





THEODOROS
PANAGIOTAKOPOULOS


Ph.D Computational Physicist


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 TheoPhD

SUMMARY

Experienced **Ph.D.** in **Computational Physics** specializing in **Machine Learning** and Data Analysis, seeking a role to drive impactful solutions.

SKILLS

Languages: Python, Julia, R, C/C++, C#, SQL, Bash

AI Tools: Neural Networks, Decision Trees, Convolutional Neural Networks

Platforms: Linux, Git, HPC

EDUCATION

08/2019 - present

Ph.D: Physics/Material Science
GPA: 4.0/4.0

University of Central Florida

10/2017 - 07/2019

M.S.: Physics
GPA: 9.2/10, Valedictorian

National and Kapodistrian University of Athens

10/2011 - 07/2017

B.S. Physics

National and Kapodistrian University of Athens

INDUSTRY EXPERIENCE

5/2024 - 8/2024

Modeling Product Engineer Intern

ASML, Silicon Valley, CA

- Optimized optical simulations for geometrical corner rounding, achieving a **5% reduction in runtime**, **10% reduction in memory usage**, and **70% reduction in rounding time**. These enhancements were integrated into ASML's latest software release and adopted by customers.
- Led electromagnetic simulations and optimized the Transition Cross Coefficient (TCC), reducing runtime by **9%** and memory usage by **34%**. These improvements were incorporated into ASML's latest software release for a major customer.
- Developed a **Python library** along with **ETL data pipelines** for data cleaning, analysis, and pattern recognition, improving the interpretability of large-scale simulation results.
- Collaborated with **cross-functional teams** to enhance the efficiency of computational lithography models.

Python / C/C++ / Bash

EXPERIENCE

8/2019 - present

Research Assistant

University of Central Florida

DOE -NSF Funded

- Engineered **numerical methods** and **algorithms** to model metal growth on **semiconductor substrates**, accelerating fabrication processes.
- Designed and implemented a **Deep Learning Neural Network** surpassing Density Functional Theory in speed, optimizing semiconductor fabrication simulations and accelerating material discovery workflows.
- Developed a **CNN model** using voxelized atomic properties to predict metal-semiconductor deposition morphology, achieving simulation-level accuracy while enabling cost-efficient **data analysis**.
- Engineered a **Graph Convolutional Neural Network (GCNN)** for data retrieval integrating it into a simulation tool to accelerate simulations of epitaxial metal growth on semiconductors.
- Built **end-to-end ETL and ML data pipelines** for automated preprocessing, feature engineering, and model training, reducing manual data handling and boosting operational efficiency.
- Developed three custom Python libraries:** one for modeling complex systems in fabrication processes, one for electrochemistry, and one for rendering and visualizing 3D simulation data as 2D images.
- Designed **Algorithms** for voltage control in electrochemical systems and integrated them into simulation tools, enabling data generation for analysis and predictive modeling.
- Optimized **simulations, gathered, cleaned, and analyzed data**, demonstrating the superior effectiveness of non-metallic cations over metallic counterparts in the CO₂ reduction reaction.
- Developed and implemented **algorithms** to analyze CO₂ reduction data, modeled equations for energy barrier calculations, and identified a novel, naturally occurring optimal reaction mechanism.
- Optimized and debugged **Software** for Material Science applications, conducted Linux-based HPC simulations, and improved software workflows, enhancing data analysis.
- Created a centralized **SQL database** for organizing and storing large datasets, improving data accessibility and enabling faster result validation across team members.

Python / Julia / C/C++ / Bash / SQL

GitHub

10/2017 - 7/2019

Research Assistant

National and Kapodistrian University of Athens

NKUA Funded

- Designed simulations and developed a **Machine Learning** approach for identifying dark matter particles.
- Taught **modeling** and applications of **Machine Learning**, focusing on **feature engineering techniques**.

Python / C/C++ / Bash

GitHub

TECHNICAL SKILLS

- **Libraries & Frameworks:** TensorFlow, PyTorch, Scikit-Learn, XGBoost, Pandas, NumPy, SciPy, StatsModels, Spark, Hadoop.
- Strong knowledge of **data structures**, designing and implementing efficient solutions for complex data challenges.
- Proficient in High-Performance Computing (HPC), specializing in Slurm for job scheduling, resource allocation, and optimization.
- Expertise in **algorithm design** and linear programming
- Experienced in **parallel programming** and **GPU acceleration**,
- Proficient in **Git**, organizing code repositories for collaborative ML projects, with **CI/CD** experience.

MANAGEMENT SKILLS

- **Supervising and independently completing projects**, consistently meeting budget and deadline goals with high-quality execution.
- Proficient in **conceptualizing, planning, and executing** end-to-end data science initiatives to solve critical business challenges.
- Thriving in **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

Effect of Ammonium-Based Cations on CO₂ Electroreduction

 Kaige Shi, Duy Le, **Theodoros Panagiotakopoulos**, Talat S. Rahman, Xiaofeng Feng

 2025  ACS

 [link](#)

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 Dalitz from the normal π^0 in the CDF detector

 **Theodoros Panagiotakopoulos**, Arkadios Manousakis

 2017  Pergamos library, National and Kapodistrian University of Athens

 [link](#)