THEODOROS PANAGIOTAKOPOULOS

Ph.D Computational Physicist

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SUMMARY

Experienced **Ph.D.** in **Computational Physics** specializing in **Machine Learning** and Data Analysis, seeking a role to drive impactful solutions.

SKILLS

Languages: Python, Julia, R, C/C++, C#, SQL, Bash
AI Tools: Neural Networks, Decision Trees, Convolutional Neural Networks
Platfroms: Linux, