

Ayush Khot

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Education

University of Illinois at Urbana-Champaign, Urbana-Champaign, IL

August 2025 - Present

Doctor of Philosophy: COMPUTER SCIENCE

GPA: na/4.00

Potential Advisor: SHAOWEN WANG

University of Illinois at Urbana-Champaign, Urbana-Champaign, IL

August 2021 - May 2025

Bachelor of Science: COMPUTER SCIENCE

GPA: 3.96/4.00

Bachelor of Science: ENGINEERING PHYSICS

Experience

National Center for Supercomputing Applications, Urbana, IL

May 2022 - Present

UNDERGRADUATE RESEARCH ASSISTANT

- Examine, identify shortcomings with, and develop improved explainable AI (xAI) methods on deep neural networks in PyTorch and TensorFlow, reaching a state-of-the-art 93.2% accuracy in top tagging
- Aggregate critical physical characteristics pertinent to top quark decay using xAI metrics like SHAP and LRP
- Compare evidential deep learning (EDL) with baseline methods for uncertainty quantification and anomaly detection in jet tagging causing an increase in AUC by 0.05 in uncertainty quantification and variable improvements in anomaly detection
- Suggest new "Confidence Tuned" variance of EDL that has more accurate uncertainty quantification and similar accuracy
- Examine EDL uncertainties in latent space and the impact of pairwise particle interactions
- Write papers as first author on both applications of XAI methods (accepted to MLST) and EDL on jet tagging (work in progress)

Brookhaven National Laboratory, Upton, NY

June 2024 - August 2024

MACHINE LEARNING GROUP INTERN

- Adopt evidential deep learning (EDL) into storm forecasting to estimate uncertainty in model predictions
- Achieve better calibrated uncertainty using EDL as compared to baseline methods like Ensemble and Monte Carlo Dropout while requiring 10 times less inference time to estimate uncertainties and sustain similar baseline MSE Loss using EDL (0.0044) as compared to baseline methods (0.0036)
- Presented a poster and oral presentation at Brookhaven National Laboratory, and wrote a NeurIPS workshop paper as first author.

National Center for Supercomputing Applications, Urbana, IL

August 2023 - May 2024

UNDERGRADUATE RESEARCH INTERN

- Employ multi-gpu training for physics-informed neural operators (PINOs) to model 2D magnetohydrodynamics (MHD) simulations
- Contributed to NVIDIA's Modulus package by implementing new PINO models for modeling MHD and nonlinear shallow water simulations

Argonne National Laboratory, Lemont, IL

May 2023 - August 2023

ADVANCED PHOTON SOURCE INTERN

- Implement machine learning models in PyTorch and new post-processing method for xylem vessel segmentation in plant, reaching 93.7% Intersection over Union
- Implement simple test code for a Universal Robot UR3e in Python for use of sample handling at beamline
- Present a poster at Argonne National Laboratory, and wrote a paper as first author

Publications

Papers

- A. Khot**, M. Neubauer, A. Roy, "A detailed study of interpretability of deep neural network based top taggers." Machine Learning: Science and Technology, July 2023.
- A. Khot**, X. Luo, A. Kagawa, S. Yoo, "Evidential deep learning for probabilistic modelling of extreme storm events." Machine Learning and the Physical Sciences Workshop at the 38th conference on Neural Information Processing Systems (NeurIPS), Dec. 2024.

Posters

- A. Khot**, X. Luo, A. Kagawa, "Using Evidential Deep Learning on Probabilistic Storm Forecasting." Poster session presented at Brookhaven National Laboratory, Upton, NY, Aug. 2024.
- A. Khot**, X. Wang, M. Neubauer, V. Kindratenko, A. Roy, "Evidential Deep Learning for Uncertainty Quantification in Deep Neural Network Based Jet Tagging." Poster session presented at the National Center for Supercomputing Applications: 2nd Annual NCSA Student Research Conference, Urbana, IL, April 2024.
- A. Khot**, Z. Finrock, C. Chang, V. Nikitin, K. Lazarski, "Implementing Machine Learning to Segment Xylem from Plant Stem." Poster session presented at Argonne National Laboratory: Learning on the Lawn 2023, Lemont, IL, Aug. 2023.
- J. Barker, S. Danthurthy, H. Kannan, An. Khot, **Ay. Khot**, S. Mohan, P. Padyala, Z. White, "Effect of Titin on Lattice Spacing in Sarcomere Structure." Poster session presented virtually as part of Argonne Exemplary Student Research Program.

