THEODOROS PANAGIOTAKOPOULOS

Ph.D Computational Physicist ∼ Quant Researcher

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SUMMARY

Experienced **Computational Physics** with a **Ph.D.**, skilled in **mathematical modeling**, adept in applying **AI/ML**, seeking a Quantitative Scientist 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** GPA: 4/4	**University of Central Florida**
10/2017 - 07/2019	**M.S. Computational Nuclear Physics** Grade: 9.2/10, Valedictorian	**National and Kapodistrian University of Athens**
10/2011 - 07/2017	**B.S. Physics** Highly focused in Computational Physics	**National and Kapodistrian University of Athens**

INTERNSHIPS

5/2024 – present — **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**, designed simulations, performed **data cleaning**, and undertook in-depth **data analysis** to investigate the impact of ammonium cations on the Bi-catalyzed CO_2 reduction reaction. Additionally, published a peer-reviewed paper exploring CO_2 reduction in small-scale systems.
- Devised a novel **Machine Learning** approach to predict CO_2 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_2 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_2 adsorption.

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Python  /  C++  /  SQL  /  Bash                                    GitHub
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10/2022 – 7/2023
scholarship holder — **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 and Physics.
- 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.

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Julia  /  SQL  /  Bash                                             GitHub
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8/2019 – 10/2022
NSF Funded — **Machine Learning for Computational Physics & Algorithm Design** — **University of Central Florida**

- Implemented **Deep Learning** 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.**
- Developed and trained 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.

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Python  /  C++  /  SQL  /  Bash                              GitHub
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10/2017 – 7/2019   **Machine Learning for Detection of Dark Mater**   **National and Kapodistrian University of Athens**
NKUA Funded
- 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**.

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Python  /  SQL  /  Bash                                      GitHub
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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