Pablo G. **Romano**

Physical Chemistry PhD Candidate · Guenza Lab

Eugene, OR, 97403

pgromano | pgromano

Summary

Research focused on developing reliable theoretical/computational models to investigate the role of stochastic fluctuations in protein-DNA complexes. Analysis of large datasets such as atomistic long timescale macromolecular simulations and unsupervised classification of kinetic states via Markov State Models.

Skills

Programming	Python, Fortran+F2PY, Cython, C++, Bash, Matlab
Data Analysis	NumPy, Scikit-Learn/Image, SciPy, Pandas, Matplotlib
MD Simulations	GROMACS, Amber
Languages	Fluent English & Spanish

Education

University Of Oregon

Eugene, Oregon

Ph.D. in Physical Chemistry — *Sep. 2012 - Exp. Sep. 2017*

- Promising Scholar Award (**2012**). Award offered to a select group of incoming graduate students in recognition of their academic excellence in expectation of the unique perspectives they will bring to campus.
- Molecular Biology Biophysics Traning Grant (**2014–16**). NIH training grant awarded yearly through the University of Oregon's Institute of Molecular Biology. The objective is this award being to facilitate training to prepare graduate students to work on important problems in molecular biology and biophysics. This is accomplished by collaboration between multifaceted research programs.

St. Edward's University

Austin, Texas

B.S. in Chemistry with a minor in Mathematics — *Aug. 2008 - May. 2012*

- Welch Research Grant (**2010–11**). Given to Chemistry & Biochemistry students who perform novel research.
- Brother Daniel Lynch Research Award (**2011**). Provides support to senior students engaged in research projects who excel in academics and community service.
- President's Scholar Award (**2008–12**). For academic merit reviewed recurrently every semester.

Research Experience

University of Oregon

Eugene, Oregon

Marina Guenza Lab — *Sep. 2012 - Sep. 2017*

- Developed "Gradient Adaptive Decomposition" (*GRAD*) method to refine kinetic states by optimizing decision boundaries along gradient of the energetic distribution. Reproduced decomposition, label assignment, and transition timescales by refining undersampled Markov model.
- Modeled the conformational dynamics of DNA slow barrier crossing within stacking transitions, assessing chiral pathways involved in thermally induced breathing fluctuations critical in protein recognition.
- Developed Python API and Fortran+F2PY backend for *GRAD* method and developed Python API to Langevin Equation for Protein Dynamics (*LE4PD*) for the analysis of large all atom molecular dynamics datasets.
- Simulated several microsecond molecular dynamics simulations of various biological molecule on Extreme Scientific and Engineering Discovery Environment (XSEDE).

St. Edward's University

Austin, Texas

Eamonn Healy Lab — *Jan. 2009 - Jun. 2012*

- Analyzed structural homogeneity of ADAM10 and ADAM17 to study drug potency and selectivity. The ADAM family is a class of enzymes largely linked to inflammatory response in pathologies such as rheumatoid arthritis and metastasis in cancers.
- Designed novel inhibitors that selectively targeting ADAM17 while maximizing potency and reducing the selectivity in ADAM10 and thereby reducing liklihood of side effects.
- Performed docking studies within Accelrys Discovery Studio to structurally evaluate novel acetylenic based inhibitors and score the resulting "docked" structures.

Teaching Experience

University of Oregon Department

Eugene, Oregon

Undergraduate Research Mentor

Sep. 2012 - Sep. 2017

- Trained and mentored undergraduates in research, data analysis, and computational methods.
- Students were trained to run Molecular Dynamics (MD) simulations using Gromacs.
- Visualization used PyMol and Visual Molecular Dynamics software.
- Data analysis through Python, Fortran, and Gromacs analysis tools.
- Additional requirements for mentorship involved teaching students to use Linux operating systems, giving a 2 hour course on Research Ethics, and conducting weekly research review sessions to help students develop proper research methods.

