Julian Melendez Ph.D.

jamelendez@usf.edu

0000-0002-2304-8643

JAMelendezD

julian-melendez

813-298-8497 Tampa, FL, USA

Skills

Biophysics | Molecular Dynamics | Molecular and Structural Biology | Method Development | Coding | QM Calculations | Machine Learning | High Performance Computing | Structural Bioinformatics | Big Data | Data Analysis and Visualization | Scientific Writting and Reviewing

Strengths

Problem Solving Thinking

Ability to identify patterns, troubleshoot issues, and refine methodologies, leading to more efficient workflows

Attention to Detail

High quality work with carefully constructed, visually compelling, and informative figures that effectively communicate complex data

Technical Proficiency

Proficient in computational methods and simulation techniques, with the ability to quickly adapt to new tools and languages for solving complex biophysics problems

Collaboration

Skilled at collaborating across interdisciplinary teams and clearly communicating complex concepts to both technical and non-technical audiences

Summary

Computational biophysicist specializing in the development of advanced computational models to explore molecular and atomic-level dynamics of biological systems. Expertise in molecular dynamics (MD), force field development, and biomolecular modeling, with skills in designing and implementing robust computational pipelines using Python. Leverages tools like quantum mechanics and statistical mechanics to solve complex biological questions. Focused on cross-disciplinary collaboration, contributing to both fundamental research and translational applications, driving high-impact projects that lead to peer-reviewed publications. Passionate about integrating machine learning techniques to refine computational methodologies, enhance simulation accuracy, and accelerate insights into biophysical processes such as protein-ligand interactions, ion channel dynamics, and enzyme catalysis, ultimately advancing the understanding of biophysics in health and disease.

Research Experience

Ph.D. Researcher - University of South Florida 2020-2025

- Performed QM calculations and developed a curated dataset to improve models of ion interactions in biological systems, while automating workflows to enhance computational efficiency and accuracy in ion-binding predictions.
- Developed a polarizable force field for proteins and nucleotides with improved ion interactions, evaluated using enhanced sampling techniques and alchemical free energy methods to assess binding affinities and thermodynamic properties.
- Applied MD simulations to investigate biomedical challenges, including lithium's role in bipolar disorder and viral protein binding to host receptors, supporting the development of therapeutic strategies and drug-target interaction models.
- Collaborated on identifying key residues involved in lactamase-mediated antibiotic resistance, utilizing NMR data and automating statistical analysis of large PDB datasets to accelerate insights into resistance mechanisms.

Undergraduate Researcher - Universidad de los Andes 2017-2018

- Conducted MD simulations to investigate how specialized lipids influence the membrane biophysics of *Staphylococcus aureus*, revealing changes in membrane structure and dynamics that offer insights into bacterial resilience and potential avenues for targeted antimicrobial therapy development.

Education

Tampa, FL, USA, University of South Florida 2020-2025
Ph.D., Molecular Biosciences (Conc. Computational Biophysics)

Bogota, Colombia, Universidad de los Andes 2014-2018
Bachelor of Science in Physics. Minor in Biology

Publications

- **Delgado, J. M.**, et al. **(2025)**. Development of Phosphate and Phosphorylated amino acids for the AMOEBA-HFC polarizable Force Field. ***(in preparation)***
- **Delgado, J. M.**, et al. (**2025**). Structure and dynamics of the bioactive form of lithium. ***JACS. (submitted)***
- Arcia, E., [...], **Delgado, J. M.**, et al. **(2025)**. Dynamic signature of activity-stability tradeoff in lactamase evolution. ***Nat. Commun. (under revision)***
- Figueroa, D., [...], **Delgado, J. M.**, et al. **(2025)**. Staphyloxanthin modifies the structure of bacterial-model phosphoglycerol membranes ***(in preparation)***.
- **Delgado, J. M.**, et al **(2023)**. Polarizable AMOEBA Model for Simulating Mg^{2+}·Protein·Nucleotide Complexes. ***J. Chem. Inf. Model.*** 64, 2, 378–392. [URL]
- **Delgado, J. M.**, et al **(2022)**. Inclusion of High-Field Target Data in AMOEBA's Calibration Improves Predictions of Protein–Ion Interactions. ***J. Chem. Inf. Model.*** 62, 19, 4713–4726. [URL]
- **Delgado, J. M.**, et al **(2021)**. Molecular basis for higher affinity of SARS-CoV-2 spike RBD for human ACE2 receptor. ***Proteins: Struct., Funct., Bioinf.*** 89, 2, 1134-1144. [URL]
- Wineman-Fisher, V., **Delgado, J. M.**, et al. **(2020)**. Transferable interactions of Li^{+} and Mg^{2+} ions in polarizable models. ***J. Chem. Phys.*** 153, 10, 104-113. [URL]

