Krishnan **Raghavan**

Assistant Computational Mathematician

Mathematics and Computer Science, Argonne National Laboratory, Lemont, IL.

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Summary

My primary research agenda is to develop a mathematical characterization of machine learning (ML) models, their learning/training behavior and the associated precision achieved by them. Towards this end, I study the two broad facets of ML: theory; through the eyes of tools from systems theory, statistics and optimization; and applied; by building AI/ML models to solve key problems in nuclear physics, material science, HPC and more recently climate. I have a strong publication record in the field of ML, HPC and scientific applications with a total of 51 publications. I also have a significant track record of grants and have been involved in 23 grant proposals, many of them multi-institutional. I also have substantial experience in successfully soliciting and managing multi-million dollar multi-institutional proposals as an institutional PI.

Education

Jan '15 – May '19 | Ph.D., Computer Engineering, Missouri University of Science & Technology, Rolla, MO.
- Dissertation: *Deep Neural Network Learning-based Classifier Design for Big-data Analytics*
- Advisor: Prof. Jagannathan Sarangapani.

Aug '12 – Dec '14 | M.S., Computer Engineering, Missouri University of Science & Technology, Rolla, MO.
- Thesis: *Computer Vision Libraries for Trailer Truck Test Bed*
- Advisor: Prof. Levent Acar.

Sep '08 – Jul '12 | B.E., Instrumentation and Control, V.E.S. Institute of Technology (VESIT), University of Mumbai, India.
- Thesis: *Modbus Protocol Implementation with ARM7*
- Advisor: Prof. Deepthi Khimani.

Work Experience

Jun '22 – Present | Assistant Computational Mathematician, Mathematics and Computer Science (MCS), Argonne National Laboratory, Lemont, IL.
- Supervisor: Dr. Sven Leyffer.

Sep '19 – Jun '22 | Postdoctoral Appointee, Mathematics and Computer Science (MCS), Argonne National Laboratory, Lemont, IL.
- Supervisor: Dr. Prasanna Balaprakash.

Sep '13 – May '19 | Graduate Research Assistant, Electrical and Computer Engineering, Missouri University of Science & Technology, Rolla, MO.

Grants and Proposals

Current

5. $3M, **Thrust Co-Lead**, DOE ASCR, Privacy Preserving Federated Learning, *09/24-08/27*.
4. $1.88M, **Senior Personnel**, DOE ASCR, Energy Efficient Computing: A Holistic Methodology, *09/24-08/28*.
3. $37.50M, **Senior Personnel**, DOE ASCR, SciDAC-5 Rapids3 Institute, *10/24-09/29*.

2. $8.75M ($1.875M), **Institutional PI**, DOE ASCR, Exploring the Power of Distributed Intelligence for Resilient Scientific Workflows, *07/23-06/28*.

1. $13M ($0.525M), **Thrust Lead**, DOE ASCR, SciDAC-5 Nuclear Computational Low Energy Initiative (NUCLEI), *10/22-09/27*.

Successfully Completed

4. $28.75M, **Senior Personnel**, DOE ASCR, SciDAC-5 Rapids2 Institute, 10/22-09/25.

3. $3.75M ($1.050M), **Institutional PI**, DOE ASCR, Platform for Explainable Distributed Infrastructure (PosEiDon), 10/21-09/24.

2. $25k, **PI**, Argonne National Laboratory Directed Research and Development, Accelerating inversion of nuclear responses with uncertainty quantification, 2021.

1. $2.10M, **Co-PI**, Argonne National Laboratory Directed Research and Development, Nuclear Quantum Monte Carlo methods for ML and AI techniques, 10/20-09/23.

Unfunded

14. $2.75M, PI, DOE ASCR, Coordinate Locally, Learning Globally and Evolve Smartly: A Distributed Approach, 09/25-08/30.

13. $2.75M, Senior Personnel, DOE NP, The ATLAS AI Upgrade - Leveraging Large Language Models and Machine-Learning Methods to Address Key Operational Challenges at the ATLAS User Facility, 09/25-08/28.

