Aldo Sayeg Pasos Trejo

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Education

Freie Universität Berlin
PhD candidate, Physics Department
Dates: September 2022 - Present
Project title: "Transferable Machine-Learned Coarse Grained models for proteins"
Supervisor: Prof. Dr. Cecilia Clementi

National Autonomous University of Mexico
Master's degree in Mathematics
Dates: August 2019 - August 2022
GPA: 97.7/100
Thesis: "Locking Transition in Three Dimensional Polygonal Chains"
Supervisor: Dr. Ricardo Atahualpa Solórzano Kraemer

National Autonomous University of Mexico
Bachelor's degree in Physics
Dates: August 2013 - May 2019
GPA: 94.1/100
Thesis: "Ising-like model for the study of intermediate phase in chalcogenide glasses"
Supervisor: Dr. Ricardo Atahualpa Solórzano Kraemer.

Work Experience

Software Developer Engineer
Altair Engineering
Dates: September 2021 - July 2022
Working as part of the Meshing and Geometry department. Working maintaining a meshing and geometry engine, improving performance and implementing new features. Code is developed in C++ using Visual Studio. Agile program management with the help of JIRA.

Adjunct Professor
Faculty of Sciences. National Autonomous University of Mexico
Dates: January 2020 - July 2022
Teaching courses such as "Computational algorithms" (a basic introduction to programming and computer science) and "Computational Physics" (An applied numerical methods course, with examples focused on physics) as part of the Physics Department.

Computational skills

- Python (8 years)
  Focus on machine learning (PyTorch, Scikit-learn, Triton) and Scientific Computing (Numpy, Scipy, Matplotlib)
- Julia (4 years)
- C/C++ (3 years)
  Experience with advanced object-oriented design, polymorfism and concurrency.
- Javascript (1 year)
- Linux (6 years)
- Git (6 years)

Languages

Spanish (native), English (fluent), German (Basic), French (Basic)

Research

(September 2022 - Present) Physics Department. Freie Universität Berlin.
Research under the supervision of Prof. Dra. Cecilia Clementi. Consisting on building machine learned coarse grained models of proteins capable of running molecular dynamics and capturing processes such as protein folding, protein aggregation and interaction.

(August 2018 - July 2021) Physics Department. Faculty of Sciences, UNAM.
Research under the supervision of Prof. Atahualpa Kraemer. Mainly consisted on using Markov Chain Monte Carlo methods for sampling canonical ensembles of models to calculate macroscopical variables os systems such as amorphous solids and lattice proteins. Agent-based models for the study of disease propagation in complex networks have also been treated. All models are programmed with the minimal use of libraries in order to have more control over the simulations.

(June 2018 - August 2018) Institute for Quantum Computation University of Waterloo
Research assistant under the supervision of Prof. Kevin Resch in the Quantum Optics and Quantum Information group. Research consisted in the mounting and calibration of a Sagnac interferometer, as well as running and testing simulations about the possibility of performing experiments with the inteferometer.

(June 2017 - August 2017) Department of Mathematics and Computer Science. University of Lethbridge
Research assistant under the supervision of Prof. Jacqueline Rice researching the optimization of reversible logic circuits and documenting experimental software capable of making such optimizations. Research funded by the MITACS Globalink Research Internship. Original project name: Support for Reversible Logic Synthesis Tools.

(December 2016 - January 2017) Berkeley Energy and Climate Institute University of California, Berkeley
Research assistant under the supervision of Ph.D. Sergio Castellanos in the SWITCH-Mexico project making Data Analysis. The project aspired to make a simulation of the mexican electrical network to create an investment plan focused on renewable energy.

