THEODOROS PANAGIOTAKOPOULOS

Ph.D Physicist ~ ML Engineer

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📍 Orlando, FL, USA in 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, 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 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 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**.

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Python  /  C/C++  /  Bash
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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**.
- Built **Python libraries** and **PySpark ETL pipelines** adopted by ASML product engineering teams to standardize cleaning and preprocessing of **400+ GB** of **simulation metadata**.

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Python  /  C/C++  /  Bash
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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**.
- **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.
- **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 and modeling pipeline** for **noisy electrochemical time series** using **LSTMs** to capture **nonlinear memory effects**, yielding results instrumental in securing **DOE funding**.

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