EVARISTO VILLASECO

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EDUCATION

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

Programming & Platforms: Python, SQL, Bash, PySpark, SQLAlchemy, Fortran, Git, HPC, AWS (familiar).

Quantitative Skills: Probability, Statistical inference, A/B testing, Linear algebra, Calculus, Numerical methods.

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

Soft Skills: Problem-solving, Critical-thinking, Communication, Cross-functional Collaboration.

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

AI Engineer (Intern) | *Burnt* | February 2025–Present

- Developed a GenAI-powered Conversational Agent in Python to automate order data collection for sales representatives, enabling integration with RAG and vector database search for efficient information retrieval and data validation.
- Enabled real-time interaction via WhatsApp using Twilio and Flask improving order verification and customer communication.
- Designed AI agent workflows using BeeAI to streamline data processing and enhance automation capabilities.
- Built a multi-tenant backend using SQLAlchemy and a Flask API for secure, scalable data management across clients.

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%.

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

- Developed new methods to simulate complex molecular interactions that led to a 80 % reduction in energy deviation and an 87% improvement in molecular property predictions compared to existing standard approaches [LINK].
- Engineered an exact mathematical framework based on coupled differential equations for quantum-classical interactions, to guide the development of next-generation methods for molecular dynamics simulations.
- Published 10 papers in high-impact peer-reviewed journals and presented findings at international conferences.

Computational Physics PhD | Graduate Student Instructor | *Rutgers University* | September 2020–January 2022

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

SELECTED PROJECTS

BiteBuddy: a Nutrition Assistant Chatbot | April 2025

- Designed and deployed BiteBuddy, an AI-powered chatbot that provides personalized diet recommendations.
- Integrated natural language understanding with tool calling to ensure accurate caloric estimates and smooth conversational interactions.
- Deployed the chatbot on Streamlit Cloud, delivering an intuitive, fully web-based user experience.

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% and outperforming bookmaker implied probabilities by 24%.
- Engineered features from historical match data, including team performance metrics and situational factors.

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 QLoRA to standardize product categorization across restaurant suppliers, achieving ~92.5% classification accuracy. [LINK]

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

- Uncovered key trends in restaurant sales and consumer behavior across various conditions and time periods informing decision-making or inventory management and operational adjustments.
- Developed a predictive 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.

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.

PUBLICATIONS

- **E. Villaseco Arribas** and N. T. Maitra. "Electronic Coherences in Molecules: The Projected Nuclear Quantum Momentum as a Hidden Agent." *Phys. Rev. Lett. 133, 233201 (2024).*
- **E. Villaseco Arribas**, N. T. Maitra, and F. Agostini. "Nonadiabatic dynamics with classical trajectories: The problem of an initial coherent superposition of electronic states." *J. Chem. Phys. 160, 054102 (2024).*
- L. M. Ibele, E. Sangiogo Gil, **E. Villaseco Arribas**, and F. Agostini. "Simulations of photoinduced processes with the ex- act factorization: State of the art and perspectives." *Phys. Chem. Chem. Phys. (2024).*
- A. Pollien, **E. Villaseco Arribas**, D. Lauvergnat, and F. Agostini. "Exact-factorisation study of the photochemistry of phenol." *Mol. Phys. 0 (2024), e2378960.*
- **E. Villaseco Arribas** and N. T. Maitra. "Energy-conserving coupled trajectory mixed quantum-classical dynamics." *J. Chem. Phys. Commun. 158, 161105 (2023)*
- **E. Villaseco Arribas**, L. M. Ibele, D. Lauvergnat, N T. Maitra, and Federica Agostini. "Significance of Energy Conservation in Coupled-Trajectory Approaches to Nonadiabatic Dynamics." *J. Chem. Theory Comput. 19 (2023).*
- **E. Villaseco Arribas**, P. Vindel-Zandbergen, S. Roy, and N. T. Maitra. "Different flavors of exact-factorization-based mixed quantum-classical methods for multistate dynamics." *Phys. Chem. Chem. Phys. 25, 26380 (2023).*
- **E. Villaseco Arribas**, F. Agostini, and N. T. Maitra. "Exact Factorization Adventures: A Promising Approach for Non-Bound States." *Molecules 27 (2022), p. 13.*
- A. Emelianova, E. A. Basharova, A. L. Kolesnikov, **E. Villaseco Arribas**, E. V. Ivanova and G. Y. Gor. "Force fields for molecular modeling of sarin and its simulants: DMMP and DIMP" *J. Phys. Chem. B 125, 16, 4086-4098 (2021).*
- A.L. Ruiz, **E. Villaseco Arribas** and K. McEnnis. "Poly (lactic-co-glycolic acid) encapsulated platinum nanoparticles for cancer treatment". *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.