Nils Estuardo Mundaca Elias Strand

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Personal website

INTERNATIONAL BACKGROUND

- Dual citizenship: Norway, USA
- Languages: fluent (written and spoken) in English, Norwegian, Spanish, French

ABOUT ME

I earned my PhD degree at Northwestern University in September 2023. My PhD research involved nonequilibrium statistical mechanics. A well-timed exposure to tensor networks (TN) allowed me to successfully leverage these powerful numerical tools to study a periodically driven multiparticle Brownian ratchet. I was the first to compute, with the help of TNs and the time-dependent variational principle, steady-state currents for a classical many-body time-periodic system. With the help of transition path theory (TPT), I also successfully analyzed how species concentrations in a gene toggle switch (GTS) toy model jump to trigger stochastic switches from one metastable regime to another. My expertise in TN methods has opened my eyes to their potential applicability to high-dimensional biomolecular systems in which rare events play a pivotal role. What microscopic mechanisms underlie pattern formation in gene regulatory processes within living cells? As I transition to my postdoctoral position at the University of Chicago starting October 2023, I have been interested in devising theoretical representations of intracellular mechanisms using toy chemical reaction networks (CRNs) mimicking gene regulatory networks, modeling these CRNs as reaction-diffusion systems and incorporating stochastic noise.

EDUCATION

PhD Chemistry, September 2017 – September 2023
Northwestern University, Evanston, IL

- "Exploring Nonequilibrium Dynamics: Numerical Insights into Steady States and Reactive Pathways in Discrete Many-Body Systems"
- Thesis committee: Todd Gingrich (chair), Erik Luijten, George Schatz; degree obtained September 8, 2023
- Research: nonequilibrium statistical mechanics, rare event sampling, transition path theory, tensor networks, electronic structure theory with and without relativistic effects
- Advisors: Todd Gingrich (June 2018 – September 2023), Toru Shiozaki (September 2017 – March 2018)

BS Chemistry, Computer Science, with Honors, September 2013 – April 2017
The University of Michigan, Ann Arbor, MI

- Minor in Physics
- Cumulative GPA: 3.74
- "Computational Study of Ruthenium-Catalyzed Dimethylcarbamate Hydrogenation to Methanol: C-O and C-N Breaking Pathways"
- Advisors: Paul M. Zimmerman (September 2015 – April 2017), Bart M. Bartlett (June – August 2015), Hui Deng (June – August 2014)

AWARDS

- 2022 Best student contributed talk award, 52nd Midwest Theoretical Chemistry Conference (MWTCC), The Ohio State University
- 2016 James B. Angell Scholar, University of Michigan
- 2015 James B. Angell Scholar, University of Michigan

PEER-REVIEWED JOURNAL PAPERS

- N.E. Strand, H. Vroylandt, and T.R. Gingrich. "Computing time-periodic steady-state currents via the time evolution of tensor network states." Journal of Chemical Physics, 2022 (doi: https://doi.org/10.1063/5.0099741).
- N.E. Strand, H. Vroylandt, and T.R. Gingrich. "Using tensor network states for multi-particle Brownian ratchets." Journal of Chemical Physics [Editor's Pick], 2022 (doi: https://doi.org/10.1063/5.0097332).
- N.E. Strand, Rueih-Sheng Fu, and T.R. Gingrich. "Current inversion in a periodically driven two-dimensional Brownian ratchet." Physical Review E [Editor's Suggestion], 2020 (doi: https://doi.org/10.1103/PhysRevE.102.012141).
- J.W. Park, R. Al-Saadon, N.E. Strand, and T. Shiozaki. "Imaginary shift in CASPT2 nuclear gradient and derivative coupling theory." Journal of Chemical Theory and Computation, 2019 (doi: https://doi.org/10.1021/acs.jctc.9b00368).

CONTRIBUTED PRESENTATIONS

- *Using tensor network states for many-body far-from-equilibrium systems*, (Post)Modern Thermodynamics Workshop, Luxembourg, December 8, 2022.
- *Using tensor network states for time-periodic nonequilibrium systems*, 52nd Midwest Theoretical Chemistry Conference (MWTCC), The Ohio State University, June 3, 2022 [**Best student contributed talk award**].
- *Using tensor network states for time-periodic nonequilibrium systems*, CECAM Workshop: Numerical Techniques for Nonequilibrium Steady States, Johannes Gutenberg University of Mainz, April 19, 2022.
- *Using tensor network states for multiparticle Brownian ratchets*, APS March Meeting 2022, Chicago, IL, March 17, 2022.

POSTER PRESENTATIONS

- *Analyzing Transition Paths in Reaction-Diffusion Systems via Tensor Network States*, Berkeley Statistical Mechanics Meeting 2023, January 13, 2023.

- *Using tensor network states for multiparticle Brownian ratchets*, Berkeley Statistical Mechanics Meeting 2022, January 7, 2022.

- *Current inversion in a periodically driven two-dimensional Brownian ratchet*, Berkeley Statistical Mechanics Meeting 2020, January 10, 2020.

TEACHING

Northwestern University, Chemistry Department:

- Spring 2022: Chem 348 Physical Chemistry for ISP
  Teaching Assistant supporting Todd Gingrich and Brian Hoffman's accelerated introduction to statistical mechanics and kinetics.

- Winter 2019: Chem 350 Advanced Laboratory 1
  Teaching Assistant supervising undergraduates in advanced experiments involving atomic spectroscopy.

- Summer 2018: Chem 131/141 General Chemistry Laboratory 1
  Teaching Assistant supervising undergraduates in experiments dealing with concepts such as calorimetry and Beer's law of absorption.

- Winter 2018: Chem 182 Advanced General Physical Chemistry Laboratory
  Teaching Assistant supervising science-oriented (i.e. Chemistry, medical track) undergraduates in introductory experiments related to, but not limited to, Aluminum crystal synthesis, buffered solutions.

- Fall 2017: Chem 161 Accelerated General Chemistry Laboratory 1
  Teaching Assistant supervising undergraduates in introductory experiments related to, but not limited to, the flame test, ICP and dealing with concepts such as VSEPR and solid-state structures.

Wyzant Online Tutoring Service:

Tutored high school and undergraduate students online and in-person for a total of 150 hours in topics of Chemistry, Physics, Mathematics, and Computer Science. Overall rating: 4.7/5.0. See profile here.

COMMUNITY ENGAGEMENT

- I have played the violin as a soloist since I was 6 years old.

- I have been a member of the Philharmonia Ensemble at Northwestern since 2018, and since 2021, I am the Assistant Concert Master of this Orchestra.

- During my entire undergraduate experience, I was a member of the University of Michigan's Campus Symphony Orchestra (CSO).

- I like to run, swim, play chess and poker.

TECHNICAL SKILLS

- Operating systems: Windows, Linux, OSX
- Programming languages: C/C++, Java, Wolfram Mathematica, Python, Julia, Bash
- Programming skills: object-oriented programming, memory management, C++ Standard Template Library, dynamic programming
- Parallel programming: multithreading (pthreads, OpenMP), Message Passing Interface
- ITensor library: C++ and Julia versions
- Supercomputing/job schedulers: Slurm, Portable Batch System, Sun Grid Engine
- Version control: GitHub
- Typesetting: LaTeX, Overleaf