THEODOROS PANAGIOTAKOPOULOS

Ph.D Data Scientist ~ Computational Physicist

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in TheoPhD hackerrank

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**

Highly focused in Computational Physics

National and Kapodistrian University of Athens

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 CO₂ Reduction Reaction, treating it as a classification problem.
- · Applied Machine Learning to model CO₂ reduction to formate and CO in small-scale systems, with predictions extrapolated to large electrochemical environments.
- · Developed novel algorithms to compute CO2 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 CO₂ adsorption.

Python / C++ / SQL / Bash

GitHub

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

University of Central Florida

- scholarship holder 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

NSF Funded

1/2019 - 10/2022 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 datadriven 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 workflox/s
- · 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

· Greek (Native)

· English (Proficient)

AWARDS-FELLOWSHIPS

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

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

SELECTED - PUBLICATIONS

· German (Intermediate)

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

■ MDPI

link

Direct and indirect detection of dark matter

Theodoros Panagiotakopoulos, Vasilios Spanos

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

≅ 2022

Pergamos library, National and Kapodistrian University of Athens

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