12. Institutional PI, DOE FES, Machine Learning for Advanced Diagnostics and Accelerated Plasma Turbulence Simulations (ML-ADAPTS), 07/23-06/26.

11. Co-PI, DOE SC, Machine Learning Methods for Active target detectors at ATLAS, 09/23-08/25.

10. Senior Personnel, DOE ASCR, Randomized Algorithms for Continually-Learning Higher-Order Graph Neural Networks, 10/22-09/25.

9. Senior Personnel, DOE HEP, Advancing Uncertainty Quantification and Interpretability of AI models in HEP, 10/22-09/25.

8. Co-PI, DOE, Batch Error-driven learning for Accelerating Scientific ML, 2021.

7. Co-PI, DOE, Federated Neural Architecture Search for Privacy-Preserving AI/ML, 2021.

6. Co-PI, Argonne National Laboratory Directed Research and Development, Hybrid Mixed Integer Programming - Deep Reinforcement Learning Framework for Systematic Process Intensification, 2021.

5. Co-PI, Argonne National Laboratory Directed Research and Development, A Hybrid Approach for Interpretable Modeling of Spatiotemporal Data, 2021.

4. PI, Argonne National Laboratory Directed Research and Development, Continual Domain-adaptation for Simulation Calibration, 2021.

3. Senior Personnel, DOE ASCR, FAIR Automated Machine Learning for Scientific Data, 2020.

2. Senior Personnel, DOE SC, Machine Learning Methods for Nuclear Physics Detectors, 2020.

1. Co-PI, Argonne National Laboratory Directed Research and Development, Machine Learning-based Design Optimizer for Molten Salt Reactor, 2020.

Publications

Journal Articles

[J14] Prasanna Balaprakash, **Krishnan Raghavan**, Franck Cappello, Ewa Deelman, Anirban Mandal, Hongwei Jin, Imtiaz Mahmud, Komal Thareja, Shixun Wu, Pawel Zuk, et al. SWARM: Reimagining Scientific Workflow Management Systems in a Distributed World. In: **The International Journal of High Performance Computing Applications** (2025), p. 10943420251339317.

[J13] **Krishnan Raghavan**, George Papadimitriou, Hongwei Jin, Anirban Mandal, Mariam Kiran, Prasanna Balaprakash, and Ewa Deelman. Advancing Anomaly Detection in Computational Workflows with Active Learning. In: **Future Generation Computer Systems** 166 (2025), p. 107608.

[J12] **Krishnan Raghavan**, Melina L. Avila, Prasanna Balaprakash, Heshani Jayatissa, and Daniel Santiago-Gonzalez. Classification of Events from α-Induced Reactions in the MUSIC Detector via Statistical and ML Methods. In: **Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment** 1058 (2024), p. 168786.

[J11] **Krishnan Raghavan** and Alessandro Lovato. Uncertainty-Quantification-Enabled Inversion of Nuclear Responses. In: **Physical Review C** 110.2 (2024), p. 025504.

[J10] **Krishnan Raghavan**, Vignesh Narayanan, and Sarangapani Jagannathan. Cooperative Deep Q-Learning Framework for Environments Providing Image Feedback. In: **IEEE Transactions on Neural Networks and Learning Systems** 35.7 (2024), pp. 9549–9558.

[J9] Orcun Yildiz, **Krishnan Raghavan**, Henry Chan, Mathew J. Cherukara, Prasanna Balaprakash, Subramanian Sankaranarayanan, and Tom Peterka. Automated Defect Identification in Coherent Diffraction Imaging with Smart Continual Learning. In: **Neural Computing and Applications** 36.35 (2024), pp. 22335–22346.

[J8] Hongwei Jin, **Krishnan Raghavan**, George Papadimitriou, Cong Wang, Anirban Mandal, Mariam Kiran, Ewa Deelman, and Prasanna Balaprakash. Graph Neural Networks for Detecting Anomalies in Scientific Workflows. In: **The International Journal of High Performance Computing Applications** 37.3-4 (2023), pp. 394–411.

