free prediction*, Frontiers in Energy Research, 9: 752185, doi: 10.3389/fenrg.2021.752185, 2022.

18. Gangrade, S., **Lu, D.**, Kao, S., Painter, S., and Coon, E., *Machine learning assisted reservoir operation model for long-term water management simulation*, J. of the Amer. Water Res. Ass., https://doi.org/10.1111/1752-1688.13060, 2022.

19. Radaideh, M., Pappas, C., Walden, C., **Lu, D.**, Vidyaratne, L., Britton, T., Rajput, K., Schram, M., Cousineau, S., *Time series anomaly detection in power electronics signals with recurrent and convlstm autoencoders*, Digital Signal Processing, 130, 103704, 2022.

20. **Lu, D.**, Konapala, G., Painter, S., and Kao, S., *Streamflow simulation in data-scarce basins using Bayesian and physics-informed machine learning models*, J. of Hydrometeorology, 1421-1438, 2021.

21. Huang, X., **Lu, D.**, Ricciuto, D. M., Hanson, P. J., Richardson, A. D., Lu, X., Weng, E., Nie, S., Jiang, L., Hou, E., Steinmacher, I. F., and Luo, Y., *A model-independent data assimilation (MIDA) module and its applications in ecology*, Geoscientific Model Development, 14(8), 5217-5238, 2021.

22. Chen, A., Mao, J., Ricciuto, D., **Lu, D.**, Xiao, J., Li, X., Thornton, P. E., and Knapp, A. K., *Seasonal changes in GPP/SIF ratios and their climatic determinants across the northern hemisphere*, Global Change Biology, 1-12, 2021.

23. Zhang, P., Liu, S., **Lu, D.**, Sankaran, R., Zhang, G., *An out-of-distribution-aware autoencoder model for reduced chemical kinetics*, American Institute of Mathematical Sciences Journal, Doi: 10.3934/dcdss.2021138, 2021.

24. Walker, A., Johnson, A., Rogers, A., Anderson, J., Bridges, R., Fisher R., **Lu, D.**, Ricciuto, D., Serbin, S. and Ye M., *Multi-hypothesis analysis of photosynthesis models reveals the unexpected influence of empirical assumptions at leaf and global scales*, Global Change Biology, Doi: 10.1111/gcb.15366, 2020.

25. Konapala, G., Kao, S., Painter, S., and **Lu, D.**, *Machine learning assisted hybrid models can improve streamflow simulation in diverse catchments across the conterminous US*, Environmental Research Letter, 15(10), 2020.

26. **Lu, D.**, and Ricciuto, D., *Efficient surrogate modeling methods for large-scale Earth system models based on machine learning techniques*, Geoscientific Model Development, 12, 1791-1807, 2019.

27. Mo, S., Shi, X., **Lu, D.**, Ye, M., and Wu, J., *An adaptive Kriging surrogate method for efficient uncertainty quantification with an application to geological carbon sequestration modeling*, Computers and Geosciences, 125, 69-77, 2019.

28. Evans, K., Kennedy, J., **Lu, D.**, Forrester, M. M., Price, S., Fyke, J., Bennett, A., Hoffman, M., Tezaur, I., Zender, C., and Vizcaino, M., *LIVVkit 2.1: Automated and extensible ice sheet model validation*, Geosci. Model Dev., 12, 2019.

29. Walker A. P., Ye, M., **Lu, D.**, De Kauwe, M. G., Gu, L., Medlyn, B. E., Rogers, A., and Serbin, S. P., *The multi-assumption architecture and testbed (MAAT v1.0): R code for generating ensembles with dynamic model structure and analysis of epistemic uncertainty from multiple sources*, Geosci. Model Dev., 11, 2018.

30. **Lu, D.**, D. Ricciuto, M. Stoyanov, and L. Gu, *Calibration of the E3SM land model using surrogate based global optimization*, Journal of Advances in Modeling Earth Systems, 10, 1337–1356, 2018.

