Brian **Andrews**

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Summary

I am a computational scientist and software developer with a background in physics who wants to develop, support, and contribute to computational tools and infrastructure which support the advancement of biophysical research capabilities and lead to scientific discoveries with concrete societal benefits.

Experience

Bucher-Jackson Postdoctoral Fellow - Bryn Mawr College *2023-Present*

- Developed a production-grade software package for bi-level optimization of RNA sequence and structure using simulated hybrid classical and quantum computing workflows. The software utilizes relational databases, includes functionality for resuming optimizations, and I deployed a mini slurm cluster to facilitate long-term optimizations.
- Developed a python package to determine transport properties of 2D corals, represented as connected graphs, using differential geometry to investigate species-specific resistance to global warming.
- Taught Condensed Matter Physics, Physics of Computers, and Introductory Labs.

Research Assistant - Drexel University *2018-2023*

Installed, maintained, and managed molecular dynamics simulation and analysis software on lab servers and the university HPC. Created and documented computational workflows for lab members conducting simulation and analyses leading to multiple publications.

Open Source Contributor - GROMACS, OpenMM

Above includes hyperlinks to contributions.

Systems Administrator - Drexel University *2020-2023*

Responsible for hardware maintenance, networking, deploying, and managing backups of Physics department Linux servers.

Analytics Contributor - Pro Lacrosse Talk *2020-2022*

Constructed a machine learning model to compute in-game win probabilities.

Operations Intern - OptoQuest *2017-2018*

Deployed a logistic regression model to predict postoperative risk for eye surgery patients with patient and structural data.

Data Science Associate - MedaSync *2017-2018*

Constructed a self-updating machine learning cost prediction model in a production AWS environment.

Education

Ph.D. Physics - Drexel University *2018 - 2023*

M.S. Physics - Case Western University *2016 - 2018*

B.A. Physics - Kenyon College *2012 - 2016*

Skills

Programming Languages	Python, C(++), Bash, SQL
Dev Experience	Git, ML (sklearn, tensorflow), Unit Testing, Databases, Data Visualization (Seaborn, Labplot, Google Looker Studio), Big Data (Dask)
Computing Experience	HPC (Drexel URCF, UT XSEDE, Bryn Mawr Athena), Cloud Computing (AWS) in Linux environments, Virtual Machines (Proxmox, VirtualBox), Virtual Environments (Virtualenv, Conda, Docker), Slurm

Selected Research & Publications

4. **B. Andrews**, J. Abraham, A. Radja, D. Fox. Limitations of RNA Folding as a Quadratic Unconstrained Binary Optimization Problem: Implications for Applicability of Modern Quantum Computers. **In Progress**.
3. **B. Andrews**. Amino Acid Residue-Specific Ramachandran Distributions Derived from a Simple Mean Field Potential. *Physical Chemistry AU*, 2024, 4, 6, 707–719.
2. **B. Andrews**, T. Ruggiero, and B. Urbanc. How do salt and lipids affect conformational dynamics of Aβ42 monomers in water? *Phys. Chem. Chem. Phys.*, **25**, 2566–2583, 2023.
1. **B. Andrews**, J. Guerra, R. Schweitzer-Stenner, and B. Urbanc. Do molecular dynamics force fields accurately model ramachandran distributions of amino acid residues in water? *Phys. Chem. Chem. Phys.*, **24**, 3259-3279, 2022.