Erik Henning Thiede

Education

2013–2019 **Doctorate in Chemistry**, *University of Chicago*, GPA 3.87.
In addition to required classes, completed graduate-level coursework in probability theory and numerical analysis.

2009–2013 **Bachelors of Science in Chemistry**, *UNC Chapel Hill*, GPA 3.90.
Graduated with Honors and Highest Distinction.

Research Experience

2019– **Postdoctoral Scholar**, *University of Chicago*, Working w. Profs. Risi Kondor and Frank Noé.
- Developing machine learning architectures for molecular data.

2014– 2019 **Graduate Research Associate**, *University of Chicago*, Advisor: Aaron Dinner and Jonathan Weare.
- Developing algorithms for
  - efficiently recombining data in umbrella sampling calculations and characterizing the resulting statistical error.
  - estimating reaction rates from data collected under biased dynamics.
  - constructing long-time dynamic estimates from multiple short trajectories in the absence of good collective variables.
  - analyzing and improving Koopman modelling in the low-data limit.
- Analyzing nonequilibrium chemical data using manifold reduction and Koopman operator-theoretic techniques.

2013 **Research Associate**, *University of Chicago*, Advisor: David Mazziotti.
- Studied electron correlation effects in electron transfer between aromatics.

2010–2013 **Undergraduate Research Assistant**, *UNC Chapel Hill*, Advisor: Wei You.
- Studied the organic synthesis of photoactive polymers.
- Synthesized and characterized photovoltaic films using spectroscopic methods.

Honors and Fellowships

2017 **MolSSI Software Fellow**, *Molecular Sciences Software Institute*.
Fellowship for the development of algorithms and software for computational molecular sciences. Initially awarded for Fall 2017, successfully renewed for Spring 2018 to Summer 2019.

2013 **Freud Fellow**, *University of Chicago*.
Initial grant of $10,000 doubled to extend to 2014.

2013 **Hypercube Scholar**, *University of North Carolina at Chapel Hill*.

2012 **Award for Undergraduate Excellence in Physical Chemistry**, *University of North Carolina at Chapel Hill*.

2009 **Carolina Scholar**, *University of North Carolina at Chapel Hill*.
Highest merit-based scholarship offered by UNC Chapel Hill.

Publications

- Thiede E.H., Giannakis D., Dinner A.R., Weare J. "Galerkin Approximation of Dynamical Quantities using Trajectory Data", Journac of Chemical Physics, 150, 24411 (2019) `https://aip.scitation.org/doi/abs/10.1063/1.5063730`
- Dinner A.R., Thiede E.H., Van Koten B., Weare J. "Stratification of Markov chain Monte Carlo sampling", arXiv:1705.08445, *submitted to Journal of Uncertainty Quantification*. `https://arxiv.org/abs/1705.08445`
- Hong L., Vani B.P., Thiede E.H., Rust, M.J., Dinner A.R. "Molecular dynamics simulations of nucleotide release from the circadian clock protein KaiC reveal atomic-resolution functional insights." PNAS, 201812555 (2018). `http://www.pnas.org/content/early/2018/11/14/1812555115.short`
- Thiede E.H., Van Koten B., Weare J., Dinner A.R. "Eigenvector method for umbrella sampling enables error analysis." J. Chem. Phys., 145, 084115 (2016) `https://aip.scitation.org/doi/abs/10.1063/1.4960649`
- Thiede E., Van Koten B., Weare J. "Sharp entrywise perturbation bounds for Markov chains." SIAM J. Matrix Anal. Appl. 36, 917 (2015) `https://epubs.siam.org/doi/abs/10.1137/140987900`

Presentations

2020 **GAMM Young Researchers Minisymposium on Molecular Dynamics**, *Invited Talk*, Dynamical Galerkin Approximation: long-time rates from short-time data.

2019 **Minisymposium in SIAM Conference on Applications of Dynamical Systems**, *Invited Talk*, Long-time Dynamical Estimates from Short-time Data using Dynamical Galerkin Approximation.

2018 **Berkeley Statistical Mechanics Meeting**, *Poster*, Quantitative Information from Trajectory Data through Dynamical Galerkin Approximation.

2017 **IPAM Program: Complex High-Dimensional Energy Landscapes: Workshop III**, *Poster*, Quantitative Information from Trajectory Data through Dynamical Galerkin Approximation.

2017 **Berkeley Statistical Mechanics Meeting**, *Poster*, Estimating Dynamical Information using Diffusion Maps.

2015 **Berkeley Statistical Mechanics Meeting**, *Poster*, Umbrella Sampling: Insights from Numerical Analysis.

Teaching Experience

Mar.–Jun. 2014, Mar.–Jun. 2015 **Teaching Assistant for Computational Methods in Chemistry and Biology**, *University of Chicago*.

- Graded student work. Helped develop curricula and homework assignments.

Oct. 2013– Mar. 2014 **Teaching Assistant for General Chemistry**, *University of Chicago*.
- Graded student work, lead discussions sections and supervised laboratory work.

Outreach

2016, 2018 **SESAME Program**, *University of Chicago*.
- Taught at the SESAME program which offers professional development courses for Chicago Public School teachers.
- In 2016, give a lecture on the Statistics of Biomolecules.
- In 2018, assisted a lecture on Enzymes.

2013, 2015, 2017 **Physics with a Bang**, *University of Chicago*.
- Volunteer at Physics with a Bang, the annual open-house for the James Franck Institute.
- Performed scientific demos for elementary and middle school children on particle jamming (2013) and molecular simulation (2015).
- In 2017, performed overtone singing to demonstrate Fourier decomposition of sound.

2017 **Chicago Area Undergraduate Research Symposium**, *University of Chicago*.
- Volunteered to judge posters for the CAURS conference.

Software Development

EMUS Package Open source implementation of the **E**igenvector **M**ethod for **U**mbrella **S**ampling available at https://github.com/ehthiede/EMUS. The package provides:
- Rapid convergence to the maximum likelihood estimate of averages calculated by umbrella sampling, leading to accuracy equivalent to or surpassing WHAM.
- Support for large, high-dimensional umbrella sampling datasets. Provides support for calculating averages over the state space, as well as free energy surfaces in collective variable spaces with dimension larger than 2.
- Error analysis of free energy calculations, detailed in Thiede et al. JCP 2016.

PyDiffMap Codeveloper of an open source implementation of the Diffusion Map algorithm, available at https://github.com/DiffusionMapsAcademics/pyDiffMap. Among other features, the implementation provides
- Automatic bandwidth parameter selection.
- Variable Bandwidth Diffusion Kernels.
- Out-of-sample Extension.
- Intelligent neighborlist construction using scikit-learn's Neighbor class.
- Support of target-measure diffusion maps.

PyEDGAR Open source implementation of the Dynamical Galerkin Approximation algorithm available at https://github.com/ehthiede/PyEDGAR. The package implements Dynamical Galerkin Approximation, a novel method for estimating long-time statistics from collections of short-time trajectories detailed in Thiede et al., arXiv:1810.01841. This algorithm generalizes Markov State Modeling, and is closely related to Koopman operator methods such as the Extended Dynamic Mode Decomposition and the Variational Approach.

Cormorant Contributing author and maintainer of an implementation of the Cormorant machine learning architecture available at https://github.com/risilab/cormorant

Enhanced Sampling Toolkit

. Contributing author to the Enhanced Sampling Toolkit at https://github.com/jtempkin/enhanced_sampling_toolkit, a software package designed for rapid prototyping and implementation of enhanced sampling algorithms. Designed and developed the Walker API, which provides an easy interface for controlling Molecular Dynamics simulations.