31. **Lu, D.**, D. Ricciuto, and K. Evans, *An efficient Bayesian data-worth analysis using a multilevel Monte Carlo method*, Advances in Water Resources, 113, 223–235, 2018.

32. Shi, X., S. Finsterle, K. Zhang, and **Lu, D.**, *Advances in multiphase flow and transport in the subsurface environment.*, Geofluids, 2018.

33. Mo, S., **Lu, D.**, X. Shi, G. Zhang, M. Ye, J. Wu, and J. Wu, *A Taylor expansion-based adaptive design strategy for global surrogate modeling with applications in groundwater modeling*, Water Resources Research, 53, 10802–10823, 2017.

34. **Lu, D.**, D. Ricciuto, A. Walker, C. Safta, and W. Munger, *Bayesian calibration of terrestrial ecosystem models: a study of advanced Markov chain Monte Carlo methods*, Biogeosciences, 14, 4295–4314, 2017.

35. Xi, M., **Lu, D.**, D. Gui, Z. Qi, and G. Zhang, *Calibration of an agricultural-hydrological model (RZWQM2) using surrogate global optimization*, Journal of Hydrology, 544, 2017.

36. **Lu, D.**, G. Zhang, C. Webster, and C. Barbier, *An improved multilevel Monte Carlo method for estimating probability distribution functions in stochastic oil reservoir simulations*, Water Resources Research, 52, 9642–9660, 2016.
(*** This work was reported in *The BAKKEN Magazine in 2015* [online version])

37. Liu, P., A. S. Elshall, M. Ye, P. Beerli, X. Zeng, **Lu, D.**, and Y. Tao, *Evaluating marginal likelihood with thermodynamic integration method and comparison with several other numerical methods*, Water Resources Research, 52, 734–758, 2016.

38. Hill, M. C., D. Kavetski, M. Clark, M. Ye, M. Arabi, **Lu, D.**, L. Foglia, and S. Mehl, *Practical use of computationally frugal model analysis methods*, Ground Water, 54, 159–170, 2015.

39. **Lu, D.**, M. Ye, and G. P. Curtis, *Maximum likelihood Bayesian model averaging and its predictive analysis for groundwater reactive transport models*, Journal of Hydrology, 529(3), 1859–1873, 2015.

40. **Lu, D.**, M. Ye, M. C. Hill, E. P. Poeter, and G. P. Curtis, *A computer program for uncertainty analysis integrating regression and Bayesian methods*, Environmental Modeling & Software, 60, 41–56, 2014.

41. Zhang, G., **Lu, D.**, M. Ye, M. Gunzburger, and C. Webster, *An adaptive sparse-grid high-order stochastic collocation method of Bayesian inference in groundwater reactive transport modeling*, Water Resour. Res, 49(10), 6871–6892, 2013.

42. **Lu, D.**, M. Ye, P. D. Meyer, G. P. Curtis, X. Shi, X. Niu, and S. B. Yabusaki, *Effects of error covariance structure on estimation of model averaging weights and predictive performance*, Water Resour. Res., 49(9), 6029–6047, 2013.

43. Hill, M. C., D. Kavetski, M. Clark, M. Ye, and **Lu, D.**, *Uncertainty quantification for environmental models*, SIAM News, 45(9), 2012.

44. **Lu, D.**, M. C. Hill, and M. Ye, *Analysis of regression confidence intervals and Bayesian credible intervals for uncertainty quantification*, Water Resources Research, 48(9), 2012.
(*** This paper was selected as *Editor's Highlight* entitled new insights into faster computation of uncertainties)

45. **Lu, D.**, M. Ye, S. P. Neuman, and L. Xue, *Multimodel Bayesian analysis of data-worth applied to unsaturated fractured tuffs*, Advances in Water Resources, 35, 69–82, 2012.

46. Neuman, S. P., L. Xue, M. Ye, and **Lu, D.**, *Bayesian analysis of data-worth considering model and parameter uncertainties*, Adv. in Water Resour., 36, 75–85, 2012.
(*** *Top 10 Cited Paper* in 2012-2013 of Adv. in Water Resour. [Certificate])

47. **Lu, D.**, M. Ye, and S. P. Neuman, *Dependence of Bayesian model selection criteria and Fisher information matrix on sample size*, Mathematical Geoscience, 43, 2011.

