EdisonFlorez

Data Scientist | Computational Biophysicist
Scientific Algorithm Developer

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Profile: As a data scientist with a profound background in quantum chemistry, biophysics, and mathematics, I bring over eight years of experience to the table, having served as a scientific algorithm developer, data scientist, and team leader. My passion lies in extracting fundamental insights from data, thinking critically, and understanding the rationale behind each task. With my ability to learn quickly and motivation to take on challenges, I have excelled as an individual contributor, taking calculated risks and showing initiative. My experience spans consulting for a biotech startup and the financial industry, where I developed scientific software, validated scalable HPC algorithms, and worked collaboratively to deliver top-quality, data-driven scientific solutions and visualizations. I have a track record of solving complex problems through algorithm development in research labs in New Zealand, Argentina, and Colombia. In the role of a teacher, I've mentored students in two large universities, simplifying complex scientific concepts, methods, and theories in science, math, and computers. In my spare time, I enjoy intellectual pursuits like reading, writing, and learning new things. I am also freelance as an editor and reviewer for scientific manuscripts and research for publication.

Key Skills: Complex problem solving • Critical thinking • Creativity • Leadership • Teamwork • Project Management • Communication • Time management • Decision making

Technical Skills: Python • SQL • Git • TDD • Fortran • openMP • Bash • Linux • HPC • LaTeX • Optimization and Search Algorithms • Testing • Deployment • Machine Learning

Professional Experience

- **Computational Protein Designer** Since Aug.2021
  HelicoBio [helico.bio], New Zealand

  Scientific Algorithm developer: Leveraging in-depth knowledge of biophysics and protein design, I created and validated scalable algorithms to advance plant biology research. As a team leader, I collaborated with cross-functional groups to deliver high-quality, data-driven scientific solutions. I contributed to all phases of the software development lifecycle, including the development, testing, and deployment of new functionalities. A notable achievement was leading the development of a protein design platform using Python, C++, and GraphQL/SQL.

- **Freelancer Editor:**
  Enago [enago.com] Since Apr.2023

MDPI [mdpi.com] Apr.2018 - Dec.2018
INGE CUC [revistascientificas.cuc.edu.co/index.php/ingecuc] Dec.2015

Copy & Substantive Editing: I perform Copy Editing, refining grammar and scientific terminology; and Substantive Editing, enhancing manuscript structure and content, clarifying ambiguous text, and verifying citation relevance. This helps authors aiming for high-impact journals and those requiring extensive language assistance. This comprehensive approach aids authors aiming for high-impact journals and those needing more extensive language assistance in checking whether they adhere to the journal's style and monitoring the writing and editing activities to ensure that the content is understandable and relies on accurate facts.

- **Demonstrator:** Aug.2018 - Mar.2020
  Massey University [massey.ac.nz], New Zealand

  Physics: Instruct and advise students in workshops, with an emphasis on intricate topics such as advanced mechanics, thermodynamics, fluid dynamics, magnetic field theory, electromagnetism, and circuit analysis. My role is instrumental in enhancing students' understanding of these complex physical concepts and principles.

- **Data Scientist:** Aug.2016 - Mar.2018
  EY-ifb [ey.com], Colombia.

  SAP-Implementation and Bank-Analyzer: Develop tailored solutions based on thorough business and technical analyses, primarily within SAP or Oracle environments for Analytical Banking and Business Intelligence. I specialize in crafting complex models using SAP Bank Analyzer and implementing them, addressing economic problems through customized IT solutions. Additionally, I develop and implement mathematical models related to financial inquiries, providing detail-oriented and pragmatic solutions.

- **Graduate Teaching Assistant:** Sept.2015 - Aug.2016
  University of Antioquia [udea.edu.co], Colombia.

  Quantum & Computational Chemistry: Guide advanced college students through the intricate domain of Quantum Chemistry. I ensure students achieve proficiency in the quantum language, comprehend relevant methods, and grasp key concepts. Furthermore, I facilitate their understanding of the interpretation and application of these principles in chemically interesting systems.

