

Taiwo A. Adebiyi

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Research Interests

Scientific Foundation Models, Physical AI, Uncertainty Quantification, Adaptive Experimentation (Bayesian Optimization), Energy Systems, Digital Twin

Education

University of Houston

PhD, Civil Engineering (Focus: Probabilistic Machine Learning & Optimization)

Houston, TX, USA

August 2022—May 2027 (Expected)

- Thesis: “Enhancing Trustworthy Autonomous Systems: Bayesian Optimization, Scientific Foundation Models, and Digital Twins”
- GPA: 3.92/4.00 | Advisor: Dr. Ruda Zhang

Rice University

Inter-institutional Visiting Scholar

Houston, TX, USA

August 2024—Dec 2024

- Deep Learning Project: Uncertainty Quantification with Adversarial Physics-Informed Neural Networks
- GPA: 4.00/4.00 | Instructor: Dr. Ankit Patel

Nigerian University of Technology and Management

PG Cert., Technology, Entrepreneurship, & Design

Lagos, Nigeria

August 2021—August 2022

- Distinction | Overall Best in All-round Academic Excellence

University of Lagos

BSc., Civil Engineering

Lagos, Nigeria

December 2015—September 2021

- First Class (Honors) | Vice Chancellor’s Overall Best Student in Service Delivery

Research Experience

Los Alamos National Laboratory

Graduate Research Assistant

Los Alamos, New Mexico, USA

August 2026—Present

- Extended an offer to continue my machine learning fellowship project on Bayesian machine learning for natural gas dynamics network.
- Working with the Computational Intelligence and Modeling (A-1) and Theoretical Division on Applied Mathematics (T-5) Teams.

Applied Machine Learning (AML) Fellow

May 2026—August 2026

- Selected as one of only twelve AML Fellows for summer 2026 internship.
- Joined the Computational Intelligence and Modeling (A-1) to develop Bayesian machine learning for stochastic natural gas dynamics.

Chishiki-AI | National Science Foundation | University of Texas at Austin

Artificial Intelligence (AI) Fellow

Austin, TX, USA

May 2026—May 2027

- Selected as one of only five SCIPe Chishiki AI Fellows to receive \$49,000 in direct funding on AI integration for civil engineering systems.
- Working on “Trustworthy adaptive experimentation for civil-engineering digital twins”.

Uncertainty Quantification Lab—University of Houston

Graduate Research Assistant

Houston, TX, USA

August 2022—Present

- Conducting research in Bayesian optimization, Gaussian processes, and foundation models with applications in high-risk decision-making.
- Seven (7) publications within three years in top machine learning and engineering venues including NeurIPS, ICLR, ASME, and Elsevier.
- Contributed to two (2) research grants award and secured multiple travel grants for presentations in workshops and conferences.
- Led open-source ML libraries creation and contributions, including SOTA’s optimization package and Meta’s BoTorch platform.

Chevron | UH Energy

Graduate Research Fellow

Houston, TX, USA

August 2025—August 2026

- Applying probabilistic machine learning and optimization to quantification of geologic hydrogen.
- Integrating Bayesian models into risk and resource forecasting frameworks.

Nigerian University of Technology & Management | First E & P Development

Visiting Graduate Research Scholar

Lagos, Nigeria

May 2022—July 2022

- Investigated digital twin frameworks for large-scale engineering systems with simulation-driven decision optimization.

