THEODOROS PANAGIOTAKOPOULOS

Ph.D Physicist ~ Data Engineer

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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** — **University of Central Florida**
GPA: 4.0/4.0

10/2017 - 07/2019 **M.S.: Physics** — **National and Kapodistrian University of Athens**
GPA: 9.2/10, **Valedictorian**

10/2011 - 07/2017 **B.S. Physics** — **National and Kapodistrian University of Athens**

INDUSTRY EXPERIENCE

5/2025 – 8/2025 **Modeling Product Engineer Intern** — **ASML, Silicon Valley, CA**

- Built, and deployed a **multithreaded/multiprocessing Python** pipeline to automate data ingestion, metric computation, and visualization, reducing manual analysis time by 80% and accelerating **CNN** training and validation diagnostics.
- Engineered a **metric learning** solution using a Triplet Margin Loss **encoder** to generate image embeddings for visual similarity, and built a cosine-similarity framework that guided data reallocation, reducing overfitting, improving model generalization, and resulting in customer adoption.
- Built a **PyTorch-based Physics Informed Neural Network** with a SIREN architecture to solve the 2D Helmholtz equation, enforcing PDE residuals and Sommerfeld boundary conditions, achieving high simulation accuracy as a surrogate for traditional solvers.

`Python / C/C++ / Bash`

5/2024 – 8/2024 **Modeling Product Engineer Intern** — **ASML, Silicon Valley, CA**

- Accelerated simulation performance by **9%** and reduced memory usage by **34%** through grid search optimization, statistical analysis, and data preprocessing. These enhancements were integrated into ASML's latest release and adopted by major customers.
- Developed a **Python library** along with **ETL data pipelines** for data cleaning, analysis, and pattern recognition, improving the interpretability of large-scale simulation results.

`Python / C/C++ / Bash`

EXPERIENCE

8/2019 – present **Research Assistant** — **University of Central Florida**
DOE -NSF Funded

- Engineered **numerical methods** for large-scale data simulations, improving predictive accuracy and enabling data-driven engineering decisions.
- Implemented a **PyTorch-based Deep Learning** model that accelerated material discovery workflows, outperforming classical simulation methods in speed.
- Developed a predictive model using **PyTorch** and **CNNs** on 3D atomic voxel data to forecast adsorbate morphology and surface interactions, matching the performance of classical simulation methods.
- 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.
- Deployed **HPC simulations** and built **end-to-end data pipelines** for CO_2 reduction, encompassing data gathering, cleaning, and interpretation, resulting in accurate energy barrier estimation and discovery of novel low-energy 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`

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 **data integration techniques** with **SQL**, extracting, loading, and transforming data for efficient processes.
- Expertise in **algorithm design** and linear programming
- Effectively **translates complex data findings into business decisions** through clear communication and compelling **storytelling**.
- 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 CO_2 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 Daliz from the normal π^0 in the CDF detector

Theodoros Panagiotakopoulos, Arkadios Manousakis

2017 Pergamos library, National and Kapodistrian University of Athens link