# THEODOROS PANAGIOTAKOPOULOS

Ph.D Computational Physicist ~ Quant Researcher

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## **SUMMARY**

Experienced Ph.D. in Computational Physics, adept in mathematical modeling and applying AI/ML for quantitative research, seeking a quantitative Scientist role to tackle complex challenges and drive impactful solutions. **SKILLS** 

Python, Julia, R, C/C++, SQL, Bash, HTML. Languages: 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 M.S. Computational Nuclear Physics

**National and Kapodistrian University of Athens** 

Grade: 9.2/10, Valedictorian

10/2011 - 07/2017 **B.S. Physics** 

National and Kapodistrian University of Athens

Highly focused in Computational Physics

#### **INTERNSHIPS**

# 5/2024 - 8/2024 Modeling Product Engineer Intern

ASML, San Jose, CA

- Engineered a custom Machine Learning library specifically designed for efficient analysis of rigorously simulated Finite-Difference Time-Domain (FDTD) images, enabling faster and more accurate results.
- · Led the improvement of the data automation tool, resulting in increased data processing efficiency for data science workflows.
- Employed ASML's automation tool and conducted thorough Data Analysis, resulting in the extraction of actionable insights from the results.
- · Participated and contributed significantly in discussions, offering critical suggestions to improve the Tachyon product, increasing the efficiency of computational lithography models for mask optimization.

# EXPERIENCE

7/2023 - 5/2024 DOE Funded

# **Machine Learning for Computational Chemistry**

University of Central Florida

- Conducted mathematical modeling and executed simulations, performed data cleaning, and undertook in-depth data analysis to investigate the impact of ammonium cations on the Bi-catalyzed CO2 reduction reaction. Additionally, published a peer-reviewed paper exploring CO2 reduction in small-scale systems.
- Devised a novel Machine Learning approach to predict CO<sub>2</sub> reduction to formate and CO by manipulating large artificially generated datasets, successfully extrapolating these findings to electrochemical systems. This work directly contributed to securing DOE funding.
- Developed novel numerical methods and designed algorithms to compute CO<sub>2</sub> adsorption energy, resulting in data segmentation into two distinct regions. These findings facilitated the calculation of electric forces and charges, revealing the impact of cations on CO<sub>2</sub> adsorption.

Python / C++ / SQL / Bash

GitHub

scholarship holder

## 10/2022 - 7/2023 Graph Neural Networks and Databases

University of Central Florida

- Mathematically modeled and investigated how Graph Convolutional Neural Networks can improve the accuracy of retrieving deleted data. This facilitated collaboration between the Department of Statistics
- · 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.
- Developed two custom Python libraries enhancing the ability to create models that accurately represent complex systems in material design and electrochemistry. Utilized them for predictive machine learning and optimized research group's data science library, enhancing it's speed and performance.

Julia / SQL / Bash

GitHub

NSF Funded

# 8/2019 - 10/2022 Machine Learning for Computational Physics & Algorithm Design

University of Central Florida

- · Implemented ML and introduced a second-generation neural network potential to understand the beahavior of metals on semiconductors, outpacing Density Functional Theory (DFT) in terms of speed and accuracy. This accomplishment played a pivotal role in securing NSF funding.
- · Created a fourth-generation Neural Network potential to overcome constraints in existing machine learning models, for predicting the behavior of metals on semiconductors, 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, leading to a collaboration with UC Davis.

• 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**

National and Kapodistrian University of Athens

- Applied simulation techniques and 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

## 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.

**CONFERENCES** 

## SPOKEN LANGUAGES

## AWARDS-FELLOWSHIPS -

- · English (Proficient)
- Greek (Native)
- German (Intermediate)
- Peer Tutoring Award UCF
- Research & Teaching Assistant Fellowship UCF Physics Dept
- 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

Direct and indirect detection of dark matter

🚰 Theodoros Panagiotakopoulos, Vasilios Spanos

🗎 2019 👂 Pergamos library, National and Kapodistrian University of Athens

Description of the method development for separating the Daliz from the normal  $\pi^0$  in the CDF detector

Theodoros Panagiotakopoulos, Arkadios Manousakis

2017 Pergamos library, National and Kapodistrian University of Athens

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