[J7] Romit Maulik, Romain Egele, **Krishnan Raghavan**, and Prasanna Balaprakash. Quantifying Uncertainty for Deep Learning Based Forecasting and Flow-Reconstruction Using Neural Architecture Search Ensembles. In: **Physica D: Nonlinear Phenomena** 454 (2023), p. 133852.

[J6] **Krishnan Raghavan**, Sarangapani Jagannathan, and V. A. Samaranayake. A Game Theoretic Approach for Addressing Domain-Shift in Big-Data. In: **IEEE Transactions on Big Data** 8.6 (2022), pp. 1610–1621.

[J5] **Krishnan Raghavan**, Prasanna Balaprakash, Alessandro Lovato, Noemi Rocco, and Stefan M. Wild. Machine-Learning-Based Inversion of Nuclear Responses. In: **Physical Review C** 103.3 (2021), p. 035502.

[J4] **Krishnan Raghavan**, Shweta Garg, Sarangapani Jagannathan, and V. A. Samaranayake. Distributed Min–Max Learning Scheme for Neural Networks with Applications to High-Dimensional Classification. In: **IEEE Transactions on Neural Networks and Learning Systems** 32.10 (2021), pp. 4323–4333.

[J3] **Krishnan Raghavan**, Sarangapani Jagannathan, and V. A. Samaranayake. Direct Error-Driven Learning for Deep Neural Networks with Applications to Big Data. In: **IEEE Transactions on Neural Networks and Learning Systems** 31.5 (2020), pp. 1763–1770.

[J2] **Krishnan Raghavan**, V. A. Samaranayake, and Sarangapani Jagannathan. A Hierarchical Dimension Reduction Approach for Big Data with Application to Fault Diagnostics. In: **Big Data Research** 18 (2019), p. 100121.

[J1] **Krishnan Raghavan**, V. A. Samaranayake, and Sarangapani Jagannathan. A Multi-Step Nonlinear Dimension-Reduction Approach with Applications to Big Data. In: **IEEE Transactions on Knowledge and Data Engineering** 31.12 (2019), pp. 2249–2261.

Conference Proceedings

[C21] Komal Thareja, **Krishnan Raghavan**, Anirban Mandal, and Ewa Deelman. Bridging Speed and Optimality in Job Scheduling: A Hybrid Ant Colony Optimization Approach for Distributed Systems. In: **Proceedings of the SC '25 Workshops of the International Conference for High Performance Computing, Networking, Storage and Analysis**. ACM. 2025.

[C20] Komal Thareja, **Krishnan Raghavan**, Anirban Mandal, Pawel Zuk, Imtiaz Mahmud, Mariam Kiran, and Ewa Deelman. A Greedy Consensus-Based Approach to Distributed Job Selection: Toward Fully-Decentralized Workload Management System. In: **2025 IEEE 25th International Symposium on Cluster, Cloud and Internet Computing (CCGrid)**. IEEE. 2025, pp. 63–72.

[C19] Hongwei Jin, George Papadimitriou, **Krishnan Raghavan**, Pawel Zuk, Prasanna Balaprakash, Cong Wang, Anirban Mandal, and Ewa Deelman. Large Language Models for Anomaly Detection in Computational Workflows: From Supervised Fine-Tuning to In-Context Learning. In: **SC24: International Conference for High Performance Computing, Networking, Storage and Analysis**. IEEE Computer Society. 2024, pp. 1466–1482.

[C18] Kibaek Kim, **Krishnan Raghavan**, Olivera Kotevska, Matthieu Dorier, Ravi Madduri, Minseok Ryu, Todd Munson, Rob Ross, Thomas Flynn, Ai Kagawa, et al. Privacy-Preserving Federated Learning for Science: Challenges and Research Directions. In: **2024 IEEE International Conference on Big Data (BigData)**. IEEE. 2024, pp. 7849–7853.

