THEODOROS PANAGIOTAKOPOULOS

Ph.D Physicist ~ Data Engineer

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SUMMARY

Data Scientist and **Ph.D**. Physicist building scalable **Deep Learning** models and end-to-end **data pipelines** to accelerate scientific discovery and reduce computational cost in **HPC** environments.

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**

PROFESSIONAL EXPERIENCE

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

- Engineered a **terabyte-scale CNN** analysis **pipeline**, scaling from **ThreadPoolExecutor** for I/O and **ProcessPoolExecutor** for compute to **Dask** to overcome DataFrame limits, **cutting analysis time** by **80%** and exposing critical overfitting.
- Trained a **ResNet-18 from scratch** in **PyTorch** with **metric learning (triplet loss)** to remediate uncovered **overfitting** by detecting **redundant or near-duplicate images** and rebalancing the **train/validation split**, **achieving target performance**.
- Implemented a **Physics-Informed Neural Network** to solve the 2D Helmholtz equation 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**

- **Optimized** a geometric simulation parameter, reducing **runtime 5%** and **memory usage 10%** in production software used by **ASML customers**.
- **Designed and executed** optimization experiments for a core optical parameter, cutting **runtime 10%** and **memory usage 34%** in **ASML's commercial release**.
- Developed **Python libraries** and **ETL pipelines** that were adopted by ASML's product engineering teams, which standardized large-scale simulation **data cleaning**, **preprocessing**, and **analysis**.

`Python / C/C++ / Bash`

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

- **Engineered numerical methods** to model complex system properties and predict **critical thresholds**, establishing a **high-fidelity baseline** for predictive modeling.
- **Developed a two-stage PyTorch framework** that delivered **highly accurate energy predictions** for large-scale systems beyond traditional simulations, pivotal in securing **NSF research funding**.
- **Implemented a 3D CNN in PyTorch** on **voxelized atomic data** to predict structural outcomes of deposition processes, **accelerating simulations** by producing accurate results in **seconds instead of hours**.
- **Built a Graph Neural Network pipeline** for incomplete graphs, achieving **94% accuracy** on sparse data and reducing computational overhead in material design simulations.
- Automated **data preprocessing, feature engineering, and model training** by designing end-to-end **ETL and ML pipelines** in **Python** and **Bash**, improving iteration speed.
- **Authored and maintained three Python libraries** for fabrication modeling, electrochemical simulations, and 3D-to-2D visualization, adopted by university engineering teams.
- **Devised a voltage-control algorithm** for electrochemical simulations, **reducing computational costs** while generating **high-fidelity data** for predictive modeling.
- **Established analytical workflows** for complex **HPC** simulation data, uncovering **novel reaction mechanisms** and identifying **root causes** of enhanced catalytic performance in clean energy processes.
- **Designed and deployed an end-to-end data pipeline** to evaluate CO_2 reduction catalysts, delivering **key insights** that guided experimental work and contributed to securing **DOE funding**.
- **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 multi-GB simulation datasets, improving data accessibility and accelerating validation across research teams.

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

TECHNICAL SKILLS

- **Libraries & Frameworks:** TensorFlow, PyTorch, Scikit-Learn, XGBoost, Pandas, NumPy, SciPy, StatsModels
- **Big Data & Distributed:** Spark, Hadoop
- **Databases:** SQL (ETL, data integration, optimization)
- **Algorithms & Optimization:** Data structures, algorithm design, linear programming
- **Tools & Platforms:** Git, CI/CD, Linux, HPC

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