Kishansingh [Kishan] Rajput

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Newport News, VA
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PROFESSIONAL APPOINTMENTS

Staff Computer Scientist II Jul 2020 - Present
Thomas Jefferson National Accelerator Facility, Newport News, VA

- **PI:** Multi-objective optimization of heat load and trip rate using reinforcement learning at Jefferson Lab's Continuous Electron Beam Accelerator Facility (CEBAF)
  - Funding Agency: Jefferson Lab Directed Research and Development
  - Funding Amount: $250K
  - Project Timeline: Oct 2021 - Sept 2022
  - Mentorship: Mentored a graduate student on development of Machine Learning optimization methods
  - Developed genetic algorithm and reinforcement learning based optimization methods
  - Multi-objective optimization shown significant reduction in Heat Load in CEBAF via simulation
- **JLab PI:** Towards Self-driving NP Scientific User Facilities through an AI-based Controls Framework
  - Funding Agency: Office of Science, Department of Energy
  - Funding Amount: $2M (JLab $675K)
  - Project Timeline: Feb 2026 - Aug 2027
  - Software and Algorithmic development for ML-based optimization/control and integration with system models (to enable hybrid use of Bayesian optimization, deep reinforcement learning, and model predictive control).
- **JLab PI:** Hardware Aware Artificial Intelligence for High Energy Physics Facilities
  - Funding Agency: Office of Science, Department of Energy
  - Funding Amount: $2M (JLab $500K)
  - Project Timeline: Sept 2025 - Aug 2027
  - Continual Learning for surrogate models, digital twins, optimization and control algorithms for HEP leveraging unique hardware features.
- **JLab PI:** Digital-Twin-based autonomous control of BNL's hadron accelerator chain
  - Funding Agency: Office of Science, Department of Energy
  - Funding Amount: $3M (Jlab $650K)
  - Project Timeline: Sept 2025 - Aug 2027
  - Digital Twin, and control system development for autonomous control of accelerator.
- **Team Co-lead**: Mathematics and Algorithm Development group for Nuclear Femtography Inference at Exascale Platforms
  - Funding Agency: Department of Energy (DOE), Scientific Discoveries through Advance Computing (SciDAC), Advance Scientific Computing Research
  - Funding Amount: $6.5 Millions

  - Project Timeline: Oct 2022 - Sept 2024
  - Leading a team of computer scientists and data scientists from Jefferson lab, Argonne National lab, Virginia Tech, and Old Dominion University
  - Developing novel Machine Learning algorithms to solve the inverse problem posed by join experimental-theoretical analysis of nuclear physics data
- **Project Lead**: Machine Learning assisted charged particle tracking using graph neural networks at GlueX, and Future TDIS experiments at Jefferson Lab
  - Funding Agency: Jefferson Lab Nuclear Physics Operations
  - Funding Amount: $150K per year
  - Project Timeline: Jan 2023 - Present
  - Mentorship: Mentoring a data science postdoc, and a physics graduate student from College of William and Mary, Williamsburg, VA
  - Deploying Graph Neural Network tracking models on edge hardware (GPUs and Field Programmable Gate Arrays -FPGA) for real time inference on tracking data, estimated to significantly speed up physics analyses
  - Developing a modular toolkit that will be made open source aimed to be leveraged at upcoming Electron Ion Collider experiments at Brookhaven National Laboratory
- **JLab PI and Use-case lead:** Machine Learning for Improving Accelerator and Target Performance at Spallation Neutron Source (SNS) accelerator, Oak Ridge National Lab
  - Funding Agency: Department of Energy (DOE), Office of Science, Basic Energy Science
  - Funding Amount: $2.4M (JLab $400K)
  - Project Timeline: Sept 2023 - Aug 2026
  - Mentorship: Mentored two postdocs working on deep learning models for accelerator fault prediction and detection of equipment degradation. Mentored two graduate students on machine learning models. Currently mentoring junior staff working on reinforcement learning algorithms for accelerator beam loss minimization.
  - Leading a team of data scientists, accelerator physicists, accelerator technicians and operators to develop novel machine learning models for preemptive fault prediction in particle accelerators
  - Developed novel uncertainty quantification models for errant beam prediction
  - Developed a modular and generalizable errant beam prediction toolkit used by SNS accelerator at Oak Ridge National Laboratory to preemptively abort beam to avoid equipment damage
  - Developing novel continual learning methods for model adaptation methods to handle drifts in the accelerator data
- **Developer**: Optimization and Control Framework applied to Next Generation Compact SRF Accelerators For Industrial Applications
  - Funding Agency: Department of Energy (DOE), Office of Science, Accelerate Initiative
  - Funding Amount: $700K
  - Project Timeline: Oct 2023 - Sept 2025
  - Developing a production level diagnostics and control toolkit for compact particle accelerator used for industrial applications