[C17] Charles Macal, Abby Stevens, Sara Rimer, Jonathan Ozik, Melissa Adrian, and **Krishnan Raghavan**. Agent-Based Modeling of Communities for Understanding Equity Effects of Climate Change. In: **AGU Fall Meeting Abstracts**. Vol. 2024. 167. 2024, GC33D–0167.

[C16] Imtiaz Mahmud, Pawel Zuk, Cong Wang, Mariam Kiran, Kesheng Wu, Komal Thareja, **Krishnan Raghavan**, Anirban Mandal, and Ewa Deelman. DISTRI: Development and Integration of Simulation Tools for Resilient Infrastructure. In: **2024 IEEE International Conference on Big Data (BigData)**. IEEE. 2024, pp. 4167–4177.

[C15] Abby Stevens, Melissa Adrian, **Krishnan Raghavan**, Jonathan Ozik, and Charles Macal. A Lightweight Decision Support Framework for Community Climate Resilience in Chicago. In: **AGU Fall Meeting Abstracts**. Vol. 2024. 2024, GC41A–03.

[C14] Manisha Garg, Tyler H. Chang, and **Krishnan Raghavan**. SF-SFD: Stochastic Optimization of Fourier Coefficients to Generate Space-Filling Designs. In: **2023 Winter Simulation Conference (WSC)**. IEEE. 2023, pp. 3636–3646.

[C13] Jan Hückelheim, Tadbhagya Kumar, **Krishnan Raghavan**, and Pinaki Pal. Forward Gradients for Data-Driven CFD Wall Modeling. In: **NeurIPS Machine Learning and the Physical Sciences Workshop**. 2023.

[C12] Daniel Santiago-Gonzalez, Melina Avila, Prasanna Balaprakash, Heshani Jayatissa, **Krishnan Raghavan**, and Nathan Callahan. CARIBU-matic and the MUSIC ML Project: Examples of Machine-Learning Applications for Beam Tuning and Experimental Data Analysis/Classification. In: **APS Meeting Abstracts**. 2023, pp. L08–004.

[C11] Romain Egele, Romit Maulik, **Krishnan Raghavan**, Bethany Lusch, Isabelle Guyon, and Prasanna Balaprakash. AutoDEUQ: Automated Deep Ensemble with Uncertainty Quantification. In: **2022 26th International Conference on Pattern Recognition (ICPR)**. IEEE. 2022, pp. 1908–1914.

[C10] Hongwei Jin, **Krishnan Raghavan**, George Papadimitriou, Cong Wang, Anirban Mandal, Patrycja Krawczuk, Loïc Pottier, Mariam Kiran, Ewa Deelman, and Prasanna Balaprakash. Workflow Anomaly Detection with Graph Neural Networks. In: **2022 IEEE/ACM Workshop on Workflows in Support of Large-Scale Science (WORKS)**. IEEE. 2022, pp. 35–42.

[C9] **Krishnan Raghavan** and Prasanna Balaprakash. Continual Learning via Dynamic Programming. In: **2022 26th International Conference on Pattern Recognition (ICPR)**. IEEE. 2022, pp. 1350–1356.

[C8] Orcun Yildiz, Henry Chan, **Krishnan Raghavan**, William Judge, Mathew J. Cherukara, Prasanna Balaprakash, Subramanian Sankaranarayanan, and Tom Peterka. Automated Continual Learning of Defect Identification in Coherent Diffraction Imaging. In: **2022 IEEE/ACM International Workshop on Artificial Intelligence and Machine Learning for Scientific Applications (AI4S)**. IEEE. 2022, pp. 1–6.

[C7] **Krishnan Raghavan** and Prasanna Balaprakash. Formalizing the Generalization-Forgetting Trade-Off in Continual Learning. In: **Advances in Neural Information Processing Systems**. Vol. 34. 2021, pp. 17284–17297.

[C6] Rohollah Moghadam, Pappa Natarajan, **Krishnan Raghavan**, and Sarangapani Jagannathan. Online Optimal Adaptive Control of a Class of Uncertain Nonlinear Discrete-Time Systems. In: **2020 International Joint Conference on Neural Networks (IJCNN)**. IEEE. 2020, pp. 1–6.