Conference Presentations

1. **A. Khot**, X. Luo, A. Kagawa, "Evidential Deep Learning for Probabilistic Storm Detection." Presented at Brookhaven National Laboratory, Upton, NY, Aug. 2024.
2. **A. Khot**, X. Wang, M. Neubauer, V. Kindratenko, A. Roy, "Uncertainty Quantification and Anomaly Detection with Evidential Deep Learning." Presentation at National Center for Supercomputing Applications: Students Pushing Innovation project, Urbana, IL, April 2024.
3. M. Neubauer, A. Roy, **A. Khot**, X. Wang, D. Zhong, "Uncertainty Quantification and Anomaly Detection with Evidential Deep Learning" Paper presented in AI and the Uncertainty Challenge in Fundamental Physics Workshop, SCAI, Paris and Institut Pascal Paris-Saclay, France, Nov. 2023.
4. M. Neubauer, A. Roy, **A. Khot**, "Explainable AI for Interpretability of Deep Neural Networks : the High Energy Physics perspective." Paper presented in AI and the Uncertainty Challenge in Fundamental Physics Workshop, SCAI, Paris and Institut Pascal Paris-Saclay, France, Nov. 2023.
5. A. Roy, M. Neubauer, **A. Khot**, "Interpretability Inspires: How explainable AI helps improve Top Tagging." Paper presented in APS Meeting Abstracts, April 2023.
6. A. Roy, **A. Khot**, M. Neubauer, "Exploring Interpretability of Deep Neural Networks in Top Tagging" Paper presented in 26th International Conference on Computing in High Energy & Nuclear Physics, Norfolk, VA, May 2023.

Grants and Funding

1. 2023 Delta Allocation for UIUC Projects. "Interpretable, anomaly-aware deep learning models for proton=proton collision events at the Large Hadron Collider", Computer allocation at National Center for Supercomputing Applications. 3,000 GPU node-hours. Undergraduate Research Student.
2. 2023 Delta Allocation for UIUC Projects. "Confluence of Numerical Relativity and Physics Inspired Artificial Intelligence for Multi-Messenger Astrophysics Discovery with NCSA Delta", Computer allocation at National Center for Supercomputing Applications. 600,000 CPU node-hours. Undergraduate Research Student.

Interviews and Media

1. "EOH 2024 at NCSA", Press Release, <https://www.ncsa.illinois.edu/eoh-2024-at-ncsa/>
2. "24 students from three area high schools chosen to work on research with Argonne scientists", Press Release, <https://www.chicagotribune.com/2020/07/08/24-students-from-three-area-high-schools-chosen-to-work-on-research-with-argonne-scientists/>

Honors & Awards

2024	Philip J. and Betty M. Anthony Undergraduate Summer Research Scholarship , University of Illinois Department of Physics	<i>Urbana, IL</i>
2021 - 2024	Shelton M&R Matthews Scholarship , University of Illinois	<i>Urbana, IL</i>
2021 - 2022	Illinois Engineering Freshman Scholarship , University of Illinois College of Engineering	<i>Urbana, IL</i>
2021 - 2025	James Scholar , University of Illinois College of Engineering	<i>Urbana, IL</i>
2021 - 2024	Dean's List , University of Illinois College of Engineering	<i>Urbana, IL</i>
2021 - 2022	Swami Vivekananda Scholarship , Community Foundation of the Fox River Valley	<i>Aurora, IL</i>

Leadership Experience

NetMath at University of Illinois at Urbana-Champaign	<i>Feb 2022 - August 2023</i>
MENTOR	
<ul style="list-style-type: none">• Facilitate weekly communication and oversee a group of over 20 Multivariable Calculus students• Utilize Mathematica to meticulously grade homework assignments and deliver comprehensive feedback to students• Conduct thorough reviews of exam results to ensure accurate assessment and continuous improvement in their understanding of the material	
Illini Strings (UIUC Orchestra)	<i>August 2021 - May 2025</i>
CORE MEMBER	
Society of Physics Students	<i>August 2023 - May 2024</i>
MEMBER	

Skills

Programming	Python, C/C++, JAVA, TeX , Linux, Parallel Computing (CUDA, DDP, Horovod), Machine Learning (PyTorch, TF)
Relevant Courses	Num. Analysis, Machine Learning, Parallel Programming, Linear Algebra, Data Structures and Algorithms
HPC Experience	NERSC Perlmutter, NCSA Delta, NCSA HAL, ALCF Polaris