Peer-reviewed Publications

- **Flórez, Edison**; Zapata-Escobar, Andy; Ferraro, Franklin; Ibarguen-Becerra, César; Chamorro, Yuly; and Maldonado, Alejandro F. "Coordination of Mercury (II) in Water Promoted over Hydrolysis in Solvated Clusters $[Hg(H_2O)_{1-6}]^{2+}_{(aq)}$: Insights from Relativistic Effects and Free Energy Analysis." Submitted

- **Flórez, Edison**; Reuvers, Tom; Schwarz, WH Eugen and Peter Schwerdtfeger."The Stability of the Noble Gas Fluorides from Nonrelativistic and Relativistic Density Functional and Coupled Cluster Studies." Submitted

- **Flórez, Edison**; Helgaker, Trygve; Klopper, Wim; Teale, Andrew; Stopkowicz, Stella; Pahl, Elke. "Melting of Neon Under Extreme Conditions: Ab Initio Monte Carlo Simulations in High Magnetic Fields." Submitted

- **Flórez, Edison**; Odile R. Smits; Jan-Michael Mewes; Paul Jerabek; and Peter Schwerdtfeger. "From the gas phase to the solid state: The chemical bonding in the superheavy element flerovium." The Journal of Chemical Physics 157, no. 6 (2022): 064304.DOI: 10.1063/5.0097642

- Chamorro, Yuly; **Flórez, Edison**; Alejandro F. Maldonado; Gustavo A. Aucar; and Albeiro Restrepo. "Microsolvation of heavy halides." International Journal of Quantum Chemistry 121, no. 7 (2021): e26571. DOI: 10.1002/qua.26571

- **Flórez, Edison**; Alejandro F. Maldonado; Gustavo A. Aucar; Jorge David; and Albeiro Restrepo. "Microsolvation of methylmercury: structures, energies, bonding and NMR constants (^{199}Hg, ^{13}C and ^{17}O)." Physical Chemistry Chemical Physics 18, no. 3 (2016): 1537-1550. DOI: 10.1039/c5cp04826e

Open-Source Contributions

- **Parallel Tempering Monte Carlo (PTMC):** This project introduces an advanced Fortran (2003) code that uses the Parallel Tempering Monte Carlo (PTMC) method for an accurate and efficient analysis of phase transitions in atomic and molecular clusters. Our application includes studying melting transitions of noble gases and water clusters, even in ultra-high magnetic fields. The code is parallelized using OpenMP and it is optimized for HPC architectures. The code is open-source and available on github.com/e-florez/PTMC

- **Atomic and Molecular Cluster Energy Surface Sampler (AMCESS):** An open-source Python package that automates the exploration of the Potential Energy Surface (PES) for atomic and molecular clusters. AMCESS uses advanced optimization techniques to generate candidate structures for critical points on the PES, enhancing research accuracy and efficiency. Its user-friendly design and integration with popular quantum chemistry packages make it a valuable tool for researchers in molecular physics, chemistry, and materials science. AMCESS code is available on gitlab.com/ADanianZE/amcess

- **Cluster Compare (pyCC):** Python project designed to analyze and compare atomic and molecular clusters. The main script is created to orchestrate a rigorous and insightful comparison of cluster data, facilitating a deeper understanding of their intrinsic properties and interactions. pyCC uses a range of data analysis and machine learning modules to derive key cluster features from atomic coordinates and bond patterns, including radial and angular distributions, and various similarity descriptors. By harnessing libraries like numpy, scipy, pandas, and scikit-learn, it provides a specialized, versatile framework for a comparative study of atomic and molecular clusters. The code is open-source and available on github.com/e-florez/pyCC

Academic Background

- **Doctor of Philosophy** (Candidate) December 2022
  Computational Physics, Massey University, New Zealand
- **Master of Science** December 2014
  Computational Chemistry, University of Antioquia, Colombia
- **Bachelor of Science** July 2012
  Computational Chemistry, University of Antioquia, Colombia

Fellowships and Awards

- **PhD in Physics:** Massey University Doctoral Scholarship (full-time) 2018, 2019, 2020
- **MSc in Chemistry:** Honours and research work with meritorious award.

Yours sincerely,

Edison Florez
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