

James Afful

DOCTORAL RESEARCHER | APPLIED MACHINE LEARNING SCIENTIFIC COMPUTING

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SUMMARY

PhD researcher in Mechanical Engineering and Applied Scientific Computing with experience building scalable computational and machine learning pipelines for engineering and environmental systems. Background includes high-performance computing, reinforcement learning, symbolic regression, Neural Radiance Field (NeRF)-based reconstruction, data-driven modeling, and research software development across cloud and supercomputing environments. Published researcher with experience translating complex scientific problems into robust computational pipelines/workflows and decision-support tools.

EDUCATION

Iowa State University (ISU), Ames, IA

Ph.D. in Mechanical Engineering (and Applied Scientific Computing), from 2024 , and expected in December 2026

Dissertation: Computational and Artificial Intelligence Methods for Flow Simulations in the Built Environment.

Iowa State University (ISU), Ames, IA

Master of Engineering, Mechanical Engineering from 2022 completed in December, 2025

Kwame Nkrumah University of Science & Technology (KNUST), Kumasi, Ghana

B.Sc. Mechanical Engineering, June 2021

Dissertation: Design and construction of a solar-powered cocoa pod breaker and bean separator.

RESEARCH & WORK EXPERIENCE

Iowa State University (ISU), Ames, IA

Researcher, Aug 2022 – Present

Supervised by Prof. Baskar Ganapathysubramanian, Prof. Ulrike Passe, Prof. Jan Thompson, Prof. Adarsh Krishnamurthy, and Dr. Zaki Jubery

Computational Physics and Mechanics Laboratory (ComPM), Center for Building Energy Research (CBER), and Translational AI Center (TrAC)

- Developed scalable CFD pipelines for K–12 school building ventilation (HVAC design) analysis using an in-house C++ finite element code (Dendrite) based on the incompressible Navier-Stokes and heat transfer equations, supporting an Iowa Economic Development Authority state-funded study. Flow over 2D and 3D complex CAD geometries (computational physics and mechanics). Point cloud data extraction, surface reconstruction with Gaussian Splats and Nerfs, SAM v3 vision model for segmentation tasks. Using gmsh software and STL files. Computational Multiphysics modeling.
- Conducted strong- and weak-scaling HPC studies on Frontera, Nova, Stampede3, and Azure and AWS cloud computing servers using Docker and Singularity containers to determine optimal mesh and compute-node configurations.
- Used ParaView and TecPlot for scientific visualization and analysis of large-scale simulation outputs i.e., over 50 million degrees of freedom, for large-eddy simulations and RANS simulations.
- Developed a controls-based reinforcement learning framework for identifying on/off states of classrooms using airflow and temperature sensor data.
- Co-led AI-enabled environmental modeling frameworks under NSF INFEWS and AIIRA using weather/time-series forecasting and prediction techniques.
- Worked with terrestrial laser scanning (TLS) and drone thermal/LiDAR imaging for vegetation/tree surface reconstruction and related downstream computational tasks.
- Developed a Neural Radiance Field (NeRF)-based plant geometry reconstruction pipeline and digital twin.

- Developing an agentic AI pipeline for the prediction of biological threats to the United States agricultural landscape using weather data for BioSHIELD (Left-of-Boom), a DARPA-funded project. Tool integration with LangGraph and Orchestration of agents.
- Applied symbolic regression methods, including AI Feynman and PySR, for empirical approximation of environmental features in EnergyPlus (E+) and DOE-2. Used SQL databases during this project and also performed classification and regression machine learning tasks.
- Mentored and evaluated NSF REU students in weather-data collection, evapotranspiration and microclimate analysis, Python-based analysis and visualization, and related federally funded research projects.
- Modeled and simulated the evapotranspiration and cooling effects of trees and tree canopies on buildings using EnergyPlus and an in-house massively parallel C++ octree-based Navier-Stokes and heat-transfer finite element CFD code.
- Used Bayesian optimization and compared model performance using mean absolute error, R-squared, and root mean squared error across XGBoost, decision trees, and neural networks. Vision models for object detection. Design of Experiments (DOE).
- Nuclear reactor cooling system two-phase and 3-phase modeling and simulations in ANSYS.
- Time-series forecasting using multiple regression techniques and LSTM for temperature and other weather/climate effects on houses in hot and arid zones of the world.
- Co-principal investigator for an NSF ACCESS allocation supporting development of a physics simulation vision transformer (PhySiVit) using The Well dataset; presented at Supercomputing (SC'25). Allocation: CIS250757. Work was done in collaboration with the Pittsburgh Supercomputing Center.
- Teaching assistant and exam proctor for Engineering Dynamics (ME 3450), including grading, office hours, and student support for complex problem solving.
- Lead AI Engineer for the Agentic APSIM project; where I worked with a team of engineers, research scientists and agronomists to create a platform/product interface, taking away several layers of abstraction for users (farmers and scientists) to be able to use a scientific tool like APSIM to run simulations using a RAG-based (LLM GPT 5.5) and knowledge graph framework. This project was deployed on AWS and a research paper is being collated.
- Attended classes and got certificates in Natural Language Processing (Large Language Models), Nvidia CUDA Programming, Scientific Machine Learning (physics-based / physics informed learning and solvers), Agentic AI, Parallel Programming with OpenMP and MPI, Computer Vision, Deep Learning, Statistics (descriptive and inferential), Game Theory, Quantum Computing, Advanced Heat Transfer, Advanced Fluid Flow, Finite Element Method, Finite Difference Method, and Computational Mathematics. Licensed FAA drone pilot. Six Sigma White Belt.

