JASON M. SWAILS, PH.D.

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Education

2008–2013 UNIVERSITY OF FLORIDA
Gainesville, FL, 32611
Ph.D. in Computational Chemistry, August 2013

2005–2008 BINGHAMTON UNIVERSITY
Binghamton, NY 13851
Bachelor of Arts in Chemistry, May 2008
Summa cum Laude

2004–2005 ROCHESTER INSTITUTE OF TECHNOLOGY
Rochester, NY 14623
Transfer to Binghamton University, GPA 4.0

Research Experience

August 2013–Present
Postdoctoral Researcher with Prof. David Case, Rutgers University, BioMaPS

- Developing empirical and density functional-based models for predicting chemical shifts in the NMR spectra of nucleic acids
- Evaluating and improving the AMOEBA polarizable force field and developing tools that implement it efficiently

June–July 2014
OpenMM Visiting Scholar with Prof. Vijay Pande's, Stanford University, Simbios

- Expanded OpenMM's capacity to implement various force fields with the aim of aiding X-ray crystallography refinement

August 2012–August 2013
Visiting Researcher with Prof. Darrin York, Rutgers University, BioMaPS

- Developed a novel method for simulating complex biological systems at constant pH

Summer 2012
Summer Intern, GlaxoSmithKline

- Programmed an efficient, free energy-based water mapping technique called SPAM for use in drug discovery
- Implemented performance-critical aspects of SPAM in the *AmberTools* program *cpptraj* using C++
- Programmed a user-friendly interface in Python for performing full SPAM analysis (*SPAM.py*)
  - *SPAM.py* can be operated via a command-line interface for batch processing
  - *SPAM.py* can be operated via a GUI written with the *Tkinter* toolkit for easy use

August, 2008–August, 2013
Research Assistant, University of Florida

- Developed new methods to treat *pH* effects explicitly in models of biological systems at an atomic level of detail.
- Supported and extended the *AMBER* program suite, one of the most popular suites of programs used for biomolecular simulation

February–May, 2011
Visiting Researcher with Prof. Ross Walker, University of California at San Diego, SDSC

- Implemented feature enhancements in a high-performance, *GPU*-accelerated molecular dynamics program in *AMBER* called *pmemd.*
- Implemented an efficient version of *Replica Exchange Molecular Dynamics* in *pmemd.*

October–December, 2010
Visiting Graduate Student with Prof. Darrin York, Rutgers University, BioMaPS

- Developed and implemented a new method for simulating biological systems at constant *pH* in a molecular dynamics program in *AMBER.*

June–August, 2008
Undergraduate Researcher, Unversidad de Buenos Aires, Química Inorgánica, Analítica y Química Física

- Modeled the nitrous oxide release mechanism of the heme protein *Nitrophorin-2.*

June–August, 2007
Undergraduate Researcher, University of Florida

- Analyzed the mechanism of Trypanosoma Cruzi's Trans-sialidase enzyme using mixed quantum-mechanical and classical-mechanical methods.

March–August, 2006
Analytical Laboratory Technician, Sanmina-SCI, Owego, NY

- Analyzed chemical baths used for circuit board printing to maintain a strict level of quality control for the manufacturing process.

Teaching Experience

2014
Instructor for AMBER Workshop, Rutgers University, New Jersey

- Developed materials to help new students learn how to carry out computational biochemistry experiments
- Helped develop interactive tutorials demonstrating how to use AMBER

2012
Instructor for AMBER Workshop, CECAM, Lausanne, Switzerland

- Developed and presented lectures on various topics relating to both the theory and practice of running biomolecular simulations with AMBER programs to a diverse set of students, graduate students, and postdoctoral researchers
- Developed interactive tutorials to demonstrate various computational techniques
- Provided assistance when necessary during the hands-on tutorials

2011
Instructor for AMBER Workshop, Barcelona Supercomputing Center, Barcelona, Spain

- Developed and presented lectures on various topics of biomolecular simulation using the AMBER software suite to a diverse set of students, graduate students, and postdoctoral researchers
- Developed a variant of a *Linux* operating system to provide the workshop attendees with a hands-on tutorial experience.
- Developed several hands-on tutorials to demonstrate various simulation techniques
- Provided assistance when necessary during the hands-on tutorials

2011
Developed and Maintained Instructional Wiki Website

- Developed an educational Wiki to serve as a tutorial and a resource for installing and using a variety of computational programs and APIs (http://jswails.wikidot.com)
- Featured on the Amber website, http://ambermd.org

2008–09
Teaching Assistant for Physical Chemistry, University of Florida

- Held office hours for students to provide assistance out of class.
- Developed problems for homework assignments as well as quizzes and exams.
- Graded homework assignments, quizzes, and exams.
- Developed and presented lecture material when Professor was absent.

2007–08
Teaching Assistant for General Chemistry, Binghamton University

- Held office hours for students to provide assistance out of class.
- Instructed students regarding proper laboratory procedures.
- Graded laboratory reports, quizzes, and exams.

