

Karan Shah — Curriculum Vitæ

CONTACT INFORMATION

E-mail: k.shah@hzdr.de *Phone:* +49 1522-7693857
Web: <https://www.karan.sh> || *GitHub:* [karanprime](#) || *Twitter:* [@ReKarantNetwork](#)

EDUCATION

PhD Candidate, Computer Science *August 2021 - Present*
Center for Advanced Systems Understanding (CASUS), Görlitz, Germany
Technische Universität Dresden, Dresden, Germany

MS Computational Science & Engineering *December 2020*
Primary Focus: Machine Learning applied to data-intensive *Physics* problems
BS Computer Science (Threads: Intelligence, Modeling-Simulation) *May 2018*
BS Physics
Thesis: *“Analysis of Uncertainty Quantification of Machine Learned Density Functionals”*
Georgia Institute of Technology, Atlanta, GA USA

EXPERIENCE

Center for Advanced Systems Understanding (CASUS), Görlitz, Germany
Helmholtz-Zentrum Dresden-Rossendorf e.V. (HZDR)
Supervisor: Dr. Attila Cangi
Machine Learning for Materials Design Department
Doctoral Researcher *Aug 2021 - Present*
Project: A simulation framework for quantum dynamics based on physics informed neural networks. Subprojects include ML accelerated PDE solvers, synthetic ML generated data to accelerate surrogate model training. Funded by Helmholtz AI.

Roblox Corporation, San Mateo, CA USA
Managers: Dr. Brian Lockwood, Dr. Nick Burgess
Physics - Solid Mechanics Team, Engine Group
Research Intern *Sept 2024 - Dec 2024*
Project: Developing ML techniques for rigid body simulations in the game engine. Using generative ML models for reduced-order modeling to accelerate 3D engine performance.

Lawrence Livermore National Laboratory, Livermore, CA USA
Hosted by: Dr. Michael Schneider
Astronomy and Astrophysics Analytics Group
Graduate Intern, Physics Division *May 2019 - Aug 2019*
Technical Scholar, Physics Division *Aug 2017 - May 2019*
Intern, Data Science Summer Institute *May 2017 - Aug 2017*
Projects: 1) Gaussian Processes with neural network equivalent kernels to estimate cosmological parameters from mass density fields with uncertainty quantification
2) Probabilistic Inference of Cosmic Shear & Intrinsic Galaxy Properties through Hierarchical Graphical Models. Used MCMC techniques to determine cosmic shear and galaxy morphology (for LSST)

Georgia Institute of Technology, Atlanta, GA USA

Medford Group, School of Chemical & Biomolecular Engineering *Jan 2017 - Aug 2019*
Advisor: Dr. Andrew Medford
Project: Determination of Exchange Correlation Functionals through Deep Learning
Using ensembles of neural networks to build surrogate density functionals