[C5] Shweta Garg, **Krishnan Raghavan**, Sarangapani Jagannathan, and V. A. Samaranayake. Distributed Learning of Deep Sparse Neural Networks for High-Dimensional Classification. In: **2018 IEEE International Conference on Big Data (Big Data)**. IEEE. 2018, pp. 1587–1592.

[C4] **Krishnan Raghavan**, Sarangapani Jagannathan, and V. A. Samaranayake. A Minimax Approach for Classification with Big-Data. In: **2018 IEEE International Conference on Big Data (Big Data)**. IEEE. 2018, pp. 1437–1444.

[C3] **Krishnan Raghavan**, Sarangapani Jagannathan, and V. A. Samaranayake. Direct Error Driven Learning for Deep Neural Networks with Applications to Bigdata. In: **International Conference on Big Data and Deep Learning (INNS)**. Vol. 144. Elsevier, 2018, pp. 89–95.

[C2] **Krishnan Raghavan**, Sarangapani Jagannathan, and V. A. Samaranayake. Deep Learning Inspired Prognostics Scheme for Applications Generating Big Data. In: **2017 International Joint Conference on Neural Networks (IJCNN)**. IEEE. 2017, pp. 3296–3302.

[C1] **Krishnan Raghavan** and Sarangapani Jagannathan. Hierarchical Mahalanobis Distance Clustering Based Technique for Prognostics in Applications Generating Big Data. In: **2015 IEEE Symposium Series on Computational Intelligence**. IEEE. 2015, pp. 516–521.

Manuscripts

[P10] Karen Medlin, Sven Leyffer, and **Krishnan Raghavan**. Sampling Imbalanced Data with Multi-Objective Bilevel Optimization. 2025.

[P9] Ganesh Sivaraman, Nicholas Jackson, and **Krishnan Raghavan**. LifeLong Learning for Large Language Models in Predicting Chemical Reaction Yields. 2025.

[P8] Chih-Hsuan Yang, Tanwi Mallick, Le Chen, **Krishnan Raghavan**, Azton Wells, Amal Gueroudji, Ian T. Foster, and Rajeev Thakur. Who Gets the Reward, Who Gets the Blame? Evaluation-Aligned Training Signals for Multi-LLM Agents. 2025.

[P7] Supriyo Chakraborty and **Krishnan Raghavan**. On Understanding of the Dynamics of Model Capacity in Continual Learning. 2024.

[P6] Karen Medlin, Sven Leyffer, and **Krishnan Raghavan**. A Bilevel Optimization Framework for Imbalanced Data Classification. 2024.

[P5] Shixun Wu, **Krishnan Raghavan**, Sheng Di, Zizhong Chen, and Franck Cappello. DGRO: Diameter-Guided Ring Optimization for Integrated Research Infrastructure Membership. 2024.

[P4] Hongwei Jin, **Krishnan Raghavan**, George Papadimitriou, Cong Wang, Anirban Mandal, Ewa Deelman, and Prasanna Balaprakash. Self-Supervised Learning for Anomaly Detection in Computational Workflows. 2023.

[P3] George Papadimitriou, Hongwei Jin, Cong Wang, Rajiv Mayani, **Krishnan Raghavan**, Anirban Mandal, Prasanna Balaprakash, and Ewa Deelman. Flow-Bench: A Dataset for Computational Workflow Anomaly Detection. 2023.

[P2] **Krishnan Raghavan** and Prasanna Balaprakash. Learning Continually on a Sequence of Graphs – The Dynamical System Way. 2023.

[P1] **Krishnan Raghavan**, Vignesh Narayanan, and Sarangapani Jagannathan. Learning to Control Using Image Feedback. 2021.

