





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: Computational Physics
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

DOE -NSF Funded

Research Assistant

University of Central Florida

- Developed numerical methods** to model epitaxial **metal growth on semiconductors**, reducing defects and improving junction performance.
- Architected and optimized a **Deep Learning** model in **PyTorch** that outperformed Density Functional Theory in speed, accelerating semiconductor fabrication simulations and material discovery workflows.
- Implemented **CNN** models in **PyTorch** using 3D atomic voxel data to predict adsorbate morphology and surface interactions, reducing simulation costs while preserving high predictive accuracy.
- Constructed a **graph convolutional neural network (GCNN)** in **Flux.jl** for rapid data retrieval, integrated into a production-grade simulation tool to accelerate material growth predictions.
- Designed and built** end-to-end **ETL** and **ML pipelines** using **Python** and **Bash**, automating data preprocessing, feature engineering, and model training to improve iteration speed.
- Developed and maintained **three Python libraries** adopted by university engineering teams for modeling fabrication systems, simulating electrochemical processes, and visualizing 3D simulation data in 2D.
- Engineered** voltage control **algorithms** for electrochemical systems and integrated them into simulation platforms to generate high-quality data for predictive modeling.
- Optimized HPC simulations and conducted **end-to-end data analysis, gathering, cleaning, and interpreting** data, to demonstrate the superior performance of non-metallic cations over metallic ones in CO₂ reduction reactions.
- Designed **algorithms** for CO₂ reduction **analysis**, enabling rapid energy barrier estimation and identifying novel, low-energy reaction pathways.
- Debugged and optimized** software for materials science applications on Linux-based HPC systems, **accelerating data processing** and reducing time to results.
- 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

NKUA Funded

Research Assistant

National and Kapodistrian University of Athens

- 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](#)