EVARISTO VILLASECO

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EDUCATION

P.hD. in Physics, Rutgers University | 2020–2025 | GPA 4.0.

M.Sc. in Physics, Rutgers University | 2020-2022 | GPA 4.0.

M.Sc. in Theoretical Chemistry and Computational Modeling, Autonomous University of Madrid | 2016-2018 | 1 A+ Class Honor.

B.Sc. in Chemistry, *University of Salamanca* | 2012–2016 | 8 A+ Class Honors.

SKILLS & CERTIFICATIONS

Languages & Platforms: Python, SQL, PySpark, Bash, Fortran, SQL, Git, HPC.

Quantitative Skills: Linear algebra, Probability, Statistical inference, Numerical methods, Optimization techniques.

Machine Learning: PyTorch, Scikit-learn, Statsmodels, XGBoost, Hugging Face, Transformers.

Certificates: ColumbiaX Professional Certificate in Corporate Finance [LINK], The Erdős Institute Data Science Boot Camp [LINK],

The Erdős Institute Deep Learning Boot Camp [LINK].

EXPERIENCE

Data Scientist (Intern) | Burnt | February 2025–Present

- Developed a GenAI-powered Conversational Agent in Python to automate order data collection for sales representatives, ensuring data validation and integration with external tools using RAG for database retrieval.
- · Enabled real-time interaction via WhatsApp using Twilio and Flask improving order verification and customer communication.

Physics PhD | Researcher | Rutgers University | September 2020–Present

- Developed novel mathematical models and efficient computational schemes to simulate highly correlated dynamical systems, solving coupled differential equations governing quantum-classical interactions.
- Designed numerical algorithms for time-dependent molecular behavior, that led to a 80 % reduction in energy deviation and an 87% improvement in molecular property predictions compared to existing standard approaches [Video Presentation].
- Published 10 papers in high-impact peer-reviewed journals and presented findings at international conferences.

Open Source Contributor | g-ctmqc & QuantumModelLib | September 2022–Present

- Implemented a new molecular dynamics method in g-ctmqc [LINK] and extended the codebase with additional functionalities, expanding its simulations capabilities by 25%, and supporting 4 peer-reviewed publications.
- Integrated two new quantum models into QuantumModelLib [LINK] increasing the library's electronic structure capabilities by 5%.

Physics PhD | Instructor | Rutgers University | September 2020–Present

• Led problem-solving sessions for 100+ students, developed materials, graded assessments and provided office hour support.

SELECTED PROJECTS

LaLiga SoccerSage | Jan 2025–March 2025

- Developed and implemented a Random Forest model to predict outcomes of La Liga soccer matches achieving accuracy rate of 75%.
- Engineered features from historical match data, including team performance metrics and situational factors to enhance predictions.
- Outperformed bookmaker implied probabilities by 24%.

Restaurant Analytics & Demand Forecasting | Burnt & The Erdős Institute | May 2024—August 2024

- Uncovered key trends in restaurant sales and consumer behavior analyzing sales fluctuations across various conditions and time periods.
- Developed a forecasting model for restaurant sales and menu item demand, leveraging key external and operational factors, with a projected 15% annual savings (~\$250k) on food costs if adopted by the restaurant.[LINK]
- Ranked in the top 10 out of 70+ projects in the bootcamp, earning distinction for innovation and impact.

GenAI-powered solutions for the restaurant industry Burnt & The Erdős Institute | May 2024—August 2024

• Fine-tuned open-source LLMs (LLaMA 2, BERT, GPT-2) using efficient techniques such as LoRA to standardize product categorization across restaurant suppliers, achieving ~92.5% classification accuracy. [LINK]

GPT: Central Perk Edition | March 2025

- · Implemented a GPT language model using PyTorch, developing core components such as self-attention or positional encoding.
- Trained the model on a corpus of all Friends TV show episodes to generate realistic Friends-like dialogues.
- Used the project as a proof of concept to gain a deeper insight into the mathematical foundations of large language models (LLMs).

LIST OF PUBLICATIONS

- E. Villaseco Arribas and N. T. Maitra, Phys. Rev. Lett. 133, 233201 (2024).
- E. Villaseco Arribas, N. T. Maitra, and F. Agostini, J. Chem. Phys. 160, 054102 (2024).
- · L. M. Ibele, E. Sangiogo Gil, E. Villaseco Arribas, and F. Agostini. Phys. Chem. Chem. Phys. (2024).
- A. Pollien, E. Villaseco Arribas, D. Lauvergnat, and F. Agostini. Mol. Phys. 0 (2024), e2378960.
- E. Villaseco Arribas and N. T. Maitra. J. Chem. Phys. Commun. 158, 161105 (2023)
- E. Villaseco Arribas, L. M. Ibele, D. Lauvergnat, N T. Maitra, and Federica Agostini. J. Chem. Theory Comput. 19 (2023).
- E. Villaseco Arribas, P. Vindel-Zandbergen, S. Roy, and N. T. Maitra. Phys. Chem. Chem. Phys. 25, 26380 (2023).
- E. Villaseco Arribas, F. Agostini, and N. T. Maitra. Molecules 27 (2022), p. 13.
- A. Emelianova, E. A. Basharova, A. L. Kolesnikov, E. Villaseco Arribas, J. Phys. Chem. B 125, 16, 4086-4098 (2021).
- A.L. Ruiz, E. Villaseco Arribas and K. McEnnis. Mater. Adv., 3, 2858-2870 (2022).

SPEAKING ENGAGEMENTS AND CONFERENCES

American Conference in Theoretical Chemistry (ACS) | Palisades Tahoe, CA, USA (2022)

• Title: Exact factorization-based coupling terms for mixed quantum-classical dynamics (Contributed Talk).

ACS Northeastern Regional Meeting | Rochester, NY, USA (2022)

• Title: Mixed quantum-classical dynamics with coupled trajectories (Contributed talk).

Seminar Series, Université Paris Saclay | Paris, France (2022)

• Title: Exact factorization-based mixed quantum-classical dynamics (Invited talk).

CECAM Workshop | Lausanne, Switzerland (2022) (Contributed talk).

• Title: Energy-conserving coupled trajectories mixed quantum-classical dynamics.

Seminar Series, Universidad de Salamanca | Salamanca, Spain (2023)

• Title: Exact factorization-based mixed quantum-classical dynamics (Invited talk).

American Conference in Theoretical Chemistry (ACS) | New Orleans, LA, USA (2024)

• Title: Exact Factorization Approach of Coupled Electrons, Ions, and Photons (Invited Talk, replacement speaker).

AWARDS

- Chateaubriand Fellowship: Awarded a prestigious fellowship by the Embassy of France on the United States to lead a joint research project between Université Paris-Saclay and Rutgers University that resulted in 5 peer-reviewed publications.
- Dean Dissertation Fellowship: Awarded for outstanding research contributions in applied physics.
- ICIQ Summer Fellowship: Top 1.4% among 1,000+ applicants for a prestigious research program in one of Spain's leading chemical institutions.
- IFIMAC Grant: Awarded a full-tuition M.Sc. scholarship and living stipend by the Institute of Condensed Matter Physics.