Publications

- Swails, Jason M., Zhu, Tong, He, Xiao, and Case, David A., "AFNMR: Automated Fragment Quantum mechanical Calculation of NMR Chemical shifts for Biomolecules," **2014**, *In preparation*
- Dissanayake, Thakshila, Swails, Jason M., Roitberg, Adrian E., and York, Darrin M. "Interpretation of pH-activity Profiles for Acid-Base Catalysis from Molecular Simulations," *Biochemistry*, **2014**, *In review*
- McGibbon, Robert T., Beauchamp, Kyle A., Schwantes, Christian R., Wang, Lee-Ping, Hernández, Carlos X., Harrigan, Matthew P., Lane, Thomas J., Swails, Jason M., and Pande, Vijay S., "MDTraj: a modern, open library for the analysis of molecular dynamics trajectories," *bioRxiv*, **2014**, DOI: http://dx.doi.org/10.1101/008896
- Swails, Jason M., York, Darrin M. and Roitberg, Adrian E. "Constant pH Replica Exchange Molecular Dynamics in Explicit Solvent Using Discrete Protonation States: Implementation, Testing, and Validation," *J. Chem. Theory Comput.,* **2014**, v. 10 (3) p. 1341
- Bergonzo, Christina, Henriksen, Niel M., Roe, Daniel R., Swails, Jason M., Roitberg, Adrian E., and Cheatham III, Thomas E., "Multi-dimensional Replica Exchange Molecular Dynamics Yields a Converged Ensemble of an RNA Tetranucleotide," *J. Chem. Theory Comput.,* **2014**, v. 10 (1) p. 492
- Cui, Guanglei, Swails, Jason M., and Manas, Eric S. "SPAM: a simple approach for profiling bound water molecules," *J. Chem. Theory Comput.,* **2013**, v. 9 (12), p. 5539
- Swails, Jason M. and Roitberg, Adrian E., "Enhancing Conformation and Protonation State Sampling of Hen Egg White Lysozyme Using pH Replica Exchange Molecular Dynamics", *J. Chem. Theory Comput.*, **2012**, v. 8 (11) p. 4393
- Miller III, Bill. R., McGee, T. Dwight, Swails, Jason M., Homeyer, Nadine, Gohlke, Holger, and Roitberg, Adrian E., "MMPBSA.py: An Efficient Program for End-State Free Energy Calculations", *J. Chem. Theory Comput.*, **2012**, v. 8 (9), p. 3314

- D.A. Case, T.A. Darden, T.E. Cheatham, III, C.L. Simmerling, J. Wang, R.E. Duke, R. Luo, R.C. Walker, W. Zhang, K.M. Merz, B. Roberts, S. Hayik, A. Roitberg, G. Seabra, J. Swails, A.W. Goetz, I. Kolossváry, K.F. Wong, F. Paesani, J. Vanicek, R.M. Wolf, J. Liu, X. Wu, S.R. Brozell, T. Steinbrecher, H. Gohlke, Q. Cai, X. Ye, J. Wang, M.-J. Hsieh, G. Cui, D.R. Roe, D.H. Mathews, M.G. Seetin, R. Salomon-Ferrer, C. Sagui, V. Babin, T. Luchko, S. Gusarov, A. Kovalenko, and P.A. Kollman (2012), *AMBER 12*, University of California, San Francisco
- Jeletic, M., Lowry, R., Swails, J., Ghiviriga, I., Veige, Adam., "Synthesis and Characterization of κ-2-*bis-N*-Heterocyclic Carbene Rhodium(I) Catalysts: Application in Enantioselective Arylboronic Acid Addition to Cyclohex-2-enones," *J. Organomet. Chem.*, **2011**, v. 696 (20), p. 3127
- Swails, J., Meng, Y., Walker, A., Martí, M., Estrin, D., Roitberg, A., "Common pH Dependent Mechanism of Nitric Oxide Release in Nitrophorins 2 and 4," *J. Phys. Chem. B.,* **2009**, v. 113 (4), p. 1192
- Seabra, G., Swails, J., Roitberg, A., "Mixed Quantum-Classical Calculations in Biological Systems," Book Chapter, Editors Tai-Sung Lee, Darrin M. York, *Multi-Scale Quantum Models for Biocatalysis: Modern Techniques and Applications: A volume in CHALLENGES AND ADVANCES IN COMPUTATIONAL CHEMISTRY AND PHYSICS.* Jerzy Leszcynski (series editor), **2008**.

