THEODOROS PANAGIOTAKOPOULOS

Ph.D Computational Physicist ~ Researcher

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SUMMARY

Experienced **Ph.D.** Computational Physicist skilled in mathematical **modeling** and adept in applying **AI/ML**, seeking a 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 Stochastic Modeling for Material Design** — **University of Central Florida**
GPA: 4/4

10/2017 - 07/2019 **M.S. Nuclear Engineering** — **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

INDUSTRY EXPERIENCE

5/2024 – present **Modeling Product Engineer Intern** — **ASML, Silicon Valley, CA**

- Designed **EUV computational lithography** simulations for geometrical corner rounding optimization in the Tachyon software, reducing simulation run time by **20%**. This improvement was adopted in the latest Tachyon release and proposed to several customers.
- Worked with **Modeling Optics** team and developed **Rigorous M3D** simulations to optimize the **Transition Cross Coefficient (TCC)** number for both **high and low Numerical Aperture masks** in Tachyon software, achieving a **32%** reduction in simulation run time. This enhancement was incorporated into the latest Tachyon release and presented to multiple clients.
- **Architected** an advanced **API** for Tachyon, based on ASML standards, significantly enhancing performance and reliability for **FEM+** applications.
- As a member of **Modeling and Optics** team, 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 **Machine Learning for Computational Chemistry** — **University of Central Florida**
DOE Funded

- Pioneered **simulations** and **data analysis** demonstrating the superior effectiveness of non-metallic cations over metallic counterparts in the CO_2 reduction reaction. Findings published in a peer-reviewed journal.
- Developed an innovative **Machine Learning** model to predict CO_2 reduction to formate and CO using large, artificially generated datasets. Successfully extrapolated results to real electrochemical systems, directly securing **DOE** funding.
- Developed novel **numerical methods** and **algorithms** for CO_2 adsorption energy calculations, achieving higher precision in revealing cation effects

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

10/2022 – 7/2023 **Graph Neural Networks and Databases** — **University of Central Florida**
scholarship holder

- 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 collecting 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`

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

- Implemented **Deep Learning** and introduced a second-generation **neural network** potential to understand the behavior of **metals on semiconductors**, outpacing Density Functional Theory (DFT) in terms of speed and accuracy. This accomplishment played a pivotal role in securing
- **Developed** and **trained** a novel **Machine Learning Classifier** to predict **metal-semiconductor** interactions by modeling long-range charge transfer effects. The model significantly **accelerates computational efficiency**, addresses the shortcomings of previous methods, and **enhances** the **understanding of semiconductor** physics.

- Engineered state-of-the-art **numerical methods** and designed **cutting-edge algorithms** for chemical potential calculations of **metal-semiconductor junctions**, facilitating a collaboration with UC Davis.
- 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
- Taught **modeling** and applications of **Machine Learning** to simulation-generated datasets, emphasizing **feature engineering techniques**, including data cleaning and transformation, to improve the quality and relevance of the models.

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

10/2017 – 7/2019
NKUA Funded

Machine Learning for Detection of Dark Mater **National and Kapodistrian University of Athens**

- Designed simulations 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.

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