

# Karan N. Shah — Curriculum Vitæ

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## 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

**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>Fiedler, L., <b>Shah, K.</b>, Bussmann, M. &amp; Cangi A., ‘<i>A Deep Dive into Machine Learning Density Functional Theory for Materials Science and Chemistry</i>’ UNDER REVIEW, <a href="#">arxiv:2110.00997</a></p> <p>Dzanic, T., <b>Shah, K.</b>, Witherden, F., ‘<i>Fourier Spectrum Discrepancies in Deep Network Generated Images</i>’, Accepted to NeurIPS 2020, <a href="#">arXiv:1911.06465</a></p>
HONORS AND AWARDS	<ul style="list-style-type: none"> <li>• American Physical Society - Data Science Education &amp; Community of Practice Fellowship 2022-23</li> <li>• Datmo Applied Machine Learning Fellowship, December 2017</li> <li>• Amazon Web Services Research Grant, September 2017 (Advisor: Dr. Madden)</li> <li>• President’s Undergraduate Research Award: Fall 2017, Fall 2016</li> <li>• Fellow, Data Science Summer Institute, LLNL, Summer 2017</li> <li>• Student Travel Awards: JupyterCon 2017 (NYC), WSSSPE 2016 (Manchester, UK)</li> <li>• Top 10 percentile in Indian National Astronomy Olympiad, 2012</li> </ul>
PRESENTATIONS	<p><i>Physics Informed Neural Networks based Solvers for the Time-Dependent Schrödinger Equation</i> Feb 2022 DFT Methods for Matter Under Extreme Conditions Workshop (<i>poster</i>) Görlitz, Germany</p> <p><i>Estimation of Cosmological Parameters from n-body simulations through Gaussian Processes</i> Aug 2019 Astronomy &amp; Astrophysics Analytics Group Summer Presentation (<i>talk</i>) Livermore CA</p> <p><i>Hierarchical Probabilistic Inference of Multivariate Galaxy Properties</i> Dec 2018 Bay Area LSST &amp; Machine Learning Meeting, Berkeley CA (<i>talk</i>)</p> <p><i>Analysis of Uncertainty in Machine Learned Density Functionals</i> Apr 2018 Annual Undergraduate Research Spring Symposium, Georgia Tech, Atlanta GA (<i>poster</i>)</p> <p><i>Inferring Student Success Predictors for CS1301x Online Course at Georgia Tech</i> Nov 2017 Georgia Tech STEM Education Research Expo, Atlanta GA (<i>poster</i>)</p> <p><i>Hierarchical Bayesian Inference of Cosmic Shear &amp; Intrinsic Galaxy Properties</i> Aug 2017 LLNL Summer Symposium, Livermore CA (<i>poster</i>)</p> <p><i>Classifying Cellular Automata using Machine Learning</i> July 2016 Wolfram Summer School Symposium, Waltham MA (<i>talk, poster</i>)</p> <p><i>Cellular Automata</i> Mar 2016 Senior Seminar, School of Physics, Georgia Tech, Atlanta GA (<i>talk</i>)</p>
MEMBERSHIPS	<ul style="list-style-type: none"> <li>• Large Synoptic Survey Telescope Dark Energy Science Collaboration (LSST-DESC)</li> <li>• American Physical Society (APS)</li> <li>• Society of Industrial and Applied Mathematicians (SIAM)</li> </ul>
TEACHING EXPERIENCE	<p><b>Graduate Teaching Assistant, College of Computing, Georgia Tech</b> Aug 2018 - May 2020</p> <p>TA for Junior Level <i>CS 3510 - Design-Analysis of Algorithms</i>, under Dr. Constantine Dovrolis S’20</p> <p>TA for Graduate Level <i>CSE 6730 - Modeling &amp; Simulation</i>, under Dr. Richard Vuduc S’19</p> <p>TA for Senior Level <i>CS 4510 - Automata &amp; Complexity</i>, under Dr. Richard Peng F’18</p>

COMPUTER SKILLS	Python (Data) Science Stack, PyMC3, Keras(Tensorflow), PyTorch Mathematica, C/C++, Matlab, L <sup>A</sup> T <sub>E</sub> X, Arduino Processing	
OUTREACH AND LEADERSHIP	<b>Doctoral Representative, HZDR, Dresden, Germany</b> <b>Volunteer, ICML 2020, Remote</b> <b>Volunteer, ICLR 2019, New Orleans, LA</b>  <b>Reviewer, President's Undergraduate Research Award (PURA)</b> Reviewed Physics and CS research proposals for PURA, a competitive undergraduate research award.  <b>Senator, Graduate Student Senate, Georgia Tech</b> Representing Computational Science & Engineering in the Student Government Association.  <b>Co-founder, Bitcoin@Tech, Georgia Tech's Bitcoin Club</b>	<i>Feb 2022 - Present</i> <i>July 2020</i> <i>May 2019</i>  <i>May 2018 - Dec 2020</i>  <i>Sept 2018 - May 2019</i>  <i>Aug 2014 - May 2015</i>
SUPPLEMENTAL EXPERIENCE	<b>Student Assistant, Center for Non Linear Science, GT</b> Supervisor: Dr. Predrag Cvitanović Assisted Dr. Cvitanović in producing video lectures and maintaining website for a MOOC on non-linear dynamics. (Link: <a href="http://chaosbook.org">http://chaosbook.org</a> )  <b>Analyst and Developer, Cryptomen.com - Startup</b> Part of a five-person startup that raised \$47,000 in cryptocurrency investment.	<i>Jan 2015 - Aug 2015</i>     <i>July 2014 - Feb 2015</i>
MISC	Responsible Conduct of Research Stage 1 Certificate, CITI, License 15693882	