Publications

1. Bonneau, K. *et al.* Breaking the Barriers of Molecular Dynamics With Deep-Learning: Opportunities, Pitfalls, and How to Navigate Them. *Wiley Interdisciplinary Reviews: Computational Molecular Science* **16,** e70064 (2026).
2. Durumeric, A. E., Chen, Y., Pasos-Trejo, A. S., Noé, F. & Clementi, C. Learning data-efficient coarse-grained molecular dynamics from forces and noise. *Nature Communications* (2026).
3. Charron, N. E. *et al.* Navigating protein landscapes with a machine-learned transferable coarse-grained model. *Nature chemistry* **17,** 1284–1292 (2025).
4. Durumeric, A. E. *et al.* Machine learned coarse-grained protein force-fields: Are we there yet? *Current Opinion in Structural Biology* **79,** 102533 (2023).
5. Pasos-Trejo, A. S. & Kraemer, A. S. Microscopic Model of Intermediate Phase in Flexible to Rigid Transition. *Frontiers in Physics* **8,** 619320 (2021).
6. Castellanos, S. *et al. Modeling high-penetration of clean energy in the electrical grid: A case for Mexico* in *2018 IEEE 7th World Conference on Photovoltaic Energy Conversion (WCPEC)(A Joint Conference of 45th IEEE PVSC, 28th PVSEC & 34th EU PVSEC)* (2018), 1377–1379.

Scholarships and grants

(2024-2028) SBF TRR 186, project A12. Project titled "Molecular Switches in the Spatio-Temporal Control of Cellular Signal Transmission".

(2023-2026) SBF1114, project A04. Project titled "Efficient calculation of slow and stationary scales in molecular dynamics", providing funding for PhD.

(2019-2021) CONACYT national scholarship. Funding for living expenses for full duration of my Master's Degree program.

(2018) UNAM PAPIIT project IA106618 RA106618. Funding provided by Dr. Solórzano Kraemer for supporting the writing of my bachelor's thesis.

Academic events

(March 2026) International Membrane Biophysics Meeting: Membranes as Biological Barriers.
Presented a talk about my research in machine-learned coarse-grained models for lipids and membranes. Held in the Evangelisches Zentrum Kloster Drübeck from March 23th to March 26th in Ilsenburg, Sazony-Anhalt, Germany

(January 2026) CECAM Workshop "A roadmap for an atomistic machine learning software ecosystem"
Presented a talk about my research in machine learning for protein simulation and the software used for it. Held at the CECAM headquarters in the Ecole Polytechnique Federal de Lausanne (EPFL) from January 19th to January 21st in Lausanne, Switzerland.

(July 2025) Onassis Lectures 2025 in Biology and Chemistry
Congress about directed evolution, held at the Foundation for Research and Technology (FORTH) from July 7 to 11 in Heraklion, Greece.

(September 2024) CECAM Workshop: "Leveraging Machine Learning for Sampling Rare Events in Biomolecular Systems"
Presented a talk about machine learning for coarse-grained models for proteins. From September 17th to 19th at Max Planck Institute for Polymer Research in Mainz, Germany.

(August 2024) CECAM Workshop: "Biomolecular Simulations at the Mesoscale"
Presented a talk and participated in the panel discussions about coarse grained model for proteins and their limits. From August 26th to 29th at the University of Trento at Trento, Italy.

(April 2024) CECAM Workshop: "Frontiers of Coarse-Grained Models"
Presented a talk about the research group efforts for building transferable coarse-grained force fields. From April 3rd to 5th at the Centre Blaise Pascal of the École Normale Supérieure de Lyon in Lyon, France.

(September 2023) NHR Coneference 23
Presented a poster titled " Bottom-up machine learning models can compete with the UNRES model" about a direct comparison between our models for protein dynamics and other established coarse-grained model.

(June 2023) CECAM-Psi-k Research Conference
Congress titled "Bridging length scales with machine learning: from wavefunctions to thermodynamics", taking place at the Zuse Institute in Berlin, Germany from 19th to 23rd of July. Presented a poster in collaboration with colleagues about transferable machine learned coarse grained force fields for proteins.

(July 2022) Escuela Nacional de Optimizacion y Análisis númerico
Mexican National numerical analysis and optimization conference, taking place at the

online from 4th to 8th of July. Presented a talk about unfolding 3D polygonal chains.

