

Diego E. Kleiman

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Education

University of Illinois at Urbana-Champaign (UIUC)

Urbana, IL

Ph.D. in Biophysics and Quantitative Biology, GPA: 4.0/4.0

January 2021 – 2025 (expected)

Concentration: Computational Science and Engineering

Advisor: Diwakar Shukla

Thesis (in progress): "Accelerating Adaptive Sampling Molecular Dynamics Simulations with Machine Learning"

New York University in Abu Dhabi (NYUAD)

Abu Dhabi, UAE

Bachelor of Science, Physics + CS (minor), GPA: 3.9/4.0

August 2016 – May 2020

Honors: Magna Cum Laude, NYU Founders' Day Award, Member of Phi Beta Kappa

Escuela Normal Juan Pascual Pringles

San Luis, Argentina

Secondary School Diploma, GPA: 9.8/10

November 2014

Honors: Valedictorian

Publications

- Kleiman, D. E., & Shukla, D. (2023). Active Learning of the Conformational Ensemble of Proteins using Maximum Entropy VAMPNets. *Journal of Chemical Theory and Computation*. doi.org/10.1021/acs.jctc.3c00040
- Kleiman, D. E., & Shukla, D. (2022). Multiagent Reinforcement Learning-Based Adaptive Sampling for Conformational Dynamics of Proteins. *Journal of Chemical Theory and Computation*. doi.org/10.1021/acs.jctc.2c00683.
- He, W., Naleem, N., Kleiman, D. E., & Kirmizialtin, S. (2022). Refining the RNA Force Field with Small-Angle X-ray Scattering of Helix–Junction–Helix RNA. *The Journal of Physical Chemistry Letters*, 13(15), 3400–3408. doi.org/10.1021/acs.jpclett.2c00359
- Zhao, C., Kleiman, D. E., & Shukla, D. (2021). Intriguing Role of Water in Plant Hormone Perception. *bioRxiv*. doi.org/10.1101/2021.10.04.462894. Github (data and analysis scripts): github.com/ShuklaGroup/Water_Phytohormones

Open Source Software

- **Maximum entropy VAMPNet**. Github: github.com/ShuklaGroup/MaxEntVAMPNet.
The package implements a wide variety of adaptive sampling techniques, including the recently proposed maximum entropy VAMPNet. The code follows object-oriented programming to provide modularity and facilitate extension to new methods. It utilizes OpenMM as a simulation engine and Torch, Deep Time, and Scikit-learn for machine learning.
- **Multi-agent reinforcement learning-based adaptive sampling** Github: github.com/ShuklaGroup/MA_REAP.
This repository implements multi-agent reinforcement learning-based adaptive sampling and related methods. It provides a command-line interface that allow users to analyze trajectories to obtain input files for simulations with any molecular dynamics engine of choice.

Academic Conferences & Symposia

Oral Sessions (*=presenting author)

- *Kleiman, D. E., & Shukla, D. Deep Learning-Guided Adaptive Sampling with Uncertainty Rewards Enhances Exploration in Molecular Dynamics Simulations. **American Chemical Society Spring 2023 Meeting**. Session: Machine Learning in Chemistry: Biomolecular Dynamics and Design. Indianapolis, IN. March 26–30, 2023.
- *Kleiman, D. E., & Shukla, D. Multi-agent Reinforcement Learning Based Adaptive Sampling of Conformational Free Energy Landscapes of Proteins. **American Chemical Society Fall 2022 Meeting**. Session: Molecular Mechanics. Chicago, IL. August 21–25, 2022.

Poster Sessions (*=presenting author)

- *He, W., Naleem, N., Kleiman, D. E., & Kirmizialtin, S. Refining RNA Force Field with Small-Angle X-Ray Scattering of Helix-Junction-Helix RNA. **American Chemical Society Fall 2022 Meeting**. Chicago, IL. August 21-25, 2022.
- Zhao, C., *Kleiman, D. E., & Shukla, D. Optimization of Hydration Sites in Plant Hormone Receptors for Agrochemical Design. **66th Annual Meeting of the Biophysical Society**. San Francisco, CA. February 19-23, 2022.
- *Kleiman, D. E., Naleem, N., & Kirmizialtin, S. Exploring the Ion-Mediated RNA Interactions of a Helix-Junction-Helix RNA Model Through Well-Tempered Metadynamics Simulations. **64th Annual Meeting of the Biophysical Society**. San Diego, CA. February 16, 2020.

