# **Benjamin Jones**

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#### **Education**

Ph.D. Mathematics, Michigan State University

2021-2026

Graduate biochemistry courses in protein structure and function

M.A. Mathematics (4.0 GPA), University of Alabama at Tuscaloosa

May 2021

**Thesis:** "Adaptive pseudo-time methods for the Poisson-Boltzmann equation with Eulerian solvent excluded surface."

**Graduate computer science courses** in artificial intelligence, programming languages, and cryptography

B.S. Computer Science (4.0 GPA), University of Alabama at Tuscaloosa

Dec 2020

B.S. Mathematics (4.0 GPA), University of Alabama at Tuscaloosa

May 2020

Minor: Randall Research Scholars Program

Study Abroad: Budapest Semesters in Mathematics, Hungary

Summer 2019

# **Research Experience**

### Michigan State University

2021-Present

Principal Investigator: Guowei Wei

- Developed and implemented a mathematical data structure, called the Persistent Directed Flag Laplacian (PDFL), in **Topological Data Analysis** (TDA) to analyze directed clique/flag complexes on graphs.
- Analyzed topology of protein-ligand complex with PDFL implementation (C++ and MATLAB). We are currently collaborating to apply this to a larger set of protein-ligand complexes to **predict binding affinity** with machine learning.
- Currently generalizing the implementation of the PDFL to a C++ library with **Python** bindings for researchers to analyze multiple Persistent Laplacian models. Algorithmic and implementation improvements reduce computations from 1.5 hours to 12 seconds.

#### University of Alabama

2017-2021

Principal Investigator: Shan Zhao

• Used a Proportional Integral Derivative (PID) controller to adaptively choose the time step in the numerical solution of a nonlinear PDE, the Poisson-Boltzmann Equation, to save 84% CPU time with 0.06% relative error in computing the **solvation energy** of proteins.

## **Papers and Preprints**

- 1. **Benjamin Jones** and Guowei Wei. "Persistent Directed Flag Laplacian." <u>arXiv:2312.02099</u> [math.AT], Dec. 2023.
- 2. S. A. Ullah, X. Yang, **B. Jones**, S. Zhao, W. Geng, G.-W. Wei. "Bridging Eulerian and Lagrangian Poisson–Boltzmann solvers by ESES." *J. Comput. Chem. 2023*, *1. DOI:* <u>doi.org/10.1002/jcc.27239</u>.
- 3. **Benjamin Jones**, Sheik Ahmed-Ullah, Siwen Wang, and Shan Zhao. "Adaptive pseudo-time methods for the Poisson-Boltzmann equation with Eulerian solvent excluded surface." *Communications in Information & Systems*, (2021). DOI: <a href="https://dx.doi.org/10.4310/CIS.2021.v21.n1.a5">dx.doi.org/10.4310/CIS.2021.v21.n1.a5</a>

# **Teaching**

Graduate Machine Learning, MSU (TA)	Fall 2023
Calculus III, MSU (Instructor)	Summer 2023
Calculus II, MSU (TA)	Fall 2022

### **Professional Experience**

### Virtual Scholarship for Service Intern, NOAA Fisheries

Jan 2021 – Sept 2021

- Automated resource allocation for the National Coral Reef Monitoring Program.
- Unified SAS and R programs into an accessible R package for fish biologists.

### Computer Science Intern, U.S. Census Bureau

Aug 2020 – Jan 2021

- Developed **Python** software for processing Economic Census data.
- Improved CPU efficiency of a key data processing task by over 95%.
- Implemented robust unit testing.

# **Awards and Honors**

Michigan State University College of Natural Sciences Recruiting Fellowship	021-2022
Tau Beta Pi Engineering Honors Society	2020
Outstanding Senior, Randall Research Scholars Program	2020
Phi Beta Kappa	2020
Randall Outstanding Undergraduate Research Award, the top undergraduate research award at Alabama	
Upsilon Pi Epsilon Computer Science Honors Society	2019

### Service

MSU Graduate Employees Union Math Department Steward	2023-2024
MSU Graduate Employees Union Salary Bargaining Team	2023-2024
MSU Graduate Employees Union Retirement Benefits Bargaining Team	2023-2024
Organizing Committee, Graduate Student Geometry and Topology Conference 2024	2023-2024
MSU Summer Topology Program Mentor	2023
President, Upsilon Pi Epsilon Computer Science Honors Society	2020
President, Pi Mu Epsilon Math Honors Society	2019