THEODOROS PANAGIOTAKOPOULOS

Ph.D Data Scientist ~ Computational Physicist

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SUMMARY

Experienced **Ph.D.** in Applied Physics, adept in simulating and applying **AI/ML** for Computational Material Science, seeking a data science role to tackle complex challenges and drive impactful solutions.

SKILLS

Languages: Python, Julia, R, C/C++, SQL, Bash, HTML.
Tools: Machine Learning, Data Handling, Data Analysis, Data Visualization
Technologies: Linux, Mac OS, Windows.

EDUCATION

08/2019 - present **Ph.D Artificial Intelligence applications in Computational Physics** — **University of Central Florida**
GPA: 4/4

10/2017 - 07/2019 **Computational Nuclear Physics** — **National and Kapodistrian University of Athens**
Grade: 9.2/10, Valedictorian

10/2011 - 07/2017 **Physics** — **National and Kapodistrian University of Athens**
Highly focused in computational physics

EXPERIENCE

7/2023 – present
DOE Funded

Machine Learning for Computational Chemistry — **University of Central Florida**

- Performed **simulations**, **gathered, cleaned,** and **analyzed data** to examine the influence of ammonium cations on the Bi-catalyzed CO_2 Reduction Reaction, treating it as a classification problem.
- Applied **Machine Learning** to model CO_2 reduction to formate and CO in small-scale systems, with **predictions** extrapolated to large electrochemical environments.
- **Developed** novel **algorithms** to compute CO_2 adsorption energy, resulting in data segmentation into two distinct regions. These advancements culminated in the calculation of electric forces and revealing the impact of cations on CO_2 adsorption.

`Python / C++ / SQL / Bash` `GitHub`

10/2022 – 7/2023
scholarship holder

Graph Neural Networks and Databases — **University of Central Florida**

- Research and investigated how **graph convolutional neural networks** can enhance the accuracy of predictions on truncated datasets.
- Created a centralized **SQL database** by collating and organizing existing group member data from the server. Enhanced accessibility and facilitated result validation among team members, promoting seamless collaboration and data-driven decision-making.

`Julia / SQL / Bash` `GitHub`

1/2019 – 10/2022
NSF Funded

Machine Learning for Computational Physic & Algorithm Design — **University of Central Florida**

- Implemented **ML** and introduced a second-generation **neural-network** potential, significantly outpacing Density Functional Theory (DFT) in terms of speed and accuracy. This accomplishment played a pivotal role in securing renewed funding.
- Created a fourth-generation **Neural Network** potential to overcome constraints in existing machine learning models, focusing on long-range charge transfer. This potential was adopted by our **data science** group, accelerating computational calculations.
- Engineered state-of-the-art **numerical methods** and **designed cutting-edge algorithms** for chemical potential calculations of metal on semiconductor junctions.
- Taught physics labs with a focus on analyzing and **applying** simple **machine learning models** to artificial data generated from simulations, as well as real data collected from our laboratory. Implemented **feature engineering** techniques, including data cleaning and transformation, to enhance the quality and relevance of the datasets.

`Python / C++ / SQL / Bash` `GitHub`

10/2017 – 7/2019
NKUA Funded

Machine Learning for Detection of Dark Mater — **University of Central Florida**

- Engaged in the development of a sophisticated **Machine Learning Approach** for Dark-Matter Particle Identification, navigating the challenges presented by extremely low temperatures with **precision and ingenuity**.
- Conducted Physics labs for undergraduates, immersing students in the intricacies of **statistical data analysis** and the art of data preparation for the application of **machine learning algorithms**.

`Python / SQL / Bash` `GitHub`

DATA SCIENCE AND CODING SKILLS

- Demonstrated excellence in **Python** and R for advanced coding and data analysis, harnessing these languages to extract valuable insights from intricate datasets.
- Skilled in **optimizing and recompiling C/C++** software to enhance performance for specific research and **computational needs**.
- Proficient in applying linear regression and Support Vector Machines (SVM) to enhance decision-making and optimize strategies within the context of **reinforcement learning**.
- Demonstrated proficiency in **training** and **testing Neural Networks** in **deep learning** to enhance data modeling and support well-informed decision-making.
- Proficient in utilizing ARIMA and SARIMA models to effectively analyze and forecast temporal data patterns, contributing to informed decision-making and accurate predictions in dynamic environments
- Showcased expertise in **data analytics** through numerous Ph.D. projects, skillfully extracting insights, making data-driven decisions, and delivering meaningful solutions.

TECHNICAL SKILLS

- Exemplary knowledge of **data structures**, consistently designing and implementing efficient and optimized solutions for complex data-related challenges.
- Master **(**data integration) techniques with SQL, loading, extracting, and transforming data to ensure seamless and efficient processes.
- Expertise in **algorithm design** and **data science software architecture** for streamlined data workflows.
- Proficient in **high-performance computing cluster management**, specializing in **Slurm** for job scheduling, resource allocation, and **performance optimization**.
- Demonstrated **Git** expertise, maintaining organized code repositories for collaborative, data-driven projects.
- Proficiently creates compelling data visualizations with **Tableau, Matplotlib, and gnuplot** for clear communication of complex insights.

MANAGEMENT SKILLS

- **Supervising and independently completing projects**, consistently meeting budget and deadline goals with top-tier execution.
- Proficient in **conceptualizing, planning, and executing** end-to-end data science initiative aimed at solving critical business challenges.
- Successful in leading **diverse teams**, **fostering collaboration** and energizing **collective success**.
- Exceptional **communication and presentation skills**, bridging knowledge gaps and **ensuring clarity**.
- Excelled in **problem solving** and **analytical thinking** in dynamic evolving environments.
- **Excels in both written and verbal communication**, proficiently acquires knowledge and imparts insights with clarity.

SPOKEN LANGUAGES

- English (Proficient)
- Greek (Native)
- German (Intermediate)

AWARDS-FELLOWSHIPS

- Peer Tutoring Award UCF
- Research & Teaching Assistant Fellowship UCF Physics Dept

CONFERENCES

- American Physical Society, IL.
- American Physical Society, NV.
- STEM conference, FL.

SELECTED - PUBLICATIONS

Electronic structure of cobalt valence tautomeric molecules in different environments

Theodoros Panagiotakopoulos, Esha Mishra, Thilini K Ekanayaka, Duy Le, Talat Shahnaz Rahman, Ping Wang, Kayleigh McElveen, Jared Paul Phillips, Zaid Zaz, Saeed Yazdani, Alpha T. N'Diaye, Rebecca Y. Lai, Robert Streubel, Ruihua Cheng, Michael Shatruk and Peter A. Dowben

2022 Nanoscale link

Exploring Simulated Residential Spending Dynamics in Relation to Income Equality with the Entropy Trace of the Schelling Model

Theodoros Panagiotakopoulos,George-Rafael Domenikos , Alexander V. Mantzaris

2022 MDPI link

Direct and indirect detection of dark matter

Theodoros Panagiotakopoulos, Vasilios Spanos

2019 Pergamos library, National and Kapodistrian University of Athens link

Description of the method development for separating the Daliz from the normal π^0 in the CDF detector

Theodoros Panagiotakopoulos, Arkadios Manousakis

2017 Pergamos library, National and Kapodistrian University of Athens link