THEODOROS PANAGIOTAKOPOULOS

Ph.D Physicist ~ ML Engineer

TheoPhD.com
teosfp@hotmail.com
321 202 3216
theodorospanagiotakopoulos
Orlando, FL, USA
TheoPhD

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++.

SKILLS

Languages: Python, C/C++, Julia, SQL, Bash
ML/DL: PyTorch, Scikit-Learn, XGBoost, CNNs, GNNs, PINNs, ViTs
Data: PySpark, Dask, Pandas, NumPy, SciPy
HPC/Dev: Slurm, Kokkos, TBB, Linux, Git, CI/CD

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 – 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** in **PyTorch** on **voxelized atomic data** to predict **deposition structures**, accelerating simulations from **hours to seconds** and outperforming **3D Vision Transformer** baselines.
- **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.
- 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.
- 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 extract **descriptors**, enabling **structure–activity modeling** that identified **novel catalytic mechanisms**.

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

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