Lawrence Livermore National Laboratory (LLNL), Livermore, CA

Mechanical Engineer, National Security Engineering Division, Summer 2024

Supervised by Dr. Francisco Javier Espinosa-Loza and Mitchell Lane

- Developed and validated high-fidelity CFD models for isotope separation under ultra-high vacuum using ANSYS Fluent (AVLIS program) on LLNL's Borax supercomputer.
- Tested evaporation rates of metals of national interest under varying temperature and vacuum conditions.
- Began replicating the computational pipeline using MFEM.
- Research outputs were integrated into national-interest evaluation workflows at LLNL.
- Wrote detailed technical reports on computational pipeline setup and findings.
- Assembled linear replacement units (LRUs) for the Scorpius accelerator project.
- Used LabVIEW programming in support of engineering tasks.
- Recognized by senior staff during the summer engineering poster competition as a top-10 engineering poster presenter.

Center for Business Development, KNUST, Kumasi, Ghana

Mechanical and Design Engineer (2021 - 2022)

- Assembles 3D PLA and ABS printers for commercialization at the university
- Provided technical mentorship for startups at the business incubator
- Organized and ran training sessions for the center on 3D printing, artificial intelligence, and other technological trends

Volta River Authority, Akosombo Hydropower Generation Station

Mechanical Engineering Intern (Summer 2018)

- Carried out maintenance at different parts of the hydropower generation station, including the intake of the dam, the Francis turbines, generators, splitter vanes, gantry cranes, and oil pumps.
- I documented progress and inspected works for quality assurance.
- Supervised other engineering interns and attended safety trainings.

SELECTED OPEN-SOURCE PROJECTS

Grid-Gent: Agentic early-stage grid scenario screener

- Built and released a lightweight assistant for electricity and utility distribution-grid what-if analysis, including load, solar, and hosting-capacity scenarios.
- Supports user-uploaded feeder data in CSV and JSON formats and emphasizes transparent, non-black-box reasoning.
- Stack: Python, FastAPI, templated UI.
- GitHub: jamesafful/grid-gent

HSGR: Heat, Smoke, and Grid Reliability data pipeline

- Built a research-grade pipeline to determine the effects of heatwaves and wildfire smoke on electricity grids.
- Produces a merged panel dataset and QA figure.
- Stack: Python, Pandas/Geo stack, Make, PyTest.
- GitHub: jamesafful/heat-smoke-grid-risk

classroom-airdist: Interactive classroom airflow recommender

- Packaged a FastAPI backend and interactive web UI for classroom air-distribution examples.
- Includes documentation and a Codespaces-friendly startup workflow.
- Stack: Python (FastAPI/Uvicorn), JavaScript UI.
- GitHub: jamesafful/classroom-airdist

SafeLease-AR: Augmented reality mobile app for property inspection reports

- Created an offline-first web app and Android TWA shell for guided property inspection checklists.
- Supports optional AR snapshots and exports timestamped, address-stamped PDF reports.
- Stack: HTML/JavaScript, jsPDF, WebXR/AR (optional).
- GitHub: jamesafful/SafeLease-AR

Nimdie Legal: A retrieval augmented generation (RAG)-based chatbot for educating Ghanaians about their rights and to give non-expert legal recommendations on what to do in certain specific situations. Tested Gemini, Claude, and ChatGPT as LLM benchmarks, and my team is currently working with a focus group to refine this idea for a journal publication in Artificial Intelligence and Law. (<https://github.com/QwadwoNyamekye/law>)

PUBLICATIONS AND SCHOLARLY AUTHORSHIP

Peer-Reviewed Journal Article

- Muhammad Arbab Arshad, Talukder Jubery, James Afful, Anushrut Jignasu, Aditya Balu, Baskar Ganapathysubramanian, Soumik Sarkar, Adarsh Krishnamurthy. "Evaluating Neural Radiance Fields for 3D Plant Geometry Reconstruction in Field Conditions." Plant Phenomics, 2023.