- **Lead Developer**: Free Electron Laser tuning using reinforcement learning agents at Linac Coherent Light Source, SLAC National Accelerator Laboratory
  - Funding Agency: Data Science Department Operations, Jefferson Lab
  - Funding Amount: $80K
  - Project Timeline: Oct 2023 - Sept 2024
  - Developed Twin-Delayed Deep Deterministic Policy Gradient (TD3) agents for automated tuning of free electron laser
- **Advisor**: AI for Experimental Control; To enable automated detector control at GlueX experiment in Hall-D of Jefferson lab using AI
  - Funding Agency: Department of Energy (DOE), Office of Science - Nuclear Physics
  - Project Timeline: Oct 2020 - Sept 2022
- **Project Lead:** Adaptive Machine Learning Driven Uncertainty Aware Digital Twins for DIII-D National Fusion Facility
  - Project Timeline: Oct 2024 - Sept 2025
  - Developing novel adaptive training strategies for deep learning models used in data-driven digital twins
  - Developing a generalized framework to produce advance deep learning based uncertainty aware digital twin capable to adapt on drifting data
- **Lead Developer**: Machine Learning assisted Particle Identification in SoLID experiment at Jefferson Lab
- **Developer:** Novel Generative Reinforcement Learning for Ill-posed Optimization and Control Problems
- **Developer:** Uncertainty quantification for machine learning based surrogate model of Fermi National Accelerator Laboratory booster complex
  - Developed novel methods to quantify uncertainties in machine learning model outputs to increase trust in AI
  - Demonstrated accurate out-of-distribution uncertainties on model predictions
- **Advisor/Developer**: Real Time Data Quality Monitoring with Artificial Intelligence at Jefferson Lab
  - Enhanced ML models with Explainable AI approach - Layer-wise Relevance Propagation (LRP), and GradCAM to map regions of detector occupancy that may be causing anomalies in the data
- Mentoring young scientists, postdocs, and students at Jefferson Lab

Data Analytics Specialist May 2019 - Aug 2019
Shell, Houston, TX

- Supported well engineers' team to develop production level solutions for problems associated with drilling with statistics, data visualization and Machine Learning
- Improved detection/visualization of over/under gauge in oil well drilling and established correlation with other well logs to find potential cause and effects, which has potential to save millions of dollars
- Developed a novel deep learning architecture to detect surface formation transitions in earth crust using gamma ray signal logs
- Developed Encryption Agent to improve user experience by integrating systems running on different platforms/servers.

Graduate Research Assistant Aug 2018 - June 2020
University of Houston, Houston, TX

- Machine Assisted Human Development Lab (Advisor: Dr. Ryan Kennedy)
  - Improved Recommender system for individual forecasting problems (IFP) using Python and R programming languages.
- Data Visualization and Modeling Group (Advisor: Dr. Guoning Chen)
  - Developed a novel probabilistic envelope-based visualization and anomaly detection technique for time series data.
  - Devised visual analytical Framework on the novel visualization technique for anomaly detection in oil well drilling and detection of damages in oil wells.
  - The developed system is currently being used in practice providing assistance to well engineers.
  - Evaluated the time series data analysis technique DTW for the surface formation mapping using gamma ray data for oil well drilling.
- Pattern Analysis Laboratory (Advisor: Dr. Ricardo Vilalta)
  - Developed a framework for Explainable Deep Learning as applied to transfer of knowledge between tasks
  - Teaching Assistant in graduate level Artificial Intelligence class

