Daniel L. Parton

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Technical Skills

Python	7 years; numerical/scientific computing, data handling and analysis, parallel computing, bioinformatics, scalable code design; packages—numpy, pandas, scikit-learn, theano (some), SQLAlchemy, lxml, Flask, jinja, matplotlib, mpi4py, nosetests, setuptools, conda.
Web development	2 years; JavaScript, HTML5, CSS3, knockout.js, Bootstrap, Python Flask, MySQL, SQLite, RESTful APIs, nginx, Apache.
Other languages	bash, SQL, XPath. Some experience: C, C++, R, MATLAB, CUDA.
General	GitHub, git, svn, Travis CI, Sphinx, Docker, Amazon AWS, vim, LaTeX, OS X, Linux, Windows.

Experience

2012–pres Memorial Sloan Kettering Cancer Center, New York, NY
Postdoctoral Research Fellow, Computational Biology Center | *Advisor*: John D. Chodera

- Investigation of conformational networks in cancer-associated proteins using GPU-accelerated simulations, clustering techniques and Markov models.
- Developed MSMSeeder—pipeline for generating diverse structural ensembles as seeds for massively parallel simulations of proteins.
- Developed TargetExplorer and kinomeDB—database application for aggregating biological data for a target protein family, with RESTful API and frontend web client (in development).
- Data-driven selection of kinase sequences suitable for bacterial expression.
- 3 first-author papers in preparation.
- Closely involved with design and purchase of a HPC cluster (960 cores, 120 GPUs) and an integrated robotic platform for biological experiments.
- Attended Hacker School—a three month, self-driven, collaborative programming course. I worked primarily on my research projects, particularly focusing on scalable software design. I also completed online courses in machine learning and algorithms, a Kaggle competition, and a JavaScript game.

2011–2012 University of Chicago
Postdoctoral Scholar, Department of Chemistry | *Advisor*: Gregory A. Voth

- Applied advanced computer simulation techniques and free energy calculations to the study of the actin cytoskeleton. One paper as first author (in press).

2007–2011 University of Oxford
Graduate Student Researcher, Department of Biochemistry
Advisors: Mark S. P. Sansom (Oxford) and Ross Nobes (Fujitsu Laboratories of Europe)

- Studied complex multi-protein systems using physics-based molecular simulations, developed software tools for simulation analysis, contributed to MDAnalysis, and led organic chemistry tutorials. Co-authored 5 papers, 3 as first author. Results presented at many national and international conferences, and in national scientific magazines.

2005–2007 University of Bristol and GlaxoSmithKline, UK
Undergraduate Researcher / Industrial Placement Student | *Advisor*: Chris Willis

- Conducted the design and synthesis of drug candidates, as a member of medicinal chemistry teams at Bristol (6 months) and GSK (1 year). Co-authored one paper.

Education

2007–2011 **D.Phil. in Biochemistry, University of Oxford**
2003–2007 **M.Sci. in Chemistry with Industrial Experience, University of Bristol, UK**