Software Skills

Programming languages

Python, C/C++, CUDA C++, Mathematica.

Machine learning

PyTorch, Scikit-Learn, Keras, OpenCV.

Molecular dynamics

OpenMM, AmberTools, GROMACS, VMD.

Cheminformatics

RDKit.

Numerical computing

NumPy, SciPy.

Data visualization

Matplotlib, Seaborn, gnuplot, xmgrace.

Data mining

Beautiful soup, Pyppeteer.

Operative systems

Unix, macOS, Windows.

Web development

HTML, CSS, Flask.

Database development

MongoDB, SQL, Pandas.

Awards & Recognition

The Molecular Sciences Software Institute

MolSSI Seed Software Fellowship (NSF subaward)

Blacksburg, VA

2023-2024

University of Illinois at Urbana-Champaign

List of Teachers Ranked as Excellent by Their Students

Urbana, IL

Fall 2022

The Phi Beta Kappa Society

Inducted into Phi Beta Kappa, NYU Chapter (top 10% of class + competitive application)

New York, NY

May 2020

New York University

NYU Founders' Day Award (top 10% of class)

New York, NY

April 2020

New York University Tandon School of Engineering

Undergraduate Summer Research Program Fellowship

New York, NY

June 2018

6th Annual UAE Undergraduate Research Competition

Finalist

Abu Dhabi, UAE

April 2018

International Genetically Engineered Machine (iGEM) Competition

Gold Medal

Boston, MA

November 2017

International Biology Olympiad

Representative of Argentina (second best in country). Bronze Medal (position 105/238).

Bali, Indonesia

July 2014

Teaching

University of Illinois at Urbana-Champaign

LAS 291/292: Global Perspectives for Intercultural Learning

Teaching Assistant

Urbana, IL

Spring 2023

University of Illinois at Urbana-Champaign

BIOP 401: Introduction to Biophysics

Teaching Assistant | Inducted into List of Teachers Ranked as Excellent by Their Students

Urbana, IL

Fall 2022

Coursework-related Software

Graduate Level (UIUC)

CSE 408: Applied Parallel Programming <i>Project-based course Grade: A github.com/diegoeduardok/applied-parallel-programming</i>	Urbana, IL <i>Fall 2022</i>
STAT 542: Statistical Learning <i>Project-based course Grade: A+ github.com/diegoeduardok/statistical-learning</i>	Urbana, IL <i>Spring 2021</i>

Undergraduate Level (NYU & NYUAD)

PHYS-UA 135: Condensed Matter Physics <i>Grade: A- github.com/diegoeduardok/condensed-matter-physics</i>	New York, NY <i>Spring 2019</i>
CS-UH 1050: Data Structures <i>Grade: A github.com/diegoeduardok/data-structures</i>	Abu Dhabi, UAE <i>Spring 2018</i>

Leadership & Community Engagement

The Anchorage Society: Student-Run LGBTQ+ Organization at NYUAD <i>Treasurer</i>	Abu Dhabi, UAE <i>August 2019–May 2020</i>
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Other Work in Education & Outreach

University of Illinois at Urbana-Champaign <i>WYSE Camp Counselor, STEM outreach for underrepresented students in engineering</i>	Urbana, IL <i>July 2021 & July 2022</i>
International Biology Olympiad Group Challenge <i>Group Project Facilitator, team received Award of Excellence</i>	Nagasaki, Japan (remote position) <i>July–October 2020</i>
Addicest.com <i>SAT Tutor</i>	Rabat, Morocco (remote position) <i>June–July 2020</i>
Academic Enrichment Program at NYUAD <i>Mathematics Tutor</i>	Abu Dhabi, UAE <i>November 2019–February 2020</i>
Preparation Course for Medical School Admission Test at UNCuyo <i>Official Physics and Biology Tutor</i>	Mendoza, Argentina <i>June 2015–January 2016</i>

Short Courses & MOOCs

Molecular Sciences Software Institute <i>MoSSI Software Fellow Bootcamp</i> Best Practices in Software Engineering for the Molecular Sciences	Blacksburg, VA <i>July 2023</i>
International School for Advanced Studies (SISSA) <i>Summer School</i> Classical Molecular Dynamics for Material Science, Nanotechnology, and Biophysics	Trieste, Italy <i>June 2019</i>
Coursera <i>Online Coursework</i> Deep Learning Specialization by deeplearning.ai	Remote <i>2018</i>

Languages

English fluent. **Spanish**: native fluency. **French**: fluent (written), intermediate (oral).