48. Ye, M., **Lu, D.**, S. P. Neuman, and P. D. Meyer, *Comment on "Inverse groundwater modeling for hydraulic conductivity estimation using Bayesian model averaging and variance window" by Frank T.-C. Tsai and Xiaobao Li*, Water Resources Research, 46, W02801, 2010.

Conference Proceedings (Published)

1. Bororwiec, K., **Lu, D.**, Chandan, V., Chatterjee, S., Ramuhalli, P., Tipireddy, R., Halappanavar, M., and Liu, F., *Bi-fidelity weighted transfer learning for efficient heat transfer model simulation*, IEEE International Conference on Machine Learning and Applications, 2023.

2. Zhao, X., Puente B. M., Liu, S., Lim, S., Gurecky W., **Lu, D.**, Howell, M., Liu, F., Williams, W., and Ramuhalli, P., *Knowledge-informed uncertainty-aware machine learning for time series forecasting of dynamical engineered systems*. Proceeding of international topical meeting on nuclear plant instrumentation, control, and human-machine interface technologies, 2023.

3. **Lu, D.**, Ricciuto, D., and Zhang J., *Invertible neural networks for E3SM land model calibration and simulation*. Proceedings of ICLR AI for Earth and Space Sciences Workshop, 2022.

4. **Lu, D.**, Ricciuto, D., and Liu, S., *An interpretable machine learning model for advancing terrestrial ecosystem predictions*. Proceedings of ICLR AI for Earth and Space Sciences Workshop, 2022.

5. Fan, M., Zhang, L., Liu, S., Yang, T., and **Lu, D.**, *Identifying the hydrometeorological decision factors influencing reservoir releases over the upper Colorado region*. Proceedings of IEEE International Conference in Data Mining DMESS workshop, 2022.

6. Liu, S., **Lu, D.**, Ricciuto, D., and Walker A., *Improving net ecosystem CO2 flux prediction using memory-based interpretable machine learning*. Proceedings of IEEE International Conference in Data Mining DMESS workshop, 2022.

7. Radaideh, M., Pappas, C., **Lu, D.**, Walden, J., Cousineau, S., Britton, T., Rajput, K., Vidyaratne, L., Schram, M., *Progress on machine learning for the SNS high voltage converter modulators*, North American Particle Accelerator Conference, 2022.

8. Bororwiec, K., **Lu, D.**, Chandan, V., Chatterjee, S., Ramuhalli, P., Tipireddy, R., Halappanavar, M., and Liu, F., *Bi-fidelity weighted transfer learning for efficient heat transfer model simulation*, IEEE International Conference on Machine Learning and Applications, 2022.

9. Tran, H., **Lu, D.**, and Zhang, G., *Exploiting the local parabolic landscapes of adversarial losses to accelerate black-box adversarial attack*, European Conference on Computer Vision (ECCV), 2022.

10. Fan, M., **Lu, D.**, and Rastogi, D., *Multimodel ensemble predictions of precipitation using Bayesian neural networks*. Proceedings of ICLR AI for Earth and Space Sciences Workshop, 2022.

11. Liu, S., Zhang, P., **Lu, D.**, and Zhang, G., *PI3NN: Out-of-distribution-aware prediction intervals from three neural networks*. Proceedings of International Conference on Learning Representations (ICLR), 2022.

12. **Lu, D.**, Pierce, E., Kao, S., Womble, D., Li, L., Rempe, D., *Machine learning-enabled model-data integration for predicting subsurface water storage*. Proceedings of NeurIPS Tackling Climate Change with Machine Learning workshop, 2021.

13. **Lu, D.**, Painter, S., Azzolina N., and Burton-Kelly M., *Accurate and timely forecasts of geologic carbon storage using machine learning methods*. Proceedings of NeurIPS Tackling Climate Change with Machine Learning workshop, 2021.