University of Oregon Department of Chemistry

Eugene, Oregon

Nonequilibrium Statistical Mechanics

Sep. 2016

- Taught week long lecture series on non equilibrium statistical mechanics focused on applications Markov State Models (MSM) of biological macromolecules.
- The series presented up to date theory, development of the field, and provided a hands-on learning module using the Python and PyEMMA software package.
- Students built MSMs for protein folding simulations.

University of Oregon Department of Chemistry

Eugene, Oregon

Graduate Teaching Fellow

Sep. 2012 - Sep. 2014

- Assisted in laboratory course work for General Chemistry I, II, & III.
- Work expectations involved weekly office hours, assisting in theory based lectures, leading and lecturing course experiments, assisting in course examinations, and grading lab coursework.

St. Edward's University Department of Chemistry

Austin, Texas

Lab Teaching Assistant

Aug. 2010 - Jun. 2012

- Assisted in laboratory course work for General Chemistry, Organic Chemistry I & II, and Biochemistry.
- Responsibilities included giving lab lectures, assisting in desiging lab coursework, and preparing and standardizing stock reagent.

St. Edward's University Academic Success Center

Austin, Texas

Supplemental Instructor

Aug. 2010 - Jun. 2012

- Assisted in course work in General Chemistry, Organic Chemistry I & II, Analytical Chemistry, and Biochemistry.
- Expectations for the position involved holding office hours and leading two weekly group study lectures as a supplement to to coincide with course work.

Presentation & Workshops

American Physical Society: National Meeting

New Orleans, Louisiana

Chiral Pathways in DNA dinucleotides using gradient optimized refinement along metastable borders

Mar. 2017

- Presented talk on novel method for refining of Markov State Models. The method used underlying probability distribution to correct under-sampling while retaining crisp boundaries.

Centre Européen de Calcul Atomique et Moléculaire

Jülich, Germany

CECAM Macromolecular Simulation Software Workshop

Oct. 2015

- "Hackathon" workshop with the aim of tackling the most challenging problems within macromolecular modeling, particularly those relating to how the capabilities of and opportunities presented by future generations of massive heterogeneous, computational resources can best be leveraged in this domain of science.
- Travel expenses were funded by travel fellowship awarded to promising US candidates.

Biophysical Society: National Meeting

Baltimore, Maryland

Analyzing Small DNA Constructs via a Chromophore Model within the Point Dipole Approximation.

Mar. 2015

- Presented poster on ensemble model to predict the Circular Dichroism spectra of small oligonucleotide constructs employing a classical point dipole approximation.

American Chemical Society: National Meeting

Indianapolis, Indiana

Coarse-Graining and Multiscale Modeling in Complex Chemical Systems

Sep. 2013

- Attended conference for development of academic and research pursuits.
- Travel expenses were funded by a NSF Phase 1 Center for Chemical Innovation. Fellowship awarded to underrepresented minorities students in the STEM field.

American Chemical Society: Southwest Regional Meeting

New Orleans, Louisiana

Acetylenic inhibitors of ADAM10 and ADAM17: In silico analysis of potency and selectivity

Sep. 2012

- Presented talk on comparative study on binding potency and selectivity effects for inhibitors targeting TACE protein family.

Program Committees

Physical Chemistry Faculty Search

University of Oregon

Organizer & Host

2016

- Hosted lunch series aimed to introduce students to faculty candidates.
- Students had the opportunity to learn about research and working in Academia.

Physical Chemistry Guest Speakers

University of Oregon

Organizer & Host

2015-2016

- Hosted a series of lunches aimed to introduce students to invited Physical Chemistry Speakers.
- Students had opportunity to learn about research

Publications

The Gradient Adaptive Decomposition (GRAD) method: Optimized refinement along macrostate borders in Markov State Models

PG Romano, M Guenza; J. Chem. Info. & Mod.

Submitted

Chiral Stacking Transition Pathways in DNA Oligonucleotides

PG Romano, M Guenza; J. Chem. Phys.

In Preparation

Markov State Models for DNA using a Langevin Approach

PG Romano, M Guenza; J. Biophys.

In Preparation