Erik Henning Thiede

Research Fellow, Flatiron Institute CCM

Education

2013–2019 **Doctorate in Chemistry**, *University of Chicago*.

2009–2013 **Bachelors of Science in Chemistry**, *UNC Chapel Hill*.

Professional Appointments

2020– **Research Fellow**, *Center for Computational Mathematics, Flatiron Institute*, Working in collaboration with Prof. Risi Kondor.

2019– 2020 **Postdoctoral Scholar**, *University of Chicago*, Advised by Prof. Risi Kondor.

2014– 2019 **Graduate Research Associate**, *University of Chicago*, Jointly advised by Prof. Aaron Dinner and Prof. Jonathan Weare.

2013 **Research Associate**, *University of Chicago*, Advised by Prof. David Mazziotti.

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., Zhou, W., Kondor, R. "Autobahn: Automorphism-based Graph Neural Nets", arXiv:2103.01710 `https://arxiv.org/abs/2103.01710`
- Giraldo-Barreto, J., Ortiz S., Thiede E.H., Palacio-Rodriguez, K., Carpenter, B., Barnett, A.H., Cossio, P. "A Bayesian approach for extracting free energy profiles from cryo-electron microscopy experiments using a path collective variable", arXiv:2102.02077 `https://www.nature.com/articles/s41598-021-92621-1`

- Lorpaiboon, C., Thiede E.H., Webber, R.J., Weare J., Dinner A.R. "Integrated Variational Approach to Conformational Dynamics: A Robust Strategy for Identifying Eigenfunctions of Dynamical Operators", The Journal of Physical Chemistry B 124 (42), 9354-9364, https://pubs.acs.org/doi/abs/10.1021/acs.jpcb.0c06477
- Webber, R.J., Thiede E.H., Dow, D., Dinner A.R., Weare J. "Error bounds for dynamical spectral estimation", arXiv:2005.02248, https://epubs.siam.org/doi/abs/10.1137/20M1335984
- Antoszewski A., Feng C.J., Vani B.P., Thiede E.H., Hong L., Weare J. Tokmakoff A., Dinner A.R. "Insulin dissociates by diverse mechanisms of coupled unfolding and unbinding", The Journal of Physical Chemistry B 124 (27), 5571-5587, https://aip.scitation.org/doi/abs/10.1063/1.5063730
- Thiede, E.H., Son, H.T., Kondor, R. "The general theory of permutation equivariant neural networks and higher order graph variational encoders", arXiv:2004.03990 https://arxiv.org/abs/2004.03990
- Thiede E.H., Giannakis D., Dinner A.R., Weare J. "Galerkin Approximation of Dynamical Quantities using Trajectory Data", Journal 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 as a general variance reduction method for Markov chain Monte Carlo", SIAM/ASA Journal on Uncertainty Quantification, 8(3), 1139–1188, https://epubs.siam.org/doi/abs/10.1137/18M122964X
- 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). https://www.pnas.org/content/115/49/E11475.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 (Postponed to 2021).

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.

Scientific Leadership

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.