

XIYUAN GUO

Physics and Computer Science Double Major, University of Virginia
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RESEARCH FOCUS

Computational imaging; density functional theory (DFT); longitudinal measurement and missing data; Bayesian statistics; mathematical matrix calculus; physics-informed neural networks (PINN); reproducible statistical software; interdisciplinary computational science.

EDUCATION

University of Virginia
B.S., Physics and Computer Science

Expected May 2028
Charlottesville, VA

- **GPA:** 3.89/4.00

GRANTS AND FELLOWSHIPS

- **Double Hoo Research Grant**, University of Virginia 2026
Secured competitive grant funding to drive independent, interdisciplinary computational research alongside graduate mentorship.

PROFESSIONAL RESEARCH EXPERIENCE

Research Assistant
UVA BAL Lab (Prof. Xin Cynthia Tong's Group)

Apr 2026 – Present
Charlottesville, VA

- Formulating a quantum-inspired psychometric framework utilizing Hilbert-space probability models to map how individuals transition from cognitive uncertainty to commitment across repeated longitudinal measurements.
- Integrating construct validity and experience-sampling data with simulation-based validation to computationally formalize psychological constructs, including cognitive fluidity, ambivalence, crystallization, and re-fluidization.
- Engineered a mathematical framework for multivariate longitudinal missing data imputation that enforces the Law of Total Variation, mitigating structural covariance bias inherent in unconstrained predictive machine learning models.
- Developed a custom gradient descent solver to iteratively evaluate dual Lagrangian multipliers, ensuring the final global variance of imputed datasets converges to strict theoretical asymptotic expectations; implemented in C++17 via RcppArmadillo.

Research Assistant

Yale University (Prof. Mengxia Liu's Group)

Feb 2026 – Present

New Haven, CT

- Formulated a deep unrolled ADMM framework to solve ill-posed inverse problems in computational imaging, reconstructing multi-dimensional data encompassing spatial, spectral, and full-Stokes polarization domains.
- Implemented rigorous physics-informed constraints within deep learning optimization loops, mathematically grounding vectorial Stokes parameter representations utilizing complex numbers, trigonometric formulations, and 3D Poincaré sphere mappings.
- Engineered a specialized PyTorch pipeline utilizing a custom convolutional U-Net architecture as a learned proximal operator, specifically designed to mitigate non-Gaussian hardware sensor noise and yielding a 4.5 dB increase in PSNR.

Research Assistant

UVA (Prof. Liqin Ke's Group)

Oct 2025 – Present

Charlottesville, VA

- Applied quantum mechanics principles to engineer complex Density Functional Theory (DFT) reconstruction algorithms, bridging theoretical atomic modeling with robust software implementations to accurately catalog electronic material properties.
- Created immersive, browser-based data visualizations using Three.js and JSmol, generating interactive 3D atomic models and Kiviat diagrams to facilitate real-time structural inspection and validation.
- Engineered a cloud-native machine learning pipeline utilizing Go and Next.js, enabling global academic collaborators to securely share specialized datasets and execute pre-trained predictive models.

Research Intern

UVA Biocomplexity Institute

May 2026 – Present

Charlottesville, VA

- Formulated massive-scale network simulations to dynamically model the stochastic spread of viral pathogens (e.g., COVID-19 and Ebola), implementing SEIR compartmental cascade models to capture heterogeneous transmission dynamics.
- Engineered attention-based Graph Neural Network (GNN) architectures to predict multi-hop epidemic propagation pathways, leveraging spatiotemporal message-passing frameworks to extract predictive topological features from dynamic contact networks.

OPEN SOURCE SOFTWARE

- **smriti**: R package for automated longitudinal missing data imputation (available on CRAN). Executes a three-phase architecture combining missForest initialization with a custom C++ Lagrangian projection engine to strictly preserve the structural variance of the target covariance manifold.
- **sanjaya**: Automated academic literature extraction pipeline utilizing the OpenAlex Academic Graph API, Scrapy, and Playwright to extract bilingual data, exporting structured CSV/JSON datasets for downstream interdisciplinary research.
- **difi**: High-performance Go-based Git diff terminal user interface utilizing the Bubble Tea framework to streamline version control workflows; achieved official Homebrew Core inclusion, 342+ GitHub stars, and a #5 ranking on Hacker News.

HONORS AND AWARDS

- **Dean's List of Distinguished Students**, University of Virginia
- **Silver Division**, USA Computing Olympiad (USACO)

TECHNICAL SKILLS

- **Math & Physics** Quantum Mechanics, Density Functional Theory (DFT), Linear & Tensor Algebra, Real Analysis, ODEs
- **Machine Learning & AI:** PyTorch, TensorFlow, Keras, JAX, Scikit-Learn, XGBoost, Pandas, NumPy, OpenCV, RcppArmadillo
- **Languages:** Python, C/C++, Rust, Go, TypeScript, R, Julia, SQL, Lua, Bash, Java, \LaTeX
- **Infrastructure & Cloud:** Linux (RHEL/Fedora), AWS (EC2, S3), Docker, Kubernetes, CUDA, Slurm HPC, Git

COMMUNITY SERVICE

Volunteer Firefighter

Plainfield Fire Department

2022 – 2024

Plainfield

- Responded to over 200 emergency medical, fire, and rescue calls annually, operating effectively in high-stress environments to provide critical incident mitigation and community support.