Thesis, Book Chapters and Technical Reports

[M9] Imtiaz Mahmud, George Papadimitriou, Cong Wang, Hongwei Jin, Komal Thareja, Pawel Zuk, **Krishnan Raghavan**, Rajiv Mayani, Prasanna Balaprakash, Mariam Kiran, et al. RADT Scripts for Network Research. In: 2024.

[M8] George Papadimitriou, Hongwei Jin, Cong Wang, **Krishnan Raghavan**, Imtiaz Mahmud, Komal Thareja, Pawel Zuk, Rajiv Mayani, Prasanna Balaprakash, Mariam Kiran, et al. FlowBench Raw Data Archive. In: 2024.

[M7] Francieli Boito, Jim Brandt, Valeria Cardellini, Philip Carns, Florina M. Ciorba, Hilary Egan, Ahmed Eleliemy, Ann Gentile, Thomas Gruber, Jeff Hanson, et al. Autonomy Loops for Monitoring, Operational Data Analytics, Feedback, and Response in HPC Operations. In: **2023 IEEE International Conference on Cluster Computing Workshops (CLUSTER Workshops)**. 2023, pp. 37–43.

[M6] Yixuan Sun, **Krishnan Raghavan**, and Prasanna Balaprakash. Introduction to Reinforcement Learning. In: **Methods and Applications of Autonomous Experimentation**. Chapman and Hall/CRC, 2023, pp. 152–174.

[M5] Venkat Vishwanath, Murali Emani, Varuni Sastry, William Arnold, Rajeev Thakur, Valerie Taylor, Ian Foster, Salman Habib, Michael E. Papka, Bryce Allen, et al. 2023 AI Testbed Expeditions Report. In: 2023.

[M4] Rohollah Moghadam, Sarangapani Jagannathan, Vignesh Narayanan, and **Krishnan Raghavan**. Optimal Adaptive Control of Partially Uncertain Linear Continuous-Time Systems with State Delay. In: **Handbook of Reinforcement Learning and Control**. Springer International Publishing, 2021, pp. 243–272.

[M3] **Krishnan Raghavan**, Sarangapani Jagannathan, and V. A. Samaranayake. Direct Error Driven Learning for Classification in Applications Generating Big-Data. In: **Development and Analysis of Deep Learning Architectures**. Springer International Publishing, 2020, pp. 1–29.

[M2] **Krishnan Raghavan**. Deep Neural Network Learning-Based Classifier Design for Big-Data Analytics. In: Ph.D. Dissertation. 2019.

[M1] **Krishnan Raghavan**. Computer Vision Libraries for Trailer Truck Testbed Using Open Source Computer Vision Libraries. In: M.S. Thesis. 2014.

Invited Talks and Lectures

13. Looking at continual learning through a dynamical system point of view, AI Institute, University of South Carolina, March 2024.
12. Continual Learning – a Theoretical Primer, University of Pennsylvania, February 2024.
11. A Dynamical System View of Continual Learning, Department of Mechanical Engineering, Brown University, April 2023.
10. Continuously Detecting Workflow Anomalies using Graph Neural Networks – Lessons Learnt, Dagstuhl Seminar on Future perspectives in continuous monitoring of HPC systems, Schloss Dagstuhl, April 2023.
9. Continual learning for adapting digital twins to modifying environments, Artificial Intelligence for Robust Engineering & Science, Oak Ridge National Laboratory, April 2023.
8. Advanced Mathematical Tools and Applications, PK Honorarium lecture, Madras Institute of Technology, February 2023.
7. Model Parallelization in Deep Neural Networks, Split-learning Workshop, Massachusetts Institute of Technology, February 2021.
6. Machine Learning-based Inversion of Nuclear Responses, Advances in Many Body Theories: From First Principle Methods to Quantum Computing and Machine Learning, November 2020.
5. Generalization As a Tool to Understanding Neural Network Optimization, Keynote Lecture, Madras Institute of Technology, April 2020.
4. Introduction to Generalization, Guest Lecture on Adaptive Dynamic Programming at S & T, March 2020.
3. Distributed Learning with Deep Neural Networks, Washington University in St. Louis, March 2019.
2. Learning to Generalize through Deep Neural Network, Qualcomm AI Research in San Diego, July 2019.
1. Deep Learning-based Classifier Design, Argonne National Laboratory, July 2019.

