Daniel L. Parton

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Technical Skills

Python	7 years experience; numerical/scientific computing, data handling, parallel computing, bioinformatics, scalable code design; packages—numpy, pandas, scikit-learn, theano (some), SQLAlchemy, lxml, Flask, jinja, matplotlib, mpi4py, nosetests, setuptools, conda.
Full-stack web development	2 years experience; 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, UK**
2003–2007 **M.Sci. in Chemistry with Industrial Experience, University of Bristol, UK**