adrianlange.com

Adrian W. Lange Scientist + Developer

Employment

Software Developer

August 2013 - Present

Chicago, IL

Signal (formerly known as BrightTag)

- Develop data models and analytics algorithms to classify, merge, and analyze user profile data networks for millions
 of requests per day; distributed in NoSQL database with billions of records (~30 TB) [Java, Cassandra, Python, R]
- Research and implement scalable solutions for a hybrid real-time/batch data pipeline to evaluate user segmentation;
 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, NumPy, MongoDB]
- Built client data reporting web app to display inter-client clustering (via principal component analysis) and user interaction frequency trends (via kinetics modeling) [Python, Flask, SciPy, JavaScript, D3.js, Cassandra]

Postdoctoral Appointee

March 2012 - August 2013

Argonne National Laboratory Leadership Computing Facility / University of Chicago

Chicago, IL

- 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; developed implementation via numerical/statistical optimization techniques (simulated annealing, linear regression, swarm intelligence)

Ph.D. Student Researcher

June 2007 - March 2012

Columbus, OH

The Ohio State University

- Published 10 first author journal articles; presented at 20+ professional and academic events
- Invented physical model for screened solvent electrostatics, geometrical algorithm for constructing molecule surfaces, stochastic optimization (genetic algorithm) for load balancing numerical integrals; applications involving singular value decomposition of excited electronic quantum states in DNA

Education

Ph.D. Computational/Physical Chemistry

June 2007 - March 2012

The Ohio State University

Columbus, OH

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

Columbus, OH

Formal Coursework:

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

Supplementary Online Coursework:

Udacity: Web Development, Programming Languages, Parallel Programming (GPU, CUDA), Machine Learning Coursera: Data Science Signature Track (R, Statistics, Data Wrangling), 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, SciPy, Guava, Guice

Projects & Additional Experience

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

- MathWorkersJS (2014 Present): Open-source parallel JavaScript math and statistics library built around HTML5
 Web Workers and Node.js cluster library capable of speeding up computations on multi-core devices; accompanying
 documentation website: mathworkersjs.org [JavaScript/Node.js, HTML, CSS/SCSS, Python, Flask, Apache Server]
- Smart Alerts (2014 Present): Determine if an automated server alert requires manual intervention; comparing implementations as decision tree versus neural network [Python]
- **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): <u>adrianlange.com</u>; Back-end to front-end from scratch; dynamic content blog [HTML, CSS/SCSS, JavaScript/jQuery/Node.js/AJAX, MySQL]
- **Project Euler** (2013 Present): Recreational mathematics and programming problems from <u>projecteuler.net</u>; currently solved over 100 problems, 98th percentile [C++, Python]
- **FMO-MS-RMD** (2013): Parallel interface to Q-Chem program for propagating chemically reactive proton transport simulations with analytic gradients; demonstrated scalability to >200 CPUs [C++, C, MPI]

Open-Source & Community Contributions

- Cassandra Python Driver (2014): Simple 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; multi-dimensional communication interface for use in ensemble statistical mechanics simulations (LAMMPS Ensembles) [C++, MPI, OpenMP]

Selected Publications

- 4 of 14 total publications; 12 first author papers, 380+ citations, h-index 8 (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)

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