

Max Charles Klein

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EDUCATION

- 2013-2019 PhD in Computational Biophysics from Johns Hopkins University, MD
- 2009-2010 Postbaccalaureate Pre-Medical Program at New York University, NY
- 2004-2008 B.A. in Physics from Reed College, Portland, OR

COMPUTER SKILLS

- Core contributor to the JupyterLab project:
<https://github.com/jupyterlab/jupyterlab/commits?author=telamonian>
- Creator of JupyterLab extensions such as jupyterlab-hdf5:
<https://github.com/jupyterlab/jupyterlab-hdf5>
- 10+ years of experience writing scientific programs using C, C++, CMake, and Python
- 8+ years of experience with the parallel programming paradigm and several parallel programming environments, including CUDA and MPI
- 8+ years of experience with big data and related frameworks/concepts, including Hadoop, Spark, and SQL
- Experience with a wide variety of scientific and simulation software including AMBER, Copasi, GROMACS, MCCE, PyMOL, DelPhi, APBS, Zap, NAMD, Lattice Microbes, and Rosetta

SOFTWARE/SCIENCE EXPERIENCE

- 2019 **Software Engineer, Quansight, Austin, TX/Remote**
I'm currently working on the maintenance and development of the JupyterLab ecosystem of open source software. I also work on implementing new features in JupyterLab that have been requested by various clients.
- 2019 **Software Consultant, Primer Research, New York, NY**
Working as a researcher and software developer, I implemented various trading strategies starting from the academic literature. I also architected a live trading platform that uses multiprocessing to evaluate a number of different strategies in parallel.
- 2013-2019 **PhD Candidate in the Biophysics Lab of Dr. Elijah Roberts, Johns Hopkins University Biophysics Department, Baltimore, MD**
As a researcher, my driving goal has been to better understand how cellular phenotypes emerge from the interactions of large quantities of individual molecules. Towards that end, my PhD work has mostly focused on the development of methods for performing accurate stochastic simulations of large biochemical networks. Although stochastic simulation methods accurate down to the single molecule level have been previously established, they are so computationally expensive that even for relatively simple networks they can end up taking millennia of CPU time to run.
I have developed a novel statistical method (descended from the family of Enhanced Sampling techniques) called FFPilot that can speed up a stochastic simulation by many orders of magnitude. Unlike previously developed Enhanced Sampling techniques, FFPilot can easily be run to any arbitrary level of accuracy, and is guaranteed to do so in the most computationally efficient manner possible. Using MPI, I have written a fully parallelized implementation of FFPilot (~25,000 lines of C++ code) that is appropriate

for deployment on a high performance computing cluster. The FFPilot implementation is part of the latest version of Lattice Microbes, the Roberts Lab's stochastic simulation software package, which is available from our Git repository:

<https://robertslabjhu.info/www/lmes-public>. A related paper is in preparation for submission, and is available on BioRxiv.

Stochastic simulation of biochemical networks can easily produce hundreds of terabytes of data, so I have also worked on tools and methods for storing and analyzing these very large datasets. Myself and collaborators in the Roberts Lab have produced a generalized version of these tools, called Biospark, that works well with many diverse kinds of biologically relevant data. Based around the Hadoop and Spark big data frameworks, Biospark makes it easier to parallelize both the read/write step and the computation step of analyzing large datasets. Biospark is available from the Roberts Lab Git repository: <https://robertslabjhu.info/www/biospark-public>. A related paper has been published in the journal Bioinformatics.

In order to experimentally verify the predictions of my modeling software I am also working on the design and manufacture of several microfluidic devices. One such device that has already been created allows for the capture and easy observation of a colony of *E. coli* cells. Most recently, I have been involved in the prototyping of a device that can trap individual yeast cells and expose them to variable gradients of mating pheromones. In order to assist with the design of these microfluidic devices, I have written a new software package called MicroMake. The program is now used by all of the members of the Roberts Lab for their microfluidic designs, and is available to the public at <https://github.com/telamonian/MicroMake>.

-2010-2013 Research Assistant in the Biophysics Lab of Dr. Marilyn Gunner, CCNY Physics Department, New York, NY

When I first arrived at the lab I worked on a project that examined the pK_a s of a set of 100 mutant ionizable residues that had been introduced, using molecular cloning, into various random sites in the core of the Staphylococcal Nuclease (SNase) protein. I helped modify the lab's main software package, Multiconformer Continuum Electrostatics (MCCE), so that it could make accurate predictions of those pK_a s, and I also helped to verify these predictions. The results of this work were published in the journal Proteins: Structure, Function, and Bioinformatics.

As a follow up to this initial project, I worked on elucidating the exact structural reasons behind the difference between mutant and wild type ionizable residues. In the environment that surrounds most wild type ionizable residues, the desolvation force, which arises from the dehydration of the residue when it's inserted into the protein, exists in a precise ratio with the electrostatic force, which arises from the interactions of electric charges. However, the electrostatic force is either greatly diminished or completely absent in the immediate vicinity of most of the mutant ionizable residues that the lab has examined.

