THEODOROS PANAGIOTAKOPOULOS

Ph.D Physicist ~ ML Engineer

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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, U-Nets, GANs, RNNs
Data: PySpark, Dask, Pandas, NumPy, SciPy
HPC/Dev: Slurm, Kokkos, TBB, Linux, Git, CI/CD

EDUCATION

08/2019 - 12/2025 **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 ML evaluation pipeline** with **Dask** and **multiprocessing**, eliminating memory bottlenecks, reducing runtime by **80%**, and exposing **silent overfitting**.
- Trained a **ResNet-18** in **PyTorch** with **hard triplet loss** to learn **structure-aware embeddings**, replacing pixel comparisons and remediating **validation overfitting**.
- **Augmented ResNet-18** training datasets using **U-Net diffusion** models, selected over **GAN** and **VAE** baselines, to synthesize **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**, creating a **rapid, differentiable surrogate** that reduced reliance on **computationally expensive wave 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**.
- Architected **distributed ETL pipelines** using **PySpark** and **Spark SQL** to standardize **400+ GB** of simulation metadata, adopted by **ASML product engineering teams** for cleaning and preprocessing.

`Python / C/C++ / Bash`

8/2019 – 12/2025 **Research Assistant** — **University of Central Florida**
DOE - NSF Funded

- Developed a **two-stage PyTorch Neural Network** to predict **atomic charges** and **system energies**, capturing **thermodynamic nucleation thresholds** and 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**.
- **Developed segmentation pipelines** for **noisy experimental images** using **Faster R-CNN** and **Mask R-CNN** to **isolate atomic islands** and **extract morphological features**, supporting **deposition modeling**.
- **Built a Graph Neural Network pipeline** for incomplete graphs, achieving **94% accuracy** on sparse data and reducing computational overhead in material design simulations.
- Designed a signal processing pipeline for noisy electrochemical time series using **LSTMs**, surpassing **GRU** and **Transformer** baselines, generating findings instrumental in securing **DOE funding**.
- **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.

`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