14. Pappas, C., **Lu, D.**, Schram, M., and Vrabie D., *Machine learning for improved availability of the SNS klystron high voltage converter modulators*, 12th Int. Particle Acc. Conf. doi:10.18429/JACoW-IPAC2021-THPAB252, 2021.

15. Zhang, P., Liu, S., **Lu, D.**, and Zhang, G., *A prediction interval method for uncertainty quantification of regression models*, Proceedings of ICLR Workshop on Deep Learning for Simulation, 2021.

16. Tran, H., **Lu, D.**, and Zhang, G., *Boosting black-box adversarial attack via exploiting loss smoothness*, Proceedings of ICLR Workshop on Security and Safety in Machine Learning Systems, 2021.

17. Zhang, J., Tran, H., **Lu, D.**, and Zhang, G., *Enabling long-range exploration in minimization of multimodal functions*, Proceedings of Conference on Uncertainty in Artificial Intelligence (UAI), 2021.

18. **Lu, D.**, and Ricciuto D., *Efficient distance-based global sensitivity analysis for terrestrial ecosystem modeling*, Proceedings of IEEE International Conference on Data Mining Workshops, Doi: 10.1109/ICDMW51313.2020.00052, 2020.

19. **Lu, D.**, Liu S., and Ricciuto D., *An efficient Bayesian method for advancing the application of deep learning in earth science*. Proceedings of IEEE International Conference on Data Mining Workshops, Doi: 10.1109/ICDMW.2019.00048, 2019.

20. **Lu, D.**, and Ricciuto D., *Learning-based inversion-free model-data integration to advance ecosystem model prediction*. Proceedings of IEEE International Conference on Data Mining Workshops, Doi: 10.1109/ICDMW.2019.00049, 2019.

21. Barbier, C., **Lu, D.**, N. Collier, F. Curtis, C. G. Webster, and Y. Polsky, *High performance computing simulations for shale gas formation flow transport and uncertainty quantification analysis*, ORNL Technical Report, ORNL/TM-2015/543, 2015.

22. Zhang, G., **Lu, D.**, M. Ye, M. Gunzburger, and C. Webster, *An efficient surrogate modeling approach in Bayesian uncertainty analysis*, Proceedings of 11th International Conference of Numerical Analysis and Applied Mathematics, 2013.

23. Ye, M., **Lu, D.**, S. P. Neuman, and L. Xue , *Multimodel Bayesian analysis of data-worth applied to unsaturated fractured tuffs*, Proceedings of International Conference on Groundwater: Our Source of Security in an Uncertain Future, 2011.

24. **Lu, D.**, M. C. Hill, and M. Ye, *Analysis of regression and Bayesian predictive uncertainty measures*, Proceedings of MODFLOW and More Conference, 2011.

25. Neuman, S. P., L. Xue, M. Ye, and **Lu, D.**, *Multimodel assessment of the worth of data under uncertainty*, Proceedings of Water Management Symposium, 2011.

26. Ye, M., **Lu, D.**, G. Miller, G. P. Curtis, P. D. Meyer, and S. B. Yabusaki, *Assessment of predictive uncertainty in coupled groundwater reactive transport modeling*, Proceedings of Conference on Goldschmidt – Earth, Energy and Environ., 2010.

Lectures and Short Courses

🕮 **Machine Learning and its Applications**

Oak Ridge Continual Learning Program, Oak Ridge, March, 2023.

🕮 **Uncertainty Quantification in Earth System Modeling**

Department of Mathematics at the Federal University of Parana (UFPR), Brazil, virtually, June, 2021.

🕮 **Calibration and Uncertainty Quantification Using UCODE**

Colorado School of Mines, Golden, CO, 2017.

🕮 **Groundwater Model Calibration Using OSTRICH and UCODE**

Colorado School of Mines, Golden, CO, 2015.

🕮 **Groundwater Model Calibration Using ModelMate, ModelMuse, and UCODE**

Colorado School of Mines, Golden, CO, May 2011.