Software Developer / Data Analyst Aug 2015 - July 2018
Kilkenny Electronics, Ahmedabad, GJ, India

- Reduced operating cost of an educational institute by automating daily tasks including timekeeping, sending notifications, storing and sending grades, generating progress reports, keeping track of leaves and payroll by creating an ERP system using SQL and Java.
- Improved the follow-up process of an educational institute with students by creating an analytical tool to monitor the performance of individual students in exams. Developed an ERP system for the same.
- Mentored freelance developers and interns.

EDUCATION

Doctor of Philosophy (Ph.D.), University of Houston, Houston, TX Jan 2023 - Dec 2026 (expected)
Advisor: Dr. Sen Lin
Thesis: Adaptive Machine Learning for Science and Engineering

Master of Science (M.S.), University of Houston, Houston, TX Aug 2018 - May 2020
Advisor: Dr. Guoning Chen
Thesis: Anomaly Detection and Feature Alignment for Time Series Data
Awards: Outstanding MS Student Award, 2020

Bachelor of Engineering (B.E.), Gujarat Tech. University, Ahmedabad, India Aug 2014 - May 2018

INVITED TALKS AND LECTURES

- **Invited Talk:** ***Explainable and Differential Reinforcement Learning for Multi Objective Optimization in Particle Accelerators*** at Artificial Intelligence for Electron Ion Collider (AI4EIC) 2025, Boston, MA, USA, Oct 2025
- **Invited Talk:** ***Towards continual machine learning for your ever changing accelerator*** at International Beam Instrumentation Conference, Liverpool, UK, Sept 2025

- **Invited Lecture: Multi-objective Reinforcement Learning** at 5th ICFA Beam Dynamics Mini-workshop for Applications of Machine Learning in Particle Accelerators, CERN, Geneva, Switzerland, April 2025
- **Invited Talk:** Harnessing the power of differential simulations for multi-objective optimization in particle accelerators with reinforcement learning 4th Workshop on Applications of Machine Learning in Particle Accelerators 2025
- **Invite Talk: Errant Beam Prognostics with Machine Leaning at SNS Accelerator** at International Conference on the Application of Accelerators in Research and Industry (CAARI), Fort Worth, TX, July-2024
- **Invite Talk: Composable Optimization and Control Toolkit for Scientific Applications** at Software Infrastructure for Advance Nuclear Physics Computing, Newport News, VA, June-2024
- **Invited Talk: Machine Learning for Prognostics and Optimization of Particle Accelerators** at AI and Visualizing Large Dataset Workshop, Princeton University, New Jersey, June 2024
- **Invited Talk: Machine Learning to Improve Accelerator Operation at SNS** at 4th ICFA Beam Dynamics Mini-Workshop on Applications of ML for Particle Accelerators, South Korea, March-2024
- **Invited Tutorial: Machine Learning Model Up-keep and Continual Learning** at 4th ICFA Beam Dynamics Mini-Workshop on Applications of ML for Particle Accelerators, South Korea, March-2024
- **Invited Guest Lecture: Machine Learning for Anomaly Detection in Particle Accelerators** at Old Dominion University Graduate Class in Physics (PHYS 755), Norfolk, VA, Fall 2023
- **Tutorial: Hands on Reinforcement Learning** at 3rd ICFA Beam Dynamics Mini-Workshop on Applications of Machine Learning for Particle Accelerators, Chicago, Nov-2022 (talk)

