Adrian Lange, PhD

scientist + developer

adrian.w.lange@gmail.com
adrianlange.com

employment

Big Data Engineer, iTunes Analytics

May 2015 — Present

Apple, Inc.

Cupertino, CA

- Develop analytics infrastructure and analyses that will generate insights into customer experiences on products such as the iTunes Store, App Store, and iBookstore *[Hadoop, Splunk, Java, Python, JavaScript, R]*
- Utilize statistics, machine learning, and data mining to perform data profiling, segmentation, and hypothesis testing

Software Developer

August 2013 — April 2015

Signal (formerly known as BrightTag)

Chicago, IL

- Developed 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 (~30 TB) *[Java, Cassandra, Spark, Kafka, Python, R]*
- 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]*
- Built client data reporting web app to display inter-client clustering (via principal component analysis) and user interaction frequency trends *[Python, Flask, JavaScript, D3.js, Cassandra]*

Postdoctoral Appointee

March 2012 — July 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]*
- Implemented enhanced statistical sampling algorithms (e.g. Monte Carlo, parallel tempering) for computing energetics data
- Invented novel quantum mechanical proton transport model based on fragment electronic structure theory; model development via statistical optimization techniques (simulated annealing, multivariate regression, swarm intelligence, etc.)

Ph.D. Student Researcher

June 2007 — March 2012

The Ohio State University

Columbus, OH

- Published 10 first author journal articles (see publications); presented at 20+ professional and academic events
- Researched quantum chemistry and statistical thermodynamics; mathematical theory, computation, and algorithms
- Devised physics model for screened solvent electrostatics, geometrical algorithm for constructing continuously differentiable molecule surfaces, stochastic optimization (genetic algorithm) for load balanced numerical integrals; applications to excited electronic quantum states of DNA in simulated biological environments *[C/C++, Fortran, MPI, OpenMP]*

education

Ph.D. Computational/Physical Chemistry June 2007 — March 2012
The Ohio State University *Columbus, OH*

B.S. Chemistry with minor in Microbiology August 2003 — June 2007
The Ohio State University *Columbus, OH*

Formal Courses:

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

Supplementary Online Courses:

- **Udacity**: Web Development, Programming Languages, Parallel Programming (GPU), Machine Learning
- **Coursera**: Data Science Signature Track (R Programming, Statistics, Data Wrangling), Machine Learning, Algorithms, Databases

technical skills

Proficiency in descending order from left to right

Programming Languages	Java, Python, JavaScript, C, C++, awk, Unix/Linux shell (bash), Fortran
Databases/Storage	Cassandra, MySQL, Splunk, Kafka, Redis
Data Analysis	pandas, R, numpy, SciPy, scikit-learn
Compute Tools	Spark, Hadoop (MapReduce), MPI, OpenMP, blas/lapack, CUDA
Web Technologies	HTML, CSS/SCSS, jQuery, Flask, node.js, Markdown, web workers
Productivity Tools	git, vim, LaTeX, JIRA, svn
Machine Learning Techniques	Linear/Logistic Regression, Fourier Analysis, Clustering, k-Nearest Neighbors, Decision Trees, Random Forests, Kernel Smoothing, Bagging, Boosting, Neural Networks, SVMs

projects & additional experience

To see some code I have written, visit my GitHub account.

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, HTML5, CSS/SCSS, Python, Flask, Apache Server]*

Smart Alerts 2015

Determine if an automated server alert requires manual intervention; comparing implementations as neural network, random forest, support vector machine, and/or logistic regression *[Python, pandas, scikit-learn, Cassandra]*

PiPlayer 2014

Flask web app for streaming music from my hard drive at home, connected through a RaspberryPi computer. *[Python, Flask, JavaScript/jQuery/AJAX, HTML, CSS]*

Personal Website 2013 — present

Full stack coding, back-end to front-end. *[HTML, CSS/SCSS, JavaScript/jQuery/node.js, MySQL]*

Project Euler 2013 — present

Recreational mathematics and programming problems from Project Euler; currently solved more than 100 problems [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]*

DESMO 2011

Highly parallel solvent electrostatics model code; genetic algorithm dynamic load balancing *[C++, OpenMP, MPI]*

open source & community contributions

Cassandra Python Driver 2014

Simple error handling for input server connection list *[Python]*

Q-Chem 2007 — 2014

Lead author of PCM solvent modeling, 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

Multi-copy communication interface to open-source molecular dynamics software for parallel tempering/replica exchange (LAMMPS Ensembles); optimized compute kernel for pairwise interactions *[C++, C, MPI, OpenMP, Python]*

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 ($300)	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

publications

Google Scholar Statistics: 470+ total citations, h-index 8

14. Yihan Shao, Zhengting Gan, Evgeny Epifanovsky, Andrew T.B. Gilbert, Michael Wormit, Joerg Kussmann, **Adrian W. Lange** *et al.* Advances in molecular quantum chemistry contained in the Q-Chem 4 program package *Mol. Phys.* 1-32 (2014).
13. John M. Herbert and **Adrian W. Lange**. Book chapter: Polarizable Continuum Models for (Bio)Molecular Electrostatics: Basic Theory and Recent Developments for Macromolecules and Simulations (2014).
12. **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).
11. **Adrian W. Lange**, Gard Nelson, Christopher Knight, and Gregory A. Voth. Multiscale Molecular Simulations at the Petascale (Parallelization of Reactive Force Field Model for Blue Gene/Q): ALCF-2 Early Science Program Technical Report *Argonne National Laboratory* (2013).
10. **Adrian W. Lange** and John M. Herbert. Improving generalized Born models by exploiting connections to polarizable continuum models. II. Corrections for salt effects. *J. Chem. Theory Comput.* 8, 4381-4392 (2012).
9. **Adrian W. Lange** and John M. Herbert. Improving generalized Born models by exploiting connections to polarizable continuum models. I. An improved effective Coulomb operator. *J. Chem. Theory Comput.* 8, 1999-2011 (2012).
8. **Adrian W. Lange** and John M. Herbert. A Simple Polarizable Continuum Solvation Model for Electrolyte Solutions. *J. Chem. Phys.* 134, 204110 (2011).
7. **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).
6. **Adrian W. Lange** and John M. Herbert. Response to "Comment on 'A Smooth, Nonsingular, and Faithful Discretization Scheme for Polarizable Continuum Models: The Switching/Gaussian Approach.'". *J. Chem. Phys.* 134, 117102 (2011).
5. **Adrian W. Lange** and John M. Herbert. A Smooth, Nonsingular, and Faithful Discretization Scheme for Polarizable Continuum Models: The Switching/Gaussian Approach. *J. Chem. Phys.* 133, 244111 (2010).
4. **Adrian W. Lange** and John M. Herbert. Polarizable Continuum Reaction-field Solvation Models Affording Smooth Potential Energy Surfaces. *J. Phys. Chem. Lett.* 1, 556-561 (2010).
3. **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).
2. **Adrian W. Lange**, Mary A. Rohrdanz, and John M. Herbert. Charge-Transfer Excited States in a π-Stacked Adenine Dimer, As Predicted Using Long-Range-Corrected Time-Dependent Density Functional Theory. *J. Phys. Chem. B* 112, 6304 (2008).
1. **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).