Publications

1. **Adebiyi, T.A.***, Akash, Y.*, & Zhang, R. (2026). Calibrating Scientific Foundation Models with Inference-Time Stochastic Attention. *Under Anonymous Review* ([preprint link](#)). *Equal Contribution
2. **Adebiyi, T.A.**, Do, B., & Zhang, R. (2025). Optimizing Posterior Samples for Bayesian Optimization via Rootfinding. *In Proceedings of the Thirteenth International Conference on Learning Representations (ICLR), 2025.* ([link](#))
➤ **Average rating: 7.0 (top 8% out of over 11,000 submissions).**
3. **Adebiyi, T.A.**, Do, B., & Zhang, R. (2024). Gaussian Process Thompson Sampling via Rootfinding. *In Proceedings of the NeurIPS 2024 Workshop on Bayesian Decision-making and Uncertainty (BDU).* ([link](#))
➤ **Oral presentation (1 of 6; top 5% of accepted papers).**
4. **Adebiyi, T. A.**, Ajenifuja, N. A., & Zhang, R. (2024). Digital Twins and Civil Engineering Phases: Reorienting Adoption Strategies. *Journal of Computing and Information Science in Engineering.* ([link](#))
5. Do, B., **Adebiyi, T.A.**, & Zhang, R. (2024). Epsilon-Greedy Thompson Sampling to Bayesian Optimization. *Journal of Computing and Information Science in Engineering.* ([link](#))
➤ **Journal Editor's Award (1 of only 5 selected papers featured on the journal's front page - [link](#))**
6. Do, B., Ajenifuja, N. A., **Adebiyi, T. A.**, & Zhang, R. (2026). Sampling from Gaussian Processes: A Tutorial and Applications in Global Sensitivity Analysis and Optimization. *Springer Journal of Structural and Multidisciplinary Optimization* ([link](#))
7. Do, B., Ghalekohneh, S.J., **Adebiyi, T.A.**, Zhao, B., Zhang R. (2024). Automated Design of Nonreciprocal Thermal Emitters via Bayesian Optimization. *Journal of Quantitative Spectroscopy and Radiative Transfer.* ([link](#))
8. Do, B., Nabavi, B., Ghalekohneh, S.J., **Adebiyi, T.A.**, Zhao, B., Zhang R. (2026). Achieving high-performance polarization-independent nonreciprocal thermal radiation with pattern-free heterostructures. ([link](#))
9. Akijje I., **Adebiyi, T.A.**, (2021). An Optimized Superplasticized Microsilica Concrete for Flexible Highway Pavement. *Nigerian Research Journal of Engineering and Environmental Sciences.* ([link](#))

Software Developments & Contributions

BoTorch (Meta AI): Rebased pathwise condition sampling features for Bayesian optimization in PyTorch (GitHub link)	2025
TSRoots: Python package for efficient Gaussian process Thompson sampling in Bayesian optimization via rootfinding (Github link)	2024
LS-DYNA-GPS: Automated LS-DYNA Keyword file changes using QD Library (GitHub link)	2023
GPpyS: Gaussian Process Subspace Prediction, a Python Implementation (GitHub link)	2022

Academic Presentations

Optimizing Posterior Samples for Bayesian Optimization via Rootfinding International Conference of Learning Representation (Top 8% Poster @ Main Conference Track)	<i>Singapore Expo, Singapore</i> April 24—28, 2025
Gaussian Process Thompson Sampling via Rootfinding NeurIPS 2024 Workshop on Bayesian Decision-making and Uncertainty	<i>Vancouver, BC, Canada</i> December 10—15, 2025
Optimizing ADCIRC simulations using AI/ML-Based Surrogates NHERI Computational Academy at Texas Advanced Computing Center	<i>Austin, TX, USA</i> July 23—26, 2024
Digital Twin and Civil Engineering Phases: Reorienting Adoption Strategies Engineering Mechanics Institute Conference and Probabilistic Mechanics & Reliability Conference 2024	<i>Chicago, IL, USA</i> May 26—31, 2024

Work Experience

First Exploration and Petroleum Development Company <i>Visiting Graduate Research Scholar</i> Explored digital twin frameworks for large-scale engineering systems with simulation-driven decision optimization.	<i>Lagos, Nigeria</i> May 2022—July 2022
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SmartPharm <i>Graduate Research Analyst</i>	<i>Lagos, Nigeria</i> <i>August 2021—August 2022</i>
Conducted market research analysis and contributed to web-based product development for an upcoming pharma-tech startup.	
MO&A Engineering Consultancy <i>Engineering Intern</i>	<i>Lagos, Nigeria</i> <i>July 2019—January 2020</i>
Modelled, designed, and detailed multi-story buildings using computational tools such as Autodesk BIM and PROTA.	
Julius Berger Nigeria Limited <i>Engineering Intern</i>	<i>Lagos, Nigeria</i> <i>January—March 2019</i>
Involved in state-of-the-art mechanized construction of complex structures using high performance concrete.	