Software Development

UCODE_2014

A Computer Code for Sensitivity Analysis, Model Calibration, and Uncertainty Evaluation

Sponsor: U.S. Geological Survey

Developers: Eileen P. Poeter, Mary C. Hill, **Dan Lu**, and Steffen Mehl

Webpage: `http://igwmc.mines.edu/freeware/ucode/`

PI3NN

A Computer Code for Uncertainty Quantification of Machine Learning Model Predictions

Developers: Siyan Liu, **Dan Lu**, and Guannan Zhang

Webpage: `https://github.com/liusiyan/PI3NN`

Selected Talks

1. **(Invited)** *Machine learning in subsurface modeling: addressing small and big data challenges with uncertainty quantification*, AGU Fall Meeting, SF, CA, Dec. 13, 2023.
2. **(Invited)** *Machine learning methods for advancing earth system predictability*, SIAM MPE, Nov. 30, 2023, virtual.
3. **(Invited)** *Scale ClimaX on AMD-powered Frontier with DeepSpeed for better weather and climate solutions*, SC23, Denver, CO. Nov. 13-17, 2023.
4. **(Invited)** *Physics-informed, explainable, trustworthy AI for advancing earth system predictability*, Workshop on AI application in Earth system science, Nov. 6. 2023.
5. **(Invited)** *Explainable and trustworthy machine learning with applications in Earth and material sciences* at 2nd ORNL-VU Collaborative Workshop, Sept. 18, 2023.
6. **(Invited)** *Machine learning techniques to advance Earth system predictability* at technical meeting with Air Force, May 3, 2023.
7. **(Invited)** *Machine learning in Earth system modeling*, Florida State University, Feb. 2023.
8. **(Invited)** *Uncertainty quantification of machine learning models in scientific and engineering applications*, PNNL, Oct. 25-26, 2022.
9. *Uncertainty quantification of machine learning models to improve streamflow prediction in changing climate and environmental conditions*, AGU Fall meeting, Dec., 2022.
10. **(Invited)** *Machine learning for improving earth system predictability*, SIAM Conference on Mathematics of Planet Earth (MPE22), July 2022.
11. **(Invited)** *PI3NN-LSTM: improving machine learning model prediction of streamflow in novel climate conditions*, HydroML workshop, May 2022.
12. **(Invited)** *ML4UQ: machine learning to enable efficient uncertainty quantification in climate models*, SIAM Conference on Uncertainty Quantification, 2022
13. **(Invited)** *Physics-informed, interpretable machine learning for terrestrial ecosystem predictions*, 11th International Conference on Ecological Informatics, 2021.
14. **(Invited)** *A prediction interval method for uncertainty quantification of regression models*, Ecological Society of America Annual Meeting, August 2021.

15. **(Invited)** *Machine learning methods for improving terrestrial ecosystem predictions*, Society for Industrial and Applied Mathematics Annual Meeting, 2021.

16. **(Invited)** *An efficient bayesian machine learning method for advancing ecological forecasting*, Ecological Society of America Annual Meeting, August 2020.

17. **(Invited)** *An efficient Bayesian method for advancing the application of deep learning in earth science* in ICDM conference, Beijing, China, November 2019.

18. **(Invited)** *Learning-based inversion-free model-data integration to advance ecosystem model prediction* in ICDM conference, Beijing, China, November 2019.

19. **(Invited)** *2nd workshop on quantifying and reducing uncertainty in Earth system model projections*, University of Leeds, UK, 2019.

20. **(Invited)** *Efficient surrogate modeling methods to advance model-data integration*, American Geophysics Union annual meeting, Washington D.C., 2018.

21. **(Invited)** *Optimization of sensor networks for improving climate predictions*, DOE-BER headquarter, Germantown, Maryland, 2018.

22. **(Invited)** *A systematic Bayesian uncertainty quantification framework in environmental modeling*, Jinan University, Guangzhou, China, 2018.