OTHER SOFTWARE PROJECTS

- JupyterLab

I am extensively involved in the open source project JupyterLab, an environment for interactive and reproducible computing, based on the Jupyter Notebook. I have made a wide range of contributions to the core code, from low-level bug fixes in the build system

to a major overhaul of the UI theming system:

<https://github.com/jupyterlab/jupyterlab/commits?author=telamonian>

- **@jupyterlab/hdf5**

The first JupyterLab extension to provide a functional HDF5 viewer. Available through the JupyterLab extension manager, and at: <https://github.com/jupyterlab/jupyterlab-hdf5>

- **ocudump and OcuMOL**

A virtual reality plugin stack for PyMol, a widely used 3D modelling package for proteins: <https://github.com/telamonian/ocudump>.

- **Ecoligner**

A Python package that uses computer vision and machine learning techniques to automatically identify and track single cells in time series microscopy data:

<https://github.com/telamonian/ecoligner>.

OTHER RESEARCH EXPERIENCE

-2009-2010 **Research Assistant in the Immunology Lab of Dr. Michelle Krogsgaard, NYUMC Cancer Research Center, New York, NY**

As part of my final project at the Cancer Center, I wrote several pieces of software that assisted with the process of data acquisition and analysis from the lab's confocal microscope, and then taught my labmates how to use them.

-2007 **Laboratory Assistant in the Electrophysiology Lab of Dr. Paul Brehm, Vollum Institute at Oregon Health Sciences University, Portland, OR**

My main duty in this lab was the design and execution of a screening assay based on the electrical impulses generated by fish gills. As strange as that sounds, it was done as part of a preliminary effort to breed a zebrafish model of the human disease Rett syndrome.

-2005 **Laboratory Assistant in the Microbiology Lab of Dr. Bruce Cronstein, Bellevue Hospital, New York, NY**

In my first research posting in a laboratory, I was trained in basic molecular biological techniques, and then used those techniques to participate in a project that was searching for the genetic basis of fibromyalgia.

TEACHING EXPERIENCE

-2009-2011 **Chemistry, Physics, and Biology Tutor for Adam Wes Academics, New York, NY, Endeavor Tutoring, New York, NY, and as a freelancer, New York, NY**

I tutored a number of high school and college students in one-on-one sessions focusing on chemistry, physics and biology. In particular, students who came to me for help with the SAT math section improved their performance on both practice and actual exams by almost 200 points on average.

VOLUNTEER EXPERIENCE

-2009-2012 **Central Park Medical Unit, New York, NY**

I worked with a volunteer ambulance corps servicing Central Park and the surrounding area as a fully licensed EMT-B

-2006-2012 **Project Eye to Eye, Portland, OR and New York, NY**

I worked as a mentor with ADHD affected children from local schools. Over the course of several years this mentorship has taken on a variety of forms, from leading arts and

crafts projects, to the teaching of basic organizational skills, to helping one of the kids out with his math homework.

-2003 Youth Services Opportunity Project, New York, NY

Assisted in coordinating youth volunteer groups with local homeless service projects.

These projects ranged from a soup-kitchen run out of a synagogue to an organization that grew fruits and vegetables out on Far Rockaway, New York for those who could not buy their own.

FELLOWSHIPS AND AWARDS

- Owen Fellowship, Johns Hopkins Department of Biophysics 2013
- Bloomberg prize, Hophacks hackathon 2014
- SendGrid prize, Hophacks hackathon 2014
- Best use of peripheral prize (Oculus Rift), Hophacks hackathon 2015
- 2nd place overall jury prize, Hophacks hackathon 2016

PUBLICATIONS AND PRESENTATIONS

Gunner MR, Zhu X, Klein MC. MCCE analysis of the pKas of introduced buried acids and bases in staphylococcal nuclease. *Proteins* 2011;79:3306-3319.

Klein MC, Zhu X, Gunner MR. MCCE analysis of the pKas of buried acids and bases: the influence of the protein dielectric. Poster session presented at: CUNY Structural Biology Workshop 2011 Jun 6.

Klein MC, Gunner MR. Electrostatic characterization of naturally evolved deeply buried ionizable residues. Poster session presented at: Protons and Membrane Reactions Gordon Conference 2012 February 19.

Klein, M., Roberts, E. Using parallel enhanced sampling simulations to study rare switching events in regulatory networks. Poster session presented at: Biophysical Society Annual Meeting 2015 February 7.

Klein, M., Roberts, E. Control of Relative Error in Enhanced Sampling Simulations of Biochemical Networks. Poster session presented at: Q-Bio 2016 July 27.

Klein, M., Sharma, R., Bohrer, C. H., Avelis, C. M., Roberts, E. Biospark: scalable analysis of large numerical datasets from biological simulations and experiments using Hadoop and Spark. *Bioinformatics* 2017; 33(2), 303–305.

Klein, MC, Roberts, E. Automatic error control during forward flux sampling of rare events in master equation models. *bioRxiv* 254896; doi: <https://doi.org/10.1101/254896>