PUBLICATIONS * DENOTES EQUAL CONTRIBUTION	Shah, K. , Cangi A., ‘ <i>Accelerating Electron Dynamics Simulations through Machine Learned Time Propagators</i> ’, ICML 2024 AI for Science Workshop. Link: arXiv
	Shah, K. , Butler, J., Knaub, A., Ratcliff, W., Zenginoğlu, A., Soltanieh-ha, M., ‘ <i>Data Science Education in Undergraduate Physics: Lessons Learned from a Community of Practice</i> ’, Am. J. Phys. 1 September 2024; 92 (9): 655–662. Links: AJP , arXiv
	Martinetto, V.* , Shah, K.* , Cangi, A., Pribram-Jones, A., ‘ <i>Inverting the Kohn-Sham equations with physics-informed machine learning</i> ’, Machine Learning Science & Technology, Volume 5, Number 1, 2024. Links: MLST , arXiv
	Shah, K. , Stiller, P., Hoffmann, N., Cangi A., ‘ <i>Physics-Informed Neural Networks as Solvers for the Time-Dependent Schrödinger Equation</i> ’, NeurIPS 2022 Machine Learning and the Physical Sciences Workshop. Links: ML4PS Paper , Poster , arXiv
	Fiedler, L., Shah, K. , Bussmann, M., Cangi A., ‘ <i>Deep dive into machine learning density functional theory for materials science and chemistry</i> ’, Phys. Rev. Materials, vol. 6, p. 040301, Apr 2022. Links: PhysRevMat , arXiv
	Dzanic, T., Shah, K. , Witherden, F., ‘ <i>Fourier Spectrum Discrepancies in Deep Network Generated Images</i> ’, Accepted to NeurIPS 2020, in Advances in Neural Information Processing Systems, vol. 33, pp. 3022–3032, 2020. Links: NeurIPS , arXiv
BOOK CHAPTERS	Fiedler, L., Shah, K. , & Cangi A., Chapter ‘ <i>Machine-Learning for Static and Dynamic Electronic Structure Theory</i> ’, Book ‘Machine Learning in Molecular Sciences’, Series ‘Challenges and Advances in Computational Chemistry and Physics’, Publisher Springer Nature. Link: Springer
HONORS AND AWARDS	<ul style="list-style-type: none"> • Travel Grant, NHR (German National HPC Alliance) Conference 2023, September 2023 • Elected Member, American Physical Society-Group on Data Science (APS-GDS) Executive Committee, June 2023 - March 2025 • APS Data Science Education & Community of Practice Fellowship 2022-2023, 2023-2024 • Outstanding Reviewer Award, ML Reproducibility Challenge 2021 • Datmo Applied Machine Learning Fellowship, December 2017 • Amazon Web Services Research Grant, September 2017 (GT Data-Driven Education team) • President’s Undergraduate Research Award: Fall 2017, Fall 2016 • Fellow, Data Science Summer Institute, LLNL, Summer 2017 • Student Travel Awards: JupyterCon 2017 (NYC), WSSSPE 2016 (Manchester, UK) • Top 10 percentile in Indian National Astronomy Olympiad, 2012
TEACHING EXPERIENCE	<p>Fellow, Data Science Education Community of Practice <i>Feb 2022 - Dec 2024</i> Created multiple open-source pedagogical modules for integrating machine learning topics into the undergraduate physics curriculum, as part of a competitive APS fellowship. Link: GitHub</p> <p>Graduate Teaching Assistant, College of Computing, Georgia Tech <i>Aug 2018 - May 2020</i> TA for Junior Level <i>CS 3510 - Design-Analysis of Algorithms</i>, under Dr. Constantine Dovrolis <i>S’20</i> TA for Graduate Level <i>CSE 6730 - Modeling & Simulation</i>, under Dr. Richard Vuduc <i>S’19</i> TA for Senior Level <i>CS 4510 - Automata & Complexity</i>, under Dr. Richard Peng <i>F’18</i></p>
COMPUTER SKILLS	Python (Data) Science Stack, PyTorch Mathematica, Matlab, L ^A T _E X, Arduino Processing

SERVICE

Reviewer, ICLR 2025, NeurIPS 2024
Reviewer, New Journal of Physics (NJP) 2024
Member of Taskforce Promovierende (Graduate Student Education), HZDR, Dresden, Germany *Apr 2022 - Dec 2023*
Reviewer, ML for Physical Sciences Workshop, NeurIPS 2022
Reviewer, Synthetic Data for ML Workshop, NeurIPS 2022, 2023
Reviewer, ML Reproducibility Challenge 2021
Reviewer, President's Undergraduate Research Award (PURA) *May 2018 - Dec 2020*
Reviewed Physics and CS research proposals for PURA, a competitive undergraduate research award.

OUTREACH AND LEADERSHIP

Early Career Member-at-Large, APS GDS Executive Committee *June 2023 - Present*
Doctoral Representative, HZDR, Dresden, Germany *Feb 2022 - Present*
Volunteer, ICML 2020, Remote *July 2020*
Volunteer, ICLR 2019, New Orleans, LA *May 2019*
Senator, Graduate Student Senate, Georgia Tech *Sept 2018 - May 2019*
Representing Computational Science & Engineering in the Student Government Association.
Co-founder, Bitcoin@Tech, Georgia Tech's Bitcoin Club *Aug 2014 - May 2015*