INTERNATIONAL CONFERENCE/WORKSHOP ORGANIZATION

- **Convener:** AI/ML for Accelerators, AI for EIC workshop 2025
- **Area Chair - Technical Committee:** International Joint Conference on Neural Networks (IJCNN 2025) July 2025, Rome, Italy
- **Scientific Organizing Committee:**
  - 5th ICFA Beam Dynamics Mini-Workshop on Machine Learning for Particle Accelerators held at CERN in Geneva, Switzerland, Apr 2025
  - 4th ICFA Beam Dynamics Mini-Workshop on Applications of ML in Particle Accelerators, Gyeongju-si South Korea, March-2024
  - AI for Robust Engineering and Science, 2023, 2024, and 2025
  - AI4EIC International Hackathon-2022, College of William and Mary, Williamsburg, Virginia, USA
  - Jefferson Lab AI/ML Hackathon, 2021, Thomas Jefferson National Accelerator Facility, Newport News, Virginia, USA
- **Program Chair:**
  - AI for Robust Engineering and Science 2024, Richland, WA, USA, May-2024
- **Session Chair**
  - Field Summaries session, ICFA Beam Dynamics Workshop 2024
  - Assured Digital Twins for Robust Engineering and Science, AIRES 2023

PEER REVIEWS

- **DOE Office of Science:** Accelerator Stewardship and Accelerator Development Comparative Review Panel - [3 proposal reviews FY 2023]
- **DOE Office of Science:** Small Business Innovation Research (SBIR) - [2 proposal reviews, FY23 Phase-1 release 2]
- **DOE Office of Science:** Accelerator Stewardship and Accelerator Development applications Review Panel - [1 proposal review, FY 2024]
- **Conference/Workshop:** NeurIPS Machine Laerning and Physical Science Workshop 2025 - [4 paper reviews]
- **Conference:** 2025 International Joint Conference on Neural Networks (IJCNN 2025): Main track Area Chair [15 meta reviews plus 3 initial reviews]
- **Conference:** 2026 International Joint Conference on Neural Networks (IJCNN 2025): Main track Area Chair
- **Conference:** 27^{th} International Conference on Computing in High Energy and Nuclear Physics (CHEP 2024) [2 paper review]
- **Conference/Workshop:** AAAI 2025 Multi-Agent AI in the Real World Workshop - [3 paper reviews]
- **Conference:** 2nd International Conference on Computer Technology and Information Science - [1 paper review]
- **Conference:** 2026 IEEE International Conference on Acoustics, speed and signal processing – [10 Papers] Area Chair
- **Journal:** Machine Learning: Science and Technology - [3 paper reviews]
- **Journal:** Engineering Research Express - [2 +1 paper reviews]
- **Journal:** Journal of Computational and Cognitive Engineering - [2 paper reviews]
- **Journal:** Journal of Physics A: Mathematical and Theoretical - [1 paper review]
- **Journal:** Journal of Supercomputing - [1 paper review]
- **Journal:** Physical Review Accelerator and Beams - [1 paper review]
- **Journal:** American Journal of Neural Networks and Applications - [1 paper review]

CONFERENCE PRESENTATIONS

- Talk: Towards a Robust Adaptive Digital Twin for Fusion Applications at 67th Annual Meeting of the APS Division of Plasma Physics, San Diego, CA - Nov, 2025
- Talk: Uncertainty Aware Machine Learning Models for Particle Physics Applications at Conference on Computing in High Energy and Nuclear Physics, (CHEP) 2023
- Poster: Uncertainty Aware ML for Particle Accelerators at NeurIPS, ML for Physical Science Workshop - Dec, 2022
- Talk: Uncertainty Aware Machine Learning at 3rd ICFA Beam Dynamics Mini Workshop on ML for Particle Accelerators - Nov, 2022
- Talk: Uncertainty aware anomaly detection to predict errant beam pulses in the SNS accelerator and GradCAM Analysis at Accelerator Reliability Workshop (ARW) - Oct, 2022
- Tutorial: Machine Learning Lifecycle at AI4EIC Workshop 2022

- Flash Talk: Robust Digital Twin for Risk Averse Controller at Artificial Intelligence for Robust Engineering and Science (AIRES), 2022
- Talk: Uncertainty Aware ML-based Models for Accelerator Studies at EIC Software: AI WG Meeting 2022
- Talk: Uncertainty Quantification for Rare Events in Scientific Applications at AI@DOE Roundtable 2022
- Talk: Anomaly detection/Online data quality monitoring at AI4EIC-Exp Workshop, 2021
- Talk: Hydra: Layer-wise Relevance Propagation at Advancing Medical Care through Discoveries in Physical Sciences, 2021