Conference and Workshop Presentations

25. On the Dynamics of Neural Network Capacity, Machine Learning and Dynamical Systems, International Conference on Continuous Optimization, July 2025.
24. On the Dynamics of Neural Network Capacity, Machine Learning and Dynamical Systems, SIAM Dynamical Systems, May 2025.
23. The Effect of Uncertainty on Learning Dynamics of Neural Networks, SIAM-Computational Science and Engineering, February 2025.
22. Actively Generating Data to train better, SIAM conference on Mathematics and Data Science, February 2024.
21. The Effect of Uncertainty on Learning to Extract Response Functions, Nuclei PI meeting, May 2024.
20. Continual learning for adapting digital twins to modifying environments, SIAM conference on Parallel Processing, February 2024.
19. Learning on a small amount of data, Nuclei PI meeting, July 2023.
18. Continual Learning for Coherent Diffraction Imaging, Scientific Deep Learning, at the 17th U. S. National Congress on Computational Mechanics, July 2023.
17. The Pitfalls of Backpropagation – Some Perspectives and Alternatives, Forward Alternatives to Back-Propagation in ML and Science, SIAM-CSE, February 2023.
16. Learning as a Dynamical System, Laboratory for Applied Mathematics, Numerical Software, and Statistics Seminar, November 2021.
15. Meta-continual Learning via Dynamic Programming, Train Once Use Forever: Transferable Deep Models for Accelerating Scientific Computing Mini-symposium in SIAM Computational Science and Engineering, February 2021.

14. Machine Learning-based Inversion of Nuclear Responses, SciDAC-Nuclei Meeting, April 2021.
13. Machine Learning-based Inversion of Nuclear Responses, Advances in Many Body Theories: From First Principle Methods to Quantum Computing and Machine Learning, November 2020.
12. Distributed Learning of Deep Sparse Neural Networks for High-dimensional Classification, IEEE Conference on Big Data, December 2018.
11. A Minimax Approach for Classification with Big-data, IEEE Conference on Big Data, December 2018.
10. Mitigating Heterogeneity and Data-noise of Big-data using Deep Neural Network Learning based Analytics, Intelligent Systems Center, S&T, September 2018.
9. A Multi-step Nonlinear Dimension-reduction Approach with Applications to Big-data, International Neural Network Society's Conference on Big-data and Deep Learning, March 2018.
8. Direct Error-driven Learning for Deep Neural Networks with Applications to Big-data, International Neural Network Society's Conference on Big-data and Deep Learning, March 2018.
7. A Minimax Approach for Classification with Applications to Big-data, Intelligent Systems Center, S&T, February 2018.
6. A Direct Error-Driven Learning Approach with Applications to Big-data, Intelligent Systems Center, S&T, September 2017.
5. Deep Learning Inspired Prognostics Using Big-data, Intelligent Maintenance Systems Center – Industry Advisory Board Meeting, May 2017.
4. Introduction to Neural Networks, Lecture for EE 5320: Neural Networks Control and Application, Missouri University of Science and Technology (MST), Rolla, March 2017.
3. Camera as a Sensor for Asset Management, Intelligent Maintenance Systems Center – Industry Advisory Board Meeting, March 2017.
2. A Nonlinear Hierarchical Dimension Reduction Approach for Diagnostics in Big-data Generating Applications, Intelligent Maintenance Systems Center – Industry Advisory Board Meeting, September 2016.
1. Hierarchical Mahalanobis Distance Clustering Based Technique for Prognostics in Applications Generating Big-data, IEEE Symposium Series on Computational Intelligence, December 2015.

