Denis Mulumba

Resume

Education

2022 - present
Computing Ph.D. with emphasis in Computational Mathematics, Science and Engineering , *Boise State University*, Boise, Idaho.

Ph.D. Research

Topic one: **A three dimensional Immersed interface method for solving the Generalized Poisson equation**.

Topic two: **Tailoring Surface Topology Maps for Enhanced Catalysis Simulations** .

Topic three: **Transition Metal Dichalcogenides with Double Vacancies as Catalysts for Efficient CO_2 Reduction to Methanol**.

2020 - 2021
Masters' in Mathematical Sciences, *African Institute for Mathematical Sciences*, Remera, Rwanda.

Masters' Project

Title: **The pseudo heat equation as an estimate of the convolution integral**.

2015 - 2019
Bachelors of Science with Education in Physics and Mathematics, *Makerere University*, Kampala, Uganda.

Work Experience

Aug. 2022 – Present
Computing Ph.D. Researcher in Applied Mathematics and Materials Science, Boise State University, *Boise, Idaho, USA*.

Conducting interdisciplinary research at the intersection of numerical methods and computational materials science, with a focus on solving partial differential equations and modeling catalytic processes for CO_2 reduction.

- Developed high-accuracy solvers for elliptic PDEs on irregular domains using the Immersed Interface Method (IIM).
- Designed $3D$ numerical schemes for anisotropic jump conditions using spherical harmonics and radial basis function (RBF) interpolation.
- Simulated catalytic surfaces and reaction pathways for CO_2 conversion to methanol using density functional theory (DFT) and machine learning models.
- Analyzed catalyst stability, reaction energetics, and selectivity using Python-based computational chemistry tools.
- Integrated HPC workflows for large-scale simulations across math and material science domains.
- Presented research findings at national conferences and contributed to peer-reviewed publications.
- Mentored undergraduate researchers in applied math, numerical simulation, and computational chemistry.

Oct. 2021 - Feb 2022
VoxCroft Analytics Technology, Information and Internet, *South Africa*.
Collecting language related data and quality assurance

July 2017. - Mar. 2020	**High school Mathematics and Physics teacher, Universal High school Kisaasi**, *Kampala,Uganda*.
	Teacher or math and physics, Assistant director of studies

Certifications, Achievements and Awards

April 2025	CASCADE Rain travel award 2025
Aug. 2024	Best Oral Presenter at the symposium "Accelerating Catalytic Advancements Through the Precision of High-Throughput Experiments and Calculations" at the ACSFALL 2024 conference
2022	Events manager for Society for Industrial and Applied Mathematics Boise State Chapter.
2020 - 2021	MasterCard Foundation Scholarship awarded a fully funded Scholarship to study at African Institute for Mathematical Sciences (AIMS).
2018	Bachelors of Science with education in Physics and math

Relevant Skills

OS	Windows, Linux, macOS
Softwares	Microsoft Office, LibreOffice, Tensorflow, Pytorch LaTeX
Programming	Python, R, MatLab, C

Publications

April 2025	da Silva, T. H., Lu, J., Cortright, Z., Mulumba, D., Khan, M. S., and Andreussi, O. (2025). Automating the Analysis of Substrate Reactivity through Environment Interaction Mapping. Journal of Chemical Information and Modeling.

Languages

Luganda	Fluent (mother tongue)
English	Fluent

References

Name	Prof. Oliviero Andreussi
Position	Falculty Member, Boise State University, Boise, Idaho
Email	olivieroandreuss@boisestate.edu

Name	Prof. Donna Calhoun
Position	Falculty Member, Boise State University, Boise, Idaho
Email	donnacalhoun@boisestate.edu

Name	Prof.Grady Wright
Position	Falculty Member, Boise State University, Boise, Idaho
Email	gradywright@boisestate.edu