EdisonFlorez

Data Scientist | Computational Physicist | Scientific Algorithm Developer

edisonffh@gmail.com • github.com/e-florez • linkedin.com/in/edisonflorez

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 biotech startups and the financial industry, where I develop scientific software, validate scalable HPC algorithms, and work 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 • Testing • CI/CD • TDD • C++ • Fortran • openMP • Bash • Linux • HPC • LaTeX • Optimization and Search Algorithms

Academic Background

- **Doctor of Philosophy** (Candidate) February 2023
  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.

Professional Experience

- **Computational Physics** Aug.2021 - Apr 2022
  HelicoBio [helico.bio], New Zealand

  Computational Protein Designer: as a `TEAM LEADER`, my primary focus is driving software solutions in the field of plant biology research. My commitment to quality and scientific excellence has enabled the team's progress through all stages of the software development lifecycle, from design and development to testing and deployment. One of my key achievements as a team leader is successfully leading the creation of a novel protein design platform for running comprehensive all-atom molecular dynamics simulations. As a `DEVELOPER`, my expertise in biophysics and protein design is reflected in my development role, where I create and validate scalable algorithms that propel our research forward. My proficiency with Python, C++, and SQL has been instrumental in developing new functionalities and ensuring their seamless deployment. I have also utilized and demonstrated in-depth knowledge of various molecular dynamics packages, including GROMACS, AMBER, and OpenMM.

- **Freelancer Editor:**
  Enago [enago.com], Remote Since Apr.2023
  MDPI [mdpi.com], Remote Apr.2018 - Dec.2018

  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.

- **Course Developer:** Apr.2018 - Dec.2019
  A&E International [naeaedu.com], New Zealand

  Lesson Planner and Tutor: Develop comprehensive STEM teaching content in alignment with the New Zealand Curriculum. I meticulously prepare course materials for new classes, both for in-person and online learning environments. Additionally, I guide and mentor students to comprehend and execute relevant STEM projects and workshops, fostering their understanding and application of STEM principles in practical scenarios.

- **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 for Analytical Banking and Business Intelligence. I specialize in crafting complex models and implementing them, addressing economic problems through customized solutions. Additionally, I developed and implemented 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.

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**; 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**; Helgaker, Trygve; Klopper, Wim; Teale, Andrew; Stopkowicz, Stella; and Pahl, Elke. "Melting Under Extreme Conditions: Ab Initio Monte Carlo Simulations." In APS March Meeting Abstracts, vol. 2019, pp. C17-001. 2019. ui.adsabs.harvard.edu/abs/2019APS..MARC17001F

- **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. Code 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. Code 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. Code available on github.com/e-florez/pyCC

Supervisions

- Co-supervisor MSc thesis, computational chemistry: Apr.2018 - Feb.2020
  Microsolvation of Heavy Halides $[X(H2O)_{1-6}]^-$ (X = Br, I, At)
  University of Antioquia [udea.edu.co], Colombia.

- Co-supervisor BSc thesis, computational chemistry: Nov.2015 - Dec.2017
  Relativistic and Electron Correlation Effects on the Calculation of Nuclear Magnetic Resonance Parameters on MX Diatomic Molecules (M=Cu, Ag, Au and X=F, Cl, Br, I)
  University of Antioquia [udea.edu.co], Colombia.

Yours sincerely,

Edison Florez
edisonffh@gmail.com
May 31, 2023