Posters

7. Learning continually on a sequence of tasks, Workshop on Machine Learning and Dynamical Systems, Field Institute, Toronto, July 2024.
6. Continual learning- Robust learning on streaming tasks, Scientific Discovery (SciDAC) PI Meeting, July 2024.
5. Forward Gradients for Data-Driven CFD Wall Modeling, Neural Information Processing Systems, December 2023.
4. Formalizing the Generalization-Forgetting Tradeoff in Continual Learning, Neural Information Processing Systems, December 2021.
3. Learning as a Dynamical System, Postdoctoral Symposium, Argonne National Laboratory, November 2021.
2. Game Theory for Generalization in Machine Learning, Midwest Workshop on Control and Game Theory, Washington University at St. Louis, April 2019.
1. Deep Learning Inspired Prognostics Scheme for Applications Generating Big-data, IEEE International Joint Conference on Neural Networks, May 2015.

Professional Service

Organizing

- Special Session, International Joint Conference on Neural Networks, 2025 (with Dr. Vignesh Narayanan, Dr. Hao Xu, Dr. Avimanyu Sahoo)
- MiniSymposium, SIAM Mathematics of Data Science, 2024 (with Dr. Vignesh Narayanan)
- Panel, DOE SciDAC PI Meeting, 2024 (with Dr. Cody Balos)
- Physics Colloquium Committee Member, Argonne National Laboratory, 2024

Reviewing – Panels

- NSF PANEL number: EPCN P212071
- NSF PANEL number: EPCN P222343

Reviewing – Journals

- IEEE Transactions on Systems, Man and Cybernetics
- IEEE Transactions on Knowledge and Data Engineering
- IEEE Transactions on Neural Networks and Learning Systems
- Neural Computing and Applications
- Artificial Intelligence Review

Reviewing – Conferences

- Neural Information Processing Systems (NeurIPS)
- International Conference on Machine Learning (ICML)
- International Conference on Learning Representations (ICLR)
- International Joint Conference on Neural Networks (IJCNN)
- Super Computing Conference (SC)
- International Conference on Parallel Processing (ICPP)
- International Conference on Control, Automation, Robotics and Vision (ICARCV)
- Parallel AI and Systems for the Edge (PAISE)

Mentoring

Current

Assistant Scientist

- **Hongwei Jin**, Mathematics and Computer Science, Argonne National Laboratory, *Agentic AI.*

Post-docs

- **Allyson Hahn**, External Collaborator, *Enabling neural architecture search and hyper-parameter search in continual learning.* (external collaborator)

Ph.D. Students

- **Protik Nag**, Research Aid, *Continual Learning for Large Language Models.*

Thesis Committees

- **Prachi Jadhav**, PhD Student, University of Tennessee Knoxville, *Agentic AI for HPC Resource Management.*
- **Protik Nag**, PhD Student, AI Institute, University of South Carolina, *The effect of Task Ordering on Continual Learning.*
- **Karen Medlin**, PhD Student, University of North Carolina - Charlotte, *Addressing the Challenges of Imbalanced Data.*

Alumni

Past Post-doctoral Researchers

- **Hongwei Jin**, Mathematics and Computer Science, Argonne National Laboratory, *Graph Neural Networks.*

Past Ph.D. Students

- **Karen Medlin**, NSF-MSGI Fellow, University of North Carolina - Charlotte, *Analyzing Imbalanced-data using MCMC.*

Summer Students

- **Yuxin Zi**, Givens Fellow, *Continual Molecular Property Prediction.*
- **Haoyang Zheng**, Givens Fellow, *Thompson Sampling to Improve Sample Efficiency of Proximal Policy Gradients.*
- **Himali Kalanchige**, NSF-MSGI Fellow, *Analyzing Imbalanced-data with Neural Networks.*
- **Phanindra Raja Chava**, BS, *Indoor Localization using Bluetooth Low Energy.*
- **Shweta Garg**, BS, *Parallelized Implementation of Deep Neural Networks in Tensorflow and Python.*
- **Shameeya Airhart**, High School (ACT-SO), *Using Machine Learning to predict retention time of a molecule.*
- **Taree Evans**, High School (ACT-SO), *Is there a correlation between gut microbiota and acute stress?.*