(October 2021) LXIV Congreso Nacional de Física
Mexican National Physics congress, taking place online from 3rd to 8th of October. Presented two posters related to lattice models for protein folding (in collaboration with Diego Alam) and a simulation for alcohol-based disinfectants on a surface (in collaboration with Diana Méndez, Pablo Trinidad, Karen Hidalgo and Abigail Cabañez)

(April 2021) XIX Escuela de Probabilidad y Estadística
School organized by the Center for Research in Mathematics (CIMAT) regarding probability and statistics, taking place from April 19 to April 23.

(August 2020) III Coloquio de Simulaciones Computacionales en Ciencias
Congress organized by UNAM's Nanoscience and Nanotechnology Center. Presented a talk titled "Double phase transition in modified lattice gas model".

(November 2019) XIV Escuela Mexicana de Física Estadística
School covering statistical physics, taking place at UNAM's Faculty of Science from November 5 to November 8. Presented a poster titled "Intermediate rigid-flexible phase in a modified lattice gas model".

(October 2019) LXII Congreso Nacional de Física
Mexican National Physics congress, taking place at the Juarez Autonomous University of Tabasco from 7 to 11 of October. Presented a poster titled "Intermediate rigid-flexible phase in a modified lattice gas model".

(January 2019) XLVII Winter Meeting on Statistical Physics
International congress covering statistical physics. It was celebrated in Puebla City, Mexico, from January 9 to January 12. Presented a poster titled "Double phase transition in modified lattice gas model".

(May 2018) Undergraduate School on
Experimental Quantum Information Processing 2018
Summer School about quantum information theory and quantum computation celebrated at the Institute for Quantum Computing of the University of Waterloo from May 25 to June 5.

Teaching

Teacher Assistant — Physics Department
Statistical Physics and Thermodynamics — Freie Universität Berlin
April 2023 - September 2023
Tutoring two hours per week, elaborating homework and grading assignments. Group lectured by Prof. Dra. Cecilia Clementi.

Adjunct Professor — Physics Department
Computational Physics — Faculty of Sciences, National Autonomous University of Mexico
August 2021 - January 2022
Giving six hours of class Weekly during the Fall 2021 period at group 8446. The class was imparted remotely.

Adjunct Professor — Physics Department
Computational Algorithms — Faculty of Sciences, National Autonomous University of Mexico
January 2021 - July 2021

Giving four hours of class Weekly during the Spring 2021 period at group 8446. The class was imparted remotely.

Adjunct Professor Physics Department
Computational Physics Faculty of Sciences
National Autonomous University of Mexico

September 2020 - January 2021
Giving six hours of class Weekly during the Fall 2020 period at group 8446. The class was imparted remotely.

Adjunct Professor Physics Department
Computational Physics Faculty of Sciences
National Autonomous University of Mexico

June 2020 - September 2020
Giving six hours of class Weekly during the summer 2020 period at group 8446. The class was imparted remotely.

Adjunct Professor Physics Department
Computational Algorithms Faculty of Sciences
National Autonomous University of Mexico

January 2020 - June 2020
Giving four hours of lecture weekly at group 3009.

Teacher assistant Mathematics Department
Differential and Integral Calculus I Faculty of Sciences
National Autonomous University of Mexico

August 2019 - December 2020
Giving four hours of class weekly and grading homework during fall 2019 semester at group 4033 from M.Sc. Lauro Morales Montesinos.

Teacher assistant Mathematics Department
Differential and Integral Calculus II Faculty of Sciences
National Autonomous University of Mexico

January 2019 - May 2019
Giving five hours of lecture weekly and grading during the Spring 2019 semester on group 4058 of Prof. María de la Luz Jimena de Teresa de Oteyza.

Teacher assistant Physics Department
Computational Physics Faculty of Sciences
National Autonomous University of Mexico

August 2018 - December 2018
Assisting students in the computer lab six hour per week and grading during the Fall 2018 semester on group 8231 of Prof. David Philip Sanders.

Teacher assistant Mathematics Department
Differential and Integral Calculus I Faculty of Sciences
National Autonomous University of Mexico

January 2018 - May 2018
Giving three hours of class weekly and grading homework during the spring 2018 semester on group 4009 of Prof. Elena de Oteyza de Oteyza.