Diego E. Kleiman

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Education

University of Illinois at Urbana-Champaign (UIUC) — **Urbana, IL, USA**
Ph.D. in Biophysics and Quantitative Biology, GPA: 4.0/4.0 — *January 2021 – 2025 (expected)*
Concentration: Computational Science and Engineering

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)

- 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.
- 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)

- 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.

- 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.
- Manta Rover: an Automated System for Coral Reef Remediation. **New York University 2018 Undergraduate Research Session**. New York, NY. August 3, 2018.
- E. coLAMP: A portable device for rapid detection of Shiga toxin-producing Escherichia coli. **International Genetically Engineered Machine (iGEM) Competition**. Boston, MA. November 9-13, 2017.

Poster Sessions (coauthor)

- 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.

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

University of Illinois at Urbana-Champaign — **Urbana, IL**
List of Teachers Ranked as Excellent by Their Students — *Fall 2022*

The Phi Beta Kappa Society — **New York, NY**
Inducted into Phi Beta Kappa, NYU Chapter — *May 2020*

New York University — **New York, NY**
NYU Founders' Day Award — *April 2020*

New York University Tandon School of Engineering — **New York, NY**
Undergraduate Summer Research Program Fellowship — *June 2018*

6th Annual UAE Undergraduate Research Competition — **Abu Dhabi, UAE**
Finalist — *April 2018*

International Genetically Engineered Machine (iGEM) Competition — **Boston, MA**
Gold Medal — *November 2017*

International Biology Olympiad — **Bali, Indonesia**
Representative of Argentina (second best in country). Bronze Medal (position 105/238). — *July 2014*

Teaching

University of Illinois at Urbana-Champaign — **Urbana, IL**
LAS 291/292: Global Perspectives for Intercultural Learning — *Spring 2023*
Teaching Assistant

University of Illinois at Urbana-Champaign — **Urbana, IL**
BIOP 401: Introduction to Biophysics — *Fall 2022*
Teaching Assistant | Inducted into List of Teachers Ranked as Excellent by Their Students

Relevant Coursework

Graduate Level (UIUC)

CSE 408: Applied Parallel Programming — **Urbana, IL**
Project-based course | Grade: A | github.com/diegoeduardok/applied-parallel-programming — *Fall 2022*

IB 505: Bioinformatics & Systems Biology — **Urbana, IL**
Project-based course | Grade: A — *Spring 2022*

STAT 542: Statistical Learning — **Urbana, IL**
Project-based course | Grade: A+ | github.com/diegoeduardok/statistical-learning — *Spring 2021*

Undergraduate Level (NYU & NYUAD)

PHYS-UH 3012: Quantum Mechanics 1 — **Abu Dhabi, UAE**
Grade: A — *Fall 2019*

CSCI-UA 201: Computer Systems Organization — **New York, NY**
Grade: A- — *Spring 2019*

PHYS-UA 140: Thermal & Statistical Physics — **New York, NY**
Grade: A — *Spring 2019*

PHYS-UA 135: Condensed Matter Physics — **New York, NY**
Grade: A- | github.com/diegoeduardok/condensed-matter-physics — *Spring 2019*

CS-UH 1052: Algorithms — **Abu Dhabi, UAE**
Grade: A — *Fall 2018*

CS-UH 1050: Data Structures — **Abu Dhabi, UAE**
Grade: A | github.com/diegoeduardok/data-structures — *Spring 2018*

Leadership & Community Engagement

The Anchorage Society: Student-Run LGBTQ+ Organization at NYUAD — **Abu Dhabi, UAE**
Treasurer — *August 2019–May 2020*

Other Work in Education & Outreach

University of Illinois at Urbana-Champaign — **Urbana, IL**
WYSE Camp Counselor, STEM outreach for underrepresented students in engineering — *July 2021 & July 2022*

International Biology Olympiad Group Challenge — **Nagasaki, Japan (remote position)**
Group Project Facilitator, team received Award of Excellence — *July–October 2020*

Addictest.com — **Rabat, Morocco (remote position)**
SAT Tutor — *June–July 2020*

Academic Enrichment Program at NYUAD — **Abu Dhabi, UAE**
Mathematics Tutor — *November 2019–February 2020*

Preparation Course for Medical School Admission Test at UNCuyo — **Mendoza, Argentina**
Official Physics and Biology Tutor — *June 2015–January 2016*

Short Courses & MOOCs

International School for Advanced Studies (SISSA) — **Trieste, Italy**
Summer School — *June 2019*
Classical Molecular Dynamics for Material Science, Nanotechnology, and Biophysics

Coursera — **Remote**
Online Coursework — *2018*
Deep Learning Specialization by deeplearning.ai

Languages

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