Adrian W. Lange

Scientist + Developer

Employment

Software Developer **August 2013 – Present**

Signal (formerly known as BrightTag)

- Develop data models and algorithms to construct, merge, and analyze user profile data networks from multiple channels for millions of requests per day; stored in distributed NoSQL database with billions of records (∼20 TB) [Java, Cassandra, Python, R]
- Research and implement solutions for a scalable, hybrid real-time/batch process data pipeline for user segmentation [Python, Java, Redis, Cassandra]; experimenting with Hadoop, Spark, Kafka, and Scala
- Created real-time anomaly detection and network traffic forecasting system using Fourier analysis capable of predicting regular traffic patterns for upcoming week with >90% accuracy [Java, Python, SciPy, Storm, MongoDB]
- Built client data reporting web app to display inter-client clustering (via principal component analysis) and user interaction frequency trends [Python, Flask, SciPy, JavaScript, D3.js, Cassandra]

Postdoctoral Appointee **March 2012 – August 2013**

Argonne National Laboratory Leadership Computing Facility / University of Chicago

- Optimized and developed massively parallel physics/chemistry simulations on IBM Blue Gene/Q supercomputer; increased simulation speed more than 8x, scalability to ∼0.4 million CPU cores [C/C++, MPI, OpenMP, Python]
- Devised novel quantum mechanical proton transport model based on electronic structure theory; developed model via numerical/statistical optimization techniques (simulated annealing, linear regression, swarm intelligence)

Ph.D. Student Researcher **June 2007 – March 2012**

The Ohio State University

- Published 10 first author journal articles; presented at 20+ professional and academic events
- Invented model for screened solvent electrostatics, geometrical algorithm for constructing molecule surfaces, stochastic optimization (genetic algorithm) for load balancing numerical integrals; applied to simulate excited electrons in DNA

Education

Ph.D. Computational/Physical Chemistry **June 2007 – March 2012**

The Ohio State University

Dissertation: “Multi-layer Methods for Quantum Chemistry in the Condensed Phase: Combining Density Functional Theory, Molecular Mechanics, and Continuum Solvation Models” (view PDF)

B.S. Chemistry, minor Microbiology **August 2003 – June 2007**

The Ohio State University

Formal Coursework:

Quantum Mechanics, Statistical Thermodynamics, Molecular Biology, Computational Chemistry, Chemical Physics, Multivariable Calculus, Linear Algebra, Differential Equations, Computer Programming, Numerical Methods

Supplementary Online Coursework:

Udacity: Web Development, Programming Languages, Machine Learning
Coursera: Data Science Signature Track, Machine Learning, Algorithms, Databases

Technical Skills

Experience	Languages	Tools/Technologies
Proficient	Java, Python, C/C++, Unix/Linux shell (bash), awk	NoSQL (Cassandra), git, vim, LaTeX, MPI, OpenMP
Familiar	R, HTML, CSS, JavaScript (node.js), Fortran	SQL (MySQL), Redis, Flask, Maven, Guava, Guice

Selected Publications

5 of 14 total publications; 12 first author papers, 380+ citations, h-index 7 (see Google Scholar Citations)

- **Adrian W. Lange** and Gregory A. Voth. "Multi-state Approach to Chemical Reactivity in Fragment Based Quantum Chemistry Calculations." *J. Chem. Theory Comput.* 9, 4018-4025 (2013). (view PDF)
- **Adrian W. Lange** and John M. Herbert. "A Simple Polarizable Continuum Solvation Model for Electrolyte Solutions." *J. Chem. Phys.* 134, 204110 (2011). (view PDF)
- **Adrian W. Lange** and John M. Herbert. "Symmetric Versus Asymmetric Discretization of the Integral Equations in Polarizable Continuum Solvation Models." *Chem. Phys. Lett.* 509, 77 (2011). (view PDF)
- **Adrian W. Lange** and John M. Herbert. "Both Intra- and Interstrand Charge-Transfer Excited States in Aqueous B-DNA Are Present at Energies Comparable to or Just Above the $^1\pi\pi^*$ Excitonic Bright States." *J. Am. Chem. Soc.* 131, 3913-3922 (2009). (view PDF)
- **Adrian Lange** and John M. Herbert. "Simple Methods to Reduce Charge-Transfer Contamination in Time-Dependent Density-Functional Calculations of Clusters and Liquids." *J. Chem. Theory Comput.* 3, 1680 (2007). (view PDF)

Projects & Additional Experience

View code for my projects below on my GitHub page: github.com/awlange

- **MathWorkersJS** (2014 – Present): mathworkersjs.org; Open-source parallel JavaScript math and statistics library built around HTML5 Web Workers and node.js cluster library capable of speeding up JavaScript computations on multi-core devices; accompanying documentation website [JavaScript/node.js, HTML, CSS/SCSS, Python, Flask]
- **PiPlayer** (2014): Flask web app for streaming music from external hard drive at home, connected through a RaspberryPi computer [Python, Flask, JavaScript/jQuery/AJAX, HTML, CSS]
- **Personal Website** (2013 – Present): adrianlange.com; Back-end to front-end from scratch; dynamic content blog [HTML, CSS/SCSS, JavaScript/jQuery/node.js, MySQL]
- **Project Euler** (2013 – Present): Recreational mathematics and programming problems from projecteuler.net; currently solved over 100 problems, 98th percentile [C++, Python]
- **FMO-MS-RMD** (2013): Parallel interface to Q-Chem for propagating FMO-MS-RMD proton transport simulations with analytic gradients; demonstrated scalability to >200 CPUs [C++, C, MPI]
- **LAMMPS Ensembles** (2013): Multi-copy communication interface to molecular dynamics software, LAMMPS, for use in ensemble statistical mechanics simulations [C/C++, MPI, OpenMP, Python]

Open-Source & Community Contributions

- **Cassandra Python Driver** (2014): Error handling for input server connection list [Python]
- **KairosDB** (2014): User configurable regular expression for database keys [Java]
- **Q-Chem** (2007 – 2014): Lead author of PCM solvation, QM/MM, parallel linear algebra solvers, and Fast Multipole Method code; software design committee; 7th author of 161 co-authors on software white paper [C/C++, Fortran]
- **LAMMPS** (2013): Optimized compute kernel for pairwise interactions; debugged external interface [C++]

Honors & Awards

- Chair's Prime Choice in Computational Division at American Chemical Society Conference 2013
- Presidential Fellowship from The Ohio State University Graduate School ($33,150) 2012
- Chemical Computing Group Research Excellence Award from American Chemical Society ($1,150) 2012
- Travel Fellowship to present at American Conference on Theoretical Chemistry ($600) 2011
- Selected to attend Telluride School on Theoretical Chemistry ($850) 2011
- U.S. Department of Energy Merit Scholarship for top poster presentation ($400) 2010
- 3rd place (out of ~30) at Ohio State University Denman Undergraduate Research Forum ($300) 2006
- American Society for Microbiology Undergraduate Research Fellowship ($4,000) 2006
- Ohio State Arts & Sciences Undergraduate Honors Research Scholarship ($3,500) 2006