Fernanda Cristina Bononi (Meer)

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Education

University of California, Davis, 2021
PhD in Computational/Theoretical Chemistry. Advisor: Davide Donadio.
University of Western Ontario, 2014
MSc in Chemistry and Molecular Imaging. Advisor: Leonard Luyt.
University of São Paulo, 2009
Bachelor of Science in Pharmacy and Biochemistry.

Experience

Postdoctoral Scholar - University of North Texas Jan '21 – April '22

- Assisted with implementation and improvement of Environ, an implicit solvation plug-in for Quantum Espresso. My work included compiling, benchmarking, and debugging, with the use of version control systems (Git).
- Designed tutorials and hands-on workshop lectures directed at students and researchers on techniques available in Quantum Espresso with the Environ plugin.
- Used Bash to create workflows for molecular dynamics simulations and posterior data analysis using Python.
- Used Python to predict properties of large water systems from molecular dynamics simulation data.
- Performed and analyzed MD simulations on high-performance computing (HPC) environments.

PhD Student Researcher - University of California, Davis Sep '14 – Dec '20

- Research on predicting properties of organic molecules by using ensemble and time-series analysis using Python.
- Collaborated with the implementation of Machine Learning algorithms to model the absorption spectra of organic molecules on ice surfaces. Results published in: Atmospheric Chemistry and Physics (2022), Journal of Chemical Theory and Computation (2022) and The Journal of Physical Chemistry A (2020).
- Used open-source MD software in HPC environments. Acquired extensive experience with shared memory and distributed memory parallelism (MPI and OpenMP) and accelerators (GPU).
- Built, installed, and debugged parallel codes in local Linux machines and HPC environments.
- Performed benchmarking of application codes in HPC environments, developed regression tests.
- Contributed to numerous multidisciplinary scientific publications and presented in numerous conferences.
- Served as Instructor for organic chemistry classes.

Technical Skills

- Python (Scypy, Numpy, Pandas, Matplotlib, Plotly)
- HTML
- CSS
- JavaScript
- MD simulations (LAMMPS, GROMACS, CP2K, Quantum Espresso)
- Bootstrap, jQuery, SASS, React, Redux, Vue.js
- Flask
- SQL
- Git
- Bash

Certificates

- Responsive Web Design. freeCodeCamp.
- JavaScript Algorithms and Data Structures. freeCodeCamp.
- Learn Vue.js. Codecademy.
- Learn jQuery Course. Codecademy.