

# Daniel L. Parton

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## Technical Skills

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

## Experience

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- 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

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