Karan N. Shah — Curriculum Vitæ

CONTACT INFORMATION

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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

Fiedler, L., **Shah, K.**, Bussmann, M. & Cangi A., *'Deep dive into machine learning density functional theory for materials science and chemistry'*, Phys. Rev. Materials, vol. 6, p. 040301, Apr 2022. Links: PhysRevMat, arXiv:2110.00997

Dzanic, T., **Shah, K.**, Witherden, F., *'Fourier Spectrum Discrepancies in Deep Network Generated Images'*, Accepted to NeurIPS 2020, in Advances in Neural Information Processing Systems, vol. 33, pp. 3022–3032, 2020. Links: NeurIPS, arXiv:1911.06465

Book Chapters

Fiedler, L., **Shah, K.** & Cangi A., Chapter *'Machine Learning Surrogate Models for Materials'*, Book 'Machine Learning in Molecular Sciences', Series 'Challenges and Advances in Computational Chemistry and Physics', Publisher Springer Nature IN PREPARATION

Honors and Awards

- 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 (Advisor: Dr. Madden)
- 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

Presentations

Deep Learning the Schrödinger Equation Link — *Aug 2022*
DSECOP Data Science and Physics Workshop, College Park MD (*invited talk*)

Accelerating Time-Dependent Density Functional Theory with Physics Informed Neural Networks Link — *Mar 2022*
APS March Meeting 2022, Chicago IL (*talk*)

Physics Informed Neural Networks based Solvers for the Time-Dependent Schrödinger Equation — *Feb 2022*
DFT Methods for Matter Under Extreme Conditions Workshop (*poster*)
Görlitz Germany

Estimation of Cosmological Parameters from n-body simulations through Gaussian Processes — *Aug 2019*
Astronomy & Astrophysics Analytics Group Summer Presentation (*talk*)
Livermore CA

Hierarchical Probabilistic Inference of Multivariate Galaxy Properties — *Dec 2018*
Bay Area LSST & Machine Learning Meeting, Berkeley CA (*talk*)

Analysis of Uncertainty in Machine Learned Density Functionals — *Apr 2018*
Annual Undergraduate Research Spring Symposium, Georgia Tech, Atlanta GA (*poster*)

Inferring Student Success Predictors for CS1301x Online Course at Georgia Tech — *Nov 2017*
Georgia Tech STEM Education Research Expo, Atlanta GA (*poster*)

Hierarchical Bayesian Inference of Cosmic Shear & Intrinsic Galaxy Properties — *Aug 2017*
LLNL Summer Symposium, Livermore CA (*poster*)

Classifying Cellular Automata using Machine Learning *July 2016*
Wolfram Summer School Symposium, Waltham MA (*talk, poster*)

Cellular Automata *Mar 2016*
Senior Seminar, School of Physics, Georgia Tech, Atlanta GA (*talk*)

Memberships

- American Physical Society (APS)
- Society of Industrial and Applied Mathematicians (SIAM)
- Deutsche Physikalische Gesellschaft (DPG)

Teaching Experience

Graduate Teaching Assistant, College of Computing, Georgia Tech *Aug 2018 - May 2020*
TA for Junior Level *CS 3510 - Design-Analysis of Algorithms*, under Dr. Constantine Dovrolis *S'20*
TA for Graduate Level *CSE 6730 - Modeling & Simulation*, under Dr. Richard Vuduc *S'19*
TA for Senior Level *CS 4510 - Automata & Complexity*, under Dr. Richard Peng *F'18*

Computer Skills

Python (Data) Science Stack, PyMC3, Keras(Tensorflow), PyTorch
Mathematica, C/C++, Matlab, LaTeX, Arduino Processing

Outreach and Leadership

Doctoral Representative, HZDR, Dresden, Germany *Feb 2022 - Present*

Reviewer, ML Reproducibility Challenge 2021 *Feb 2022*
Reviewer, President's Undergraduate Research Award (PURA) *May 2018 - Dec 2020*
Reviewed Physics and CS research proposals for PURA, a competitive undergraduate research award.

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*

Supplemental Experience

Student Assistant, Center for Non Linear Science, GT *Jan 2015 - Aug 2015*
Supervisor: Dr. Predrag Cvitanović
Assisted Dr. Cvitanović in producing video lectures and maintaining website for a MOOC on non-linear dynamics. (Link: http://chaosbook.org)

Analyst and Developer, Cryptomen.com - Startup *July 2014 - Feb 2015*
Part of a five-person startup that raised $47,000 in cryptocurrency investment.

Misc

Responsible Conduct of Research Stage 1 Certificate, CITI, License 15693882