PEER-REVIEWED PUBLICATIONS [REVERSE CHRONOLOGICAL ORDER]

1. Rajput, K., Schram, M., Blokland, W., Zhukov, A., and Lin, S. Continual learning for particle accelerators. In *39th Conference on Neural Information Processing Systems (NeurIPS 2025) Machine Learning for Physical Science Workshop* (12 2025) - [Accepted; to appear]
2. Rajput, K., Lin, S., Schram, M., and Sammuli, B. Uncertainty based online ensemble on non-stationary data for fusion science. In *39th Conference on Neural Information Processing Systems (NeurIPS 2025) Machine Learning for Physical Science Workshop* (12 2025) - [Accepted; to appear]
3. Rajput, K., Schram, M., Sammuli, B., and Lin, S. Uncertainty guided online ensemble for non-stationary data streams in fusion science, 2025, url https://arxiv.org/abs/2511.02092, - under review at Engineering Applications of Artificial Intelligence
4. Rajput, K., and others. Towards continual machine learning for particle accelerators. In *Proc. IBIC 2025* (09 2025), no. 14 in IBIC2025 - 14th International Beam Instrumentation Conference, JACoW Publishing, Geneva, Switzerland, pp. 302–307
5. Rajput, K., Lin, S., Edelen, A., Blokland, W., and Schram, M. Outlook towards deployable continual learning for particle accelerators. *Machine Learning: Science and Technology 6*, 3 (jul 2025), 031001
6. Hossam Mohammed, A., Rajput, K., Taylor, S., Furletov, D., Furletov, S., and Schram, M. Geometric gnns for charged particle tracking at gluex. *Machine Learning: Science and Technology 6*, 3 (Sep 2025), 035049
7. Colen, J., Schram, M., Rajput, K., and Kasparian, A. Explainable physics-based constraints on reinforcement learning for accelerator controls, 2025 - Under review at Expert Systems with Applications
8. Rajput, K., Schram, M., Edelen, A., Colen, J., Kasparian, A., Roussel, R., Carpenter, A., Zhang, H., and Bennesch, J. Harnessing the power of gradient-based simulations for multi-objective optimization in particle accelerators. *Machine Learning: Science and Technology* (2025)
9. Lersch, D., Schram, M., Dai, Z., Rajput, K., Sato, N., Wu, X., Childers, J. T., and Goldenberg, S. Sagips: a physics-inspired scalable asynchronous generative inverse-problem solver. *Machine Learning: Science and Technology 6*, 2 (apr 2025), 025017
10. Mohammed, A. H., Jones, M., McSpadden, D., Schram, M., Hess, B., and Rajput, K. Decode the workload: Training deep learning models for efficient compute cluster representation. *EPJ Web Conf. 337* (2025)
11. Rajput, K., Schram, M., Blokland, W., Alanazi, Y., Ramuhalli, P., Zhukov, A., Peters, C., and Vilalta, R. Robust errant beam prognostics with conditional modeling for particle accelerators. *Machine Learning: Science and Technology 5*, 1 (mar 2024), 015044

12. Goldenberg, S., Schram, M., Rajput, K., Britton, T., Pappas, C., Lu, D., Walden, J., Radaideh, M. I., Cousineau, S., and Harave, S. Distance preserving machine learning for uncertainty aware accelerator capacitance predictions. *Machine Learning: Science and Technology 5*, 4 (oct 2024), 045009

13. Allaire, C., Ammendola, R., Aschenauer, E.-C., Balandat, M., Battaglieri, M., Bernauer, J., Bondì, M., Branson, N., Britton, T., Butter, A., et al. Artificial intelligence for the electron ion collider (ai4eic). *Computing and Software for Big Science 8*, 1 (Feb 2024), 5

14. Jeske, T., Britton, T., Lawrence, D., and Rajput, K. Hydra: Computer vision for online data quality monitoring. In *EPJ Web of Conferences* (2024), vol. 295, EDP Sciences, p. 02008