Awards

- **Biophysical Society (BPS) Travel Award** — 2025
- **BPS Poster Award** - Winner poster at the BPS meeting in the Theory and Computation subgroup — 2025
- **Dissertation Fellowship** - Awarded by USF to support the completion and writing of the dissertation — 2025
- **Outstanding Research Award** - USF graduate student who demonstrates strong evidence of scholarship — 2023
- **Presentation Award** - 1st at the USF Raymond. N. Castle Conference — 2023
- **1st Nationally** - Colombian standarized tests to access higher education (ICFES)/SAT equivalent — 2014

Presentations and Posters

- **Biophysical Society Meeting:** Presented research on the development and application of molecular dynamics simulations for biological systems to a specialized audience, effectively conveying technical findings through three posters, one platform talk, and one flash talk.
- **American Chemical Society Meeting:** Tailored presentations for a diverse scientific audience, communicating molecular dynamics and biophysics concepts clearly to chemists and researchers from various disciplines through two platform talks.

Coding Portfolio

- **Selective Charge Penetration in TINKER:** Modified the TINKER MD source code (Fortran) to implement selective charge penetration effects.
- **Coding Tutorials in Python and C:** Developed tutorials covering basic to intermediate programming concepts, including recursion, data structures, algorithm efficiency, and unit testing. Included optimized solutions for selected problems from **Project Euler** to demonstrate practical algorithm design.
- **Blender Plugins for Scientific Visualization:** Created two plugins for visualizing biomolecules and parametric 3D functions in Blender, combining scientific accuracy with artistic design. Sold over 500 copies.
- **Custom MD Engine and Analysis Tools:** Developed a basic MD engine and a suite of analysis tools, including contact maps, local density calculations, gradient-free optimizers, and quaternion-based rotation methods.
- **Machine Learning for Image Classification:** Applied machine learning techniques to classify images, including MNIST digit recognition and cat-dog identification, leveraging neural networks for pattern recognition.

Teaching and Mentoring Experience

Graduate Teaching Assistant - University of South Florida — 2021-2023

Led cellular and molecular biology labs, guiding student groups through experiments while effectively communicating complex concepts and fostering understanding and engagement.

Programming and Physics Tutor - Universidad de los Andes — 2016-2018

Helped STEM students with programming and introductory physics coursework

Interests and Volunteer Activities

- **Coding and Problem Solving:** Enjoy coding, tackling new challenges, and developing tools to analyze and visualize complex concepts in novel ways.
- **Sports and Teamwork:** Avid soccer player with 15+ years of experience, gaining valuable lessons in collaboration, discipline, and perseverance that I apply professionally.
- **YMCA soccer Referee and Coach:** Guided and developed youth players, ensuring fair play and teamwork. — 2019
- **SAT Math Tutor, Hillsborough County:** Improved students problem-solving skills with personalized learning strategies. — 2019

Highlights

- 6+ years of molecular dynamic simulations experience
- Experienced in QM calculations for biomolecular modeling.
- Avid coder with 10+ years of experience, 500+ plugin sales, and contributions to MD tools, coding tutorials, and ML applications.
- Strong track record with 5 publications and 8 talks & posters at national conferences.

Programming

Proficient in writing code, primarily in interpreted languages like Python, with experience in compiled languages including C and Fortran. Utilize automation in BASH and leverage HPC environments using SLURM. Experienced in version control using GIT. GitHub portfolio available for reference.

Python	●●●●●
C	●●●●○
Fortran	●●●○○
Bash	●●●●○
SLURM/HPC	●●●●○
GIT	●●●●○

Software Expertise

QM: GAUSSIAN · FHI-AIMS · PSI4

MD: GROMACS · TINKER · OPENMM

ML: TensorFlow · PyTorch · SkLearn

Graphics (vector and 3D):

Inkscape · GIMP · Matplotlib · ggplot · pymol · VMD · ChimeraX · Blender

Data analysis and writting:

Numpy · Pandas · Latex

Languages

English	●●●●●
Spanish	●●●●●
French	●●●○○

"Everything that living things do can be understood in terms of the jiggling and wigglings of atoms"

Richard Feynman