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ADRIAN W. LANGE

SCIENTIST + DEVELOPER

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EMPLOYMENT

Postdoctoral Appointee — **Argonne National Laboratory, Leadership Computing Facility** — **March 2012 – Present**

- Developed novel algorithms for massively parallel chemistry simulations on IBM Blue Gene/Q supercomputer
- Increased simulation code speed more than 8x, scalability to ∼0.4 million cores (C++, C, Python, MPI, OpenMP)
- Created quantum proton transport model, implemented in Newtonian dynamics interface code (Python, C++, MPI)
- Assisted University of Chicago research group and workshop attendees with running/improving code

Ph.D. Student Researcher — **The Ohio State University** — **June 2007 – March 2012**

- Published 10 first author journal articles, 230+ total citations, h-index 6 (for listing, see my Google Scholar Citations)
- Presented quantum chemistry research orally over 20 times at professional events/conferences
- Invented new mathematical model for solvent electrostatics, new algorithm for building molecule surfaces
- Implemented force fields, solvent models, parallel linear algebra solvers in Q-Chem (C++, C, Fortran, MPI, OpenMP)
- Led recitations and conducted exams as teaching assistant for physical chemistry courses

EDUCATION

Columbus, OH — **The Ohio State University** — **August 2003 – March 2012**

- **Ph.D.** Computational/Physical Chemistry, March 2012 (GPA: 3.65)
- **B.S.** Chemistry with minor in Microbiology, June 2007 (GPA: 3.39)

  Coursework:
  - Graduate/Undergraduate: Quantum mechanics, Statistical mechanics, Computational chemistry, Multivariable calculus, Linear algebra, Differential equations, Computer programming, Numerical methods
  - Udacity (online): Web development, GPU programming, Programming languages
  - Coursera (online): Machine learning, Data science, Algorithms, Databases

TECHNICAL SKILLS

- **Proficient**: C++, C, Python, Unix/Linux shell (csh, bash), awk, OpenMP, MPI, LaTeX
- **Familiar**: HTML, CSS, JavaScript, jQuery, SQL, Java, Fortran, Pthreads, CUDA, CVS, SVN, git

ADDITIONAL EXPERIENCE/PROJECTS

View some code I have written at GitHub: https://github.com/awlange

- **Q-Chem v4.0** (2009–2013): Lead author of polarizable continuum model and QM/MM codes in commercial software package, Q-Chem; one of six software design committee members (C++, C, Fortran)
- **LAMMPS Ensembles** (2013): Multi-copy communication interface to open-source software, LAMMPS; contributions to main LAMMPS source code (C++, C, MPI, OpenMP, Python)
- **Personal Webpage** (2013): http://scientistdeveloper.appspot.com/ (HTML, CSS, JavaScript, jQuery, Python)
- **FMO-MS-RMD** (2013): Proton transport fragment simulator; interfaced with Q-Chem (Python, C++, MPI)
- **DESMO** (2011): Highly parallel solvent model code; genetic algorithm dynamic load balancing (C++, OpenMP, MPI)

HONORS AND AWARDS

- Chair's Prime Choice presentation in Computational Division at American Chemical Society Conference (2013)
- Presidential Fellowship from The Ohio State University Graduate School (2011–2012; $33,150)
- Chemical Computing Group Research Excellence Award from American Chemical Society (2012; $1,150)
- Travel Fellowship to present at American Conference on Theoretical Chemistry (2011; $600)
- U.S. Department of Energy Merit Scholarship for top poster presentation (2010; $400)
- American Society for Microbiology Undergraduate Research Fellowship (2006; $4,000)
- Ohio State Arts & Sciences Undergraduate Honors Research Scholarship (2006; $3,500)