15. Fanelli, C., Giroux, J., McSpadden, D., Rajput, K., Suresh, K., Cisbani, E., Deconinck, W., Walter, E., Bressan, A., Diefenthaler, M., et al. Ai4eic hackathon: Pid with the epic drich. In *EPJ Web of Conferences* (2024), vol. 295, EDP Sciences, p. 08004

16. Alanazi, Y., Schram, M., Rajput, K., Goldenberg, S., Vidyaratne, L., Pappas, C., Radaideh, M. I., Lu, D., Ramuhalli, P., and Cousineau, S. Multi-module-based cvae to predict hvcm faults in the sns accelerator. *Machine Learning with Applications 13* (2023), 100484

17. Schram, M., Rajput, K., NS, K. S., Li, P., John, J. S., and Sharma, H. Uncertainty aware machine-learning-based surrogate models for particle accelerators: Study at the fermilab booster accelerator complex. *Physical Review Accelerators and Beams 26*, 4 (2023), 044602

18. Rajput, K., Schram, M., and Somayaji, K. Uncertainty aware deep learning for particle accelerators. *NeurIPS 2022 - Machine Learning and the Physical Sciences Workshop* (2022)

19. Blokland, W., Rajput, K., Schram, M., Jeske, T., Ramuhalli, P., Peters, C., Yucesan, Y., and Zhukov, A. Uncertainty aware anomaly detection to predict errant beam pulses in the oak ridge spallation neutron source accelerator. *Physical Review Accelerators and Beams 25*, 12 (2022), 122802

20. Rajput, K., and Chen, G. Probabilistic envelope based visualization for monitoring drilling well data logging. In *VISIGRAPP (3: IVAPP)* (2022), pp. 51–62

21. Radaideh, I., Pappas, C., Lu, D., Walden, J., Cousineau, S., Britton, T., Rajput, K., Vidyaratne, L., and Schram, M. Progress on machine learning for the sns high voltage converter modulators. In *5th North American Particle Accelerator Conference (NAPAC'22), Albuquerque, NM, USA, 07-12 August 2022* (2022), JACOW Publishing, Geneva, Switzerland, pp. 715–718

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

23. Britton, T., Lawrence, D., and Rajput, K. Ai enabled data quality monitoring with hydra. In *EPJ Web of Conferences* (2021), vol. 251, EDP Sciences, p. 04010

24. Rajput, K. *Anomaly Detection and Feature Alignment for Time Series Data.* PhD thesis, University of Houston, 2020

25. Rajput, K., and Mehta, V. An analytical study of hadoop and its components. *International Journal of Scientific Research and Development* (2017)

26. Rajput, K., and Oza, B. A comparative study of classification techniques in data mining. *International Journal of Creative Research Thoughts 5*, 3 (2017), 154–163

STUDENTS AND POSTDOCS ADVISED

- Ahmed Mohammed (2023-present), **Postdoc**, data science department, Jefferson Lab, Newport News, VA
- Arun Thakur (Spring 2025), **MS** capstone project at Old Dominion Univeristy, Norfolk, VA

- Ashish Verma (Spring 2025), **MS** capstone project at Old Dominion Univeristy, Norfolk, VA
- Alex Broderick (Spring 2025), **MS** capstone project at Old Dominion Univeristy, Norfolk, VA
- Denis Furletov (2021-2025), **Bachelor** student at College of William and Mary, Williamsburg, VA
- Victor Minjares Neriz (Summer 2024), **MS** student at Universidad de Sonora, Hermosillo, Mexico
- Alex Glandon (2022), **PhD student** at Old Dominion University, Norfolk, VA
- Alan Li (2021), High school student
- Daniel Khalil (2021), High school student

SOFTWARE PACKAGES

- **Core Developer:** Scientific Optimization and Control Toolkit
- **Steering Committee:** Xopt

VOLUNTEER ACTIVITIES

- Place Award Judge: Science and Engineering Fair of Houston, 2019
- Volunteer Co-ordinator: National Service Scheme-India, 2016-2018