Presentations

- Swails, J., "Simulations at Constant pH", *Memorial Sloan-Kettering Cancer Center*, Invited speaker, New York, NY, June, **2014** (Talk)
- Swails, J., "Molecular Modeling and Computational Chemistry," *Lafayette University*, Invited speaker, Easton, PA, April, **2013** (Talk)
- Swails, J., Roitberg, A. E., "Enhancing Conformation and Protonation State Sampling with Constant pH Replica Exchange Molecular Dynamics", *Joint CHARMM-Amber Meeting*, National Institute of Health, Rockville, MD, July, **2012** (Talk)
- Swails, J., Roitberg A. E., "Including pH Effects in Simulation Using Discrete Constant pH Molecular Dynamics", *Sanibel Symposium*, St. Simons Island, GA, Feb., **2012** (Poster)
- Swails, J., Miller III, Bill, Fanucci, Gail E. and Roitberg A. E., "Effect of pH on protein conformation and function in GM2-activator protein", *National ACS Meeting and Exposition*, San Francisco, CA, April, **2010** (Poster)
- Swails, J., Meng, Y., Martí, M., Estrin, D., Roitberg, A. "pH-Dependent Mechanism of Nitric Oxide Release in Nitrophorins 2 and 4," *Sanibel Symposium*, St. Simons Island, GA, Feb., **2009** (Poster)
- Swails, J., Demir, O., Seabra, G., Roitberg, A., "Mixed Quantum/Classical Studies of Trypanosoma Cruzi's Trans-sialidase," *National ACS Meeting and Exposition*, New Orleans, LA, April, **2008** (Poster)

Accomplishments and Awards

2014	OpenMM Visiting Scholar
2012	ACS Comp. Chem. Kollman Award
2010	Chemical Computing Group Excellence Award Travel Grant
2009	National Science Foundation Graduate Research Fellowship
2008	University of Florida Alumni Fellowship Award

2008 ACS Undergraduate Award—Top graduating senior at Binghamton University chosen by chemistry faculty

2007 National Science Foundation, Research Experience For Undergraduates Travel Award

2007 National Science Foundation Research Experience For Undergraduates Fellowship, University of Florida

Professional Organizations

- *American Chemical Society Member, 2008 – Present*
- *AMBER software developer, 2008 – Present (http://ambermd.org)*
- *OMNIA software developer,* 2014 – *Present (http://omnia.md)*

Role and Contributions to AMBER Software Package

- Listed as a major contributing author
- Major contributor to improving package maintenance and usability
- Major contributor to community e-mail list supporting the Amber software suites
- Active author of documentation, regression tests, and unit tests
- Added a scalable implementation of *Replica Exchange Molecular Dynamics* to the *pmemd* program in Fortran
- Added a scalable implementation of *constant pH Replica Exchange Molecular Dynamics* to the *sander* program in Fortran
- Principal author of *MMPBSA.py*: popular Python program for performing MM/PBSA free energy calculations
- Author of *parmed.py*: Python program that modifies AMBER Topology files from user command-line input
- Author of *xparmed.py*: GUI version of *parmed.py* written with the *Tkinter* GUI toolkit
- Author and architect of *update_amber*: Automatic updating script written in Python to download and apply bug fixes from the AMBER website
- Found and fixed numerous bugs in C, C++, and Fortran code written by both myself and others (both serial programs and MPI-parallelized programs)
- Generated instructional material to aid users in using Amber
- Designed and implemented an application programmer interface (API) to the *sander* molecular dynamics engine for Fortran, C, C++, and Python.
- Implemented DIIS to accelerate SCF convergence for induced dipoles in the *pmemd* program.

Role and Contributions to OpenMM Software Package

- Listed as a contributing author
- Found and fixed several bugs
- Improved integration of the Amber force field and use of AMBER files within OpenMM
- Designed and wrote support for the CHARMM force field and use of CHARMM files within OpenMM

Programming and Computer Skills

Python programming experience

- Writing production code released to the computational chemistry community since 2009
- *Python* standard library
- *Python* scientific programming ecosystem, including *numpy*, *scipy*, *matplotlib*, *pandas*, etc.
- Improving performance and linking to C/Fortran libraries by extending CPython through its C-API
- Debugging *Python* code using the *Python* debugger (*pdb*) and the interactive interpreter, including with C extensions
- Familiar with interfacing C/C++ code using *Cython* and *SWIG*
- Profiling and optimizing pure *Python* code, including with the JIT-optimized *pypy* implementation
- Python GUI programming using the *Tkinter* interface
- Supporting *Python* 2 and *Python* 3 in the same code base

Static typed language experience

- *Fortran* programming languages (Fortran 77 through modern standards), since 2008
- *C/C++* programming languages, since 2012
- Limited *CUDA C* programming language for *Graphics Processing Units*

Parallel programming experience

- *Message Passing Interface* (*MPI*) parallel programming for *Fortran* and *C/C++*
- *OpenMP* shared memory parallelism
- High performance computer clusters, queuing and scheduling systems, and UNIX environment management

Software engineering experience

- *git* distributed version control system (very experienced, since 2009)
- *Mercurial* distributed version control system to a lesser extent
- Among the most active contributors to both the OpenMM (https://github.com/pandegroup/openmm) and Amber (http://ambermd.org/contributors.html) program suites.
- Writing efficient, comprehensive unit tests
- Continuous integration (e.g., Travis-CI on Github)
- Debugging tools such as the GNU Debugger (*gdb*), Intel Debugger, and *valgrind*

Operating System, program, and scripting experience

- Shell scripting (e.g., *bash* and *tcsh*)

- *awk* processing language
- Experienced with *Linux/Unix*, *Mac OS X*, and *Windows* operating systems
- *Amber* program suite
- *OpenMM* high-performance molecular simulation library
- *Gaussian* quantum chemistry program
- *gnuplot* program
- *Visual Molecular Dynamics* (*VMD*) program