

THEODOROS PANAGIOTAKOPOULOS

Ph.D Physicist ~ ML Engineer

SUMMARY

Ph.D. Computational Physicist & ML Engineer building scalable surrogates and distributed pipelines for HPC simulations, reducing runtime by 80% using PyTorch, Dask/Spark, and C++.

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 TheoPhD

SKILLS

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

ML/DL: PyTorch, Scikit-Learn, XGBoost, CNNs, GNNs, PINNs, ViTs, U-Nets

Data: PySpark, Dask, Pandas, NumPy, SciPy

HPC/Dev: Slurm, Kokkos, TBB, Linux, Git, CI/CD

EDUCATION

08/2019 - 12/2025 **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

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**.
- Augmented the **ResNet-18 dataset** by training a **U-Net denoising diffusion model** to generate **minority-class images**, improving **class balance** and **validation generalization**.

Python / C/C++ / Bash

5/2024 – 8/2024 **Modeling Product Engineer Intern**

ASML, Silicon Valley, CA

- Implemented a **Physics-Informed Neural Network** to solve the 2D Helmholtz equation achieving high simulation accuracy as a **surrogate** for traditional solvers.
- Optimized geometric & optical simulation parameters** in production-grade **ASML software** using sensitivity analysis and benchmarking, delivering **15% faster runtime** and **34% lower memory usage**.
- Built **Python libraries** and **PySpark ETL pipelines** adopted by ASML product engineering teams to standardize cleaning and preprocessing of **400+ GB of simulation metadata**.

Python / C/C++ / Bash

8/2019 – 12/2025 **Research Assistant**

University of Central Florida

DOE - NSF Funded

- Developed a **two stage PyTorch Neural Network surrogate** for **large scale energy prediction** and **critical threshold identification**, trained on **high fidelity baselines**, **pivotal to securing NSF funding**.
- Implemented a **3D CNN** to predict atomic deposition structures from voxelized data, reducing simulation latency from **hours to seconds** and outperforming a **self-implemented 3D Vision Transformer baseline**.
- Trained a **3D U-Net denoising diffusion model** to synthesize underrepresented voxelized deposition structures for augmentation, improving **class/condition balance** and **3D CNN generalization**.
- Orchestrated a **distributed PySpark pipeline** converting **10K+ atomic configurations** into **600K+ 3D voxel tensors**, eliminating data-ingestion bottlenecks for **3D CNN training**.
- Built a **Graph Neural Network pipeline** for incomplete graphs, achieving **94% accuracy** on sparse data and reducing computational overhead in material design simulations.
- Engineered a **high-performance C++ solver**, using hierarchical parallelism with **Kokkos** and **TBB** and compile-time unit safety with **Boost.Units**, delivering **strong scaling across CPUs and GPUs**.
- Created a centralized **SQL database** for multi-GB simulation datasets, improving data accessibility and accelerating validation across research teams.
- Authored and maintained three **Python libraries** for fabrication modeling, electrochemical simulations, and 3D-to-2D visualization, adopted by university engineering teams.
- Designed a **signal-processing pipeline** for noisy **electrochemical time-series** using **Savitzky–Golay smoothing** and **IQR rejection** to extract **features**, yielding results instrumental in **DOE funding**.
- Integrated **multi-GB HPC simulation outputs** with cleaned **electrochemistry time-series** to engineer **high-dimensional features** for **predictive modeling**, improving robustness to **noise and sparsity**.

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

GitHub

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