23. **(Invited)** *Efficient surrogate modeling methods for model-data integration*, Geological Survey of Japan, Japan, 2018.

24. **(Invited)** *Efficient uncertainty quantification methods in groundwater contaminant risk assessment*, Japan Geosciences Union Annual Meeting, Japan, 2018.

25. **(Invited)** *Application of reduced-order modeling techniques for uncertainty quantification*, CSMD-CSED Cross-Divisional Seminar, 2018.

26. **(Invited)** *Potential exascale applications for quantifying uncertainty in the land-atmosphere system*, Exascale Application in Climate and Environmental Science workshop, 2018.

27. **(Invited)** *Advance climate model development, prediction, and risk assessment using artificial intelligence*, AI for Climate Sciences Seminar, 2018.

28. *An efficient Bayesian data-worth analysis using a multilevel Monte Carlo method*, American Geophysics Union Annual Meeting, New Orleans, LA, 2017.

29. *Quantum behaved particle swarm optimization for parameter estimation in terrestrial ecosystem models*, 2017 ESS PI Meeting, Washington D.C., 2017.

30. *Calibration of the Community Land Model (CLM4.5) using surrogate based global optimization*, American Geophysics Union Annual Meeting, CA, 2016.

31. *A systematic Bayesian framework for uncertainty quantification in environmental modeling*, Earth System Modeling Workshop, TN, 2015.

32. *Multilevel Monte Carlo method with application to uncertainty quantification in oil reservoir simulation*, American Geophysics Union Annual Meeting, CA, 2014.

33. *Assessment of predictive performance of Bayesian model averaging in groundwater reactive transport models*, SIAM Conference on Uncertainty Quantification, GA, 2014.

34. *Maximum likelihood Bayesian model averaging of groundwater reactive transport models*, 2014 SIAM SEAS Annual Meeting, Melbourne, FL, 2014.

Leadership and Committee

- 👍 Co-led Artificial Intelligence Initiative at ORNL, 2023
- 👍 Leadership team of Climate Change Science Institute at ORNL, 2023 – Now
- 👍 Groundwater Technique Committee for American Geophysics Union, 2016 – Now
- 👍 SIAM Activity Group on Mathematics of Planet Earth, 2021 – Now
- 👍 Review Committee for Enzyme Engineering Initiative, 2022 – Now
- 👍 Program Committee for Tackling Climate Change with Machine Learning Workshop, 2022 – Now
- 👍 Program Committee for AI for Robust Engineering and Sciences Workshop, 2021 – 2022
- 👍 Program Committee for Climate and Weather Domain of PASC19 Conference, 2019
- 👍 Co-led Artificial Intelligence Summer Institute for Students, 2019

Editorial Service

- ✎ Topic Editor: Geoscientific Model Development, 2021 – Now
- ✎ Associate Editor: Artificial Intelligence for the Earth Systems, 2021 – Now
- ✎ Associate Editor: Frontiers in Water, 2022 – Now
- ✎ Special Issue Editor: *Data-driven machine learning for advancing hydrological and hydraulic predictability*, Frontiers in Water, 2022
- ✎ Special Issue Co-editor: *Advances in multiphase flow and transport in the subsurface environment*, Geofluids, 2018

Supervising Staff, Postdocs, and Students

- ★ Dr. Siyan Liu, Early-career staff scientist
- ★ Dr. Ming Fan, Postdoc
- ★ Dr. Kshitij Tayal, Postdoc
- ★ Femi Epps, *Morgan State University*
- ★ Ahsan Jamil, *New Mexico State University*
- ★ Bear Moran, *University of Tennessee*
- ★ Xueming Zheng, *Florida State University*
- ★ Shaoxing Mo, *Nanjing University*
- ★ Siyan Liu, *University of Kansas*
- ★ Kan Zhang, *Illinois Institute of Technology*
- ★ 15 students from *diverse universities in AI Summer Institute*

Membership

Society for Industrial and Applied Mathematics (SIAM)

American Geophysical Union (AGU)

Geologic Society of America (GSA)