Core Skills

Machine / Deep Learning:	Bayesian Optimization, LLMs, Scientific Foundation Models (ViTs, Timeseries) Algorithm Development, Optimization, Probabilistic ML (GANs, VAEs, GPs, Bayesian DLs)
Programming Languages & Libraries:	Python (NumPy, Pandas, scikit-learn, PyTorch, TensorFlow, JAX), Scala/Spark (familiarity), MATLAB, Julia, R, C (familiarity)
Software Development:	Git/GitHub, HPC & distributed computing, Code Coverage and Testing, Linux
Computational Science (FEA):	LS-DYNA, Abaqus, FEniCS, Paraview, PowerBi, AutoCAD, Revit, CAD-RC, Prota

Fellowships / Grants / Awards (Selected)

NSF Strengthening Cyberinfrastructure Professional Ecosystem (SCIPE) Chishiki AI Fellowship – <i>(Research Grant)</i>	2026
Andrea Prosperetti Research Computing Student Award <i>(UH College of Engineering Most Distinguished Computing Award)</i>	2026
Los Alamos National Laboratory – Applied Machine Learning Fellowship <i>(Summer Internship)</i>	2026
Argonne National Laboratory – Given Associates <i>(Summer Internship – Declined)</i>	2026
Silver’s Reviewer Award – International Conference of Machine Learning <i>(ICML’s Top Reviewer)</i>	2026
Chevron – UH Energy Graduate Fellowship <i>(Research Fellowship)</i>	2025
ICLR Travel Award <i>(Travel Grant)</i>	2025
NeurIPS BDU Google Travel Award <i>(Travel Grant)</i>	2024
Jimmie A. Schindewolf Academic and Research Scholarship <i>(Study Grant)</i>	2024
NSF DesignSafe CI Travel Grant, University of Texas at Austin <i>(Travel Grant)</i>	2024
Cullen Fellowship Travel Grant, University of Houston <i>(Travel Grant)</i>	2024
Fellow, Blue Innovation Partnerships Consortium, Purdue University & University of Puerto Rico <i>(Research Fellowship)</i>	2023
Inclusive Excellence Admission Scholarship, University of Toronto <i>(Study Grant)</i> – Declined	2022
Winner, Circular Economy Innovation Partnership Looplab Incubation Challenge <i>(Business Grant)</i>	2022
NUTM Scholar Program <i>(Fully Funded Postgraduate Fellowship)</i>	2021
Winner, Sixth Annual Millennium Oceans Prize <i>(Research Grant)</i>	2021
NNPC/Chevron JV Scholarship <i>(Study Grant)</i>	2017–2021
Federation of Construction Scholarship <i>(Study Grant)</i>	2017–2021

Academic Affiliations and Services

United States Association for Computational Mechanics (USACM). <i>Graduate Student Member.</i>
Society for Industrial and Applied Mathematics (SIAM). <i>Graduate Student Member.</i>
Reviewer: <i>NeurIPS, ICLR, ICML, Springer, Elsevier, ASCE</i>
Undergraduate Research Mentor: <i>Sahran Ashoor (UH Electrical and Computer Engineering)</i>
Teaching Assistant: Structural Analysis (CIVE 3337); Transportation Engineering (CIVE 4337); Professional Practice in Engineering (CIVE 4311)

Volunteering / Leadership Experience

Media Coordinator, Redeemed Christian Church of God JPFAN (University of Houston)	2026
Vice President, Civil Engineering Graduate Students Organization (University of Houston)	2024–2025
Tertiary Officer, Redeemed Christian Church of God JPFAN (University of Houston)	2024
Lead, Nigerian University of Technology and Management Research Competition Team	2022
Global Admission Team Lead, United Nations Academic Impact Millennium Fellowship	2020
Campus Director, United Nations Academic Impact Millennium Fellowship	2019
Co-founder and President, Sustainable Development Advocates (University of Lagos)	2019