

Karan N. 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)

Supervisors: Dr. Attila Cangi (CASUS), Prof. Dr. Ivo Sbalzarini (TU Dresden)

Matter Under Extreme Conditions Group

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, etc. Funded by Helmholtz AI.

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

Otte Lab, Center for Relativistic Astrophysics

Jan 2016 - May 2018

Advisor: Dr. A. Nepomuk Otte

Project: Segmented Schwarzschild-Couder Telescope Model for GrOptics ray tracing package

Open Source Contrib.: Added telescope model to GrOptics, written in C++(with CERN ROOT)

PUBLICATIONS	<p>Shah, K., Stiller, P., Hoffmann, N. & Cangi A., ‘<i>Physics-Informed Neural Networks as Solvers for the Time-Dependent Schrödinger Equation</i>’, Accepted to the Machine Learning and the Physical Sciences Workshop, NeurIPS 2022. Links: ML4PS Paper, Poster, arXiv:2210.12522</p> <p>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:2110.00997</p> <p>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:1911.06465</p>
BOOK CHAPTERS	<p>Shah, K., Fiedler, L., & 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 (Accepted)</p>
HONORS AND AWARDS	<ul style="list-style-type: none"> • American Physical Society - Data Science Education & Community of Practice Fellowship 2022-23 • 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>Graduate Teaching Assistant, College of Computing, Georgia Tech Aug 2018 - May 2020</p> <p>TA for Junior Level <i>CS 3510 - Design-Analysis of Algorithms</i>, under Dr. Constantine Dovrolis <i>S’20</i></p> <p>TA for Graduate Level <i>CSE 6730 - Modeling & Simulation</i>, under Dr. Richard Vuduc <i>S’19</i></p> <p>TA for Senior Level <i>CS 4510 - Automata & Complexity</i>, under Dr. Richard Peng <i>F’18</i></p>
COMPUTER SKILLS	<p>Python (Data) Science Stack, PyMC3, Keras(Tensorflow), PyTorch</p> <p>Mathematica, C/C++, Matlab, L^AT_EX, Arduino Processing</p>
SERVICE	<p>Program Committee, JupyterCon 2023 <i>Dec 2022 - Present</i></p> <p>Reviewer, ML for Physical Sciences Workshop, NeurIPS 2022 <i>Nov 2022</i></p> <p>Reviewer, Synthetic Data for ML Workshop, NeurIPS 2022 <i>Nov 2022</i></p> <p>Reviewer, ML Reproducibility Challenge 2021 <i>Feb 2022</i></p> <p>Reviewer, President’s Undergraduate Research Award (PURA) <i>May 2018 - Dec 2020</i></p> <p>Reviewed Physics and CS research proposals for PURA, a competitive undergraduate research award.</p>
OUTREACH AND LEADERSHIP	<p>Doctoral Representative, HZDR, Dresden, Germany <i>Feb 2022 - Present</i></p> <p>Volunteer, ICML 2020, Remote <i>July 2020</i></p> <p>Volunteer, ICLR 2019, New Orleans, LA <i>May 2019</i></p> <p>Senator, Graduate Student Senate, Georgia Tech <i>Sept 2018 - May 2019</i></p> <p>Representing Computational Science & Engineering in the Student Government Association.</p> <p>Co-founder, Bitcoin@Tech, Georgia Tech’s Bitcoin Club <i>Aug 2014 - May 2015</i></p>