Conference and Workshop Publication

- Anushrut Jignasu, Ethan Herron, Talukder Zaki Jubery, James Afful, Aditya Balu, Baskar Ganapathysubramanian, Soumik Sarkar, Adarsh Krishnamurthy. "Plant Geometry Reconstruction from Field Data using NeRFs." AAAI AI for Agriculture & Food Systems Workshop, 2023.

Preprints

- James Afful. "ExplainBench: A Benchmark Framework for Local Model Explanations in Fairness-Critical Applications." arXiv.
- James Afful. "A Review of HPC-Accelerated CFD in National Security and Defense." arXiv.

- James Afful and David Oppong Nkrumah. “Performance Analysis of a Digital Legal-Literacy System in Ghana” ResearchSquare
- James Afful. “The Many Faces of a Mean–Square Identity” ResearchSquare

Manuscripts under Development

- High-Fidelity CFD Simulations for Evaluating Ventilation in K–12 Classrooms (Lead Author).
- CFD-EnergyPlus [E+] Coupled Algorithm for Urban Vegetation Microclimates (Co-Author).
- BIO-SHIELD: Agentic AI for Agricultural Biological Threat Surveillance and Risk Assessment (Co-Author)
- Semi-automated reconstruction of indoor geometry from 360-degree video for CFD-based airflow analysis in classrooms (Co-Author)

Selected Presentations

- 18th U.S. National Congress on Computational Mechanics (USNCCM18), 2025 — High-Fidelity CFD for K–12 Ventilation
- The International Conference for High Performance Computing, Networking, Storage, and Analysis (SC '25) — PhySiVit: A Physics Simulation Vision Transformer

Reviewer Roles:

- Honorary ACM member resulting from reviewing articles submitted to PEARC in 2025 & 2026
- Reviewer for the US-RSE (United States Research Software Engineering) Conference 2025 & 2026
- Reviewer for IndabaX Conference in 2024

TECHNICAL SKILLS

Programming and Scripting: Python, C++, MATLAB, LabVIEW

Machine Learning and AI: reinforcement learning, symbolic regression, neural networks, XGBoost, decision trees, Neural Radiance Fields (NeRF), Bayesian optimization, agentic AI pipelines

Scientific Computing and Visualization: ANSYS Fluent, MFEM, OpenFOAM, StarCCM+, TRACE, ParaView, TecPlot, EnergyPlus, DOE-2, COMSOL

Cloud, HPC, and Reproducibility: AWS, Azure, Docker, Singularity, Frontera, Stampede3, Nova, Borax

Data and Geospatial Tools: NumPy, matplotlib, scikit, pandas, ArcGIS

Design and Modeling Tools: SolidWorks, AutoCAD, Rhino, Grasshopper, Revit, Siemens NX

ADDITIONAL LEADERSHIP

Engineers Without Borders (EWB)

Vice President / Project Lead, 2018 – 2021

- Directed sustainable energy and water projects impacting rural communities in Ullo, Ghana.
- Helped raise close to \$45,000 for community clinic construction.
- Managed technical design reviews, funding proposals, and student-faculty teams as Projects Coordinator in Ghana.

Center for Computational Research and Education (CCRE)

Founder

- Gathered a team of African researchers in the diaspora to begin frequent training programs for students in engineering and the sciences in African Universities, to introduce them to computational research, high-performance computing, computer simulations, and other emerging technologies in the world.
- Presented at the 1st Research Software Africa Conference: On Building a Sustainable Research Software and HPC Training Pipeline in West Africa
- i. Volunteer Orientation Leadership Training Member at Large with the American Society of Mechanical Engineers (ASME 2025 - 2027)
- ii. President, Mechanical Engineering Graduate Student Organization, ISU (2024–2025)
- iii. Vice President, Emerging Leaders in Engineering (2023–2025)

- iv. Director, Student Advocacy Committee, ISU International Student Council (2023)
- v. Service Chair, Leo District 418 (2023)
- vi. Vice President, Kumasi Adehyee Leo Club (2022)
- vii. Member, Ames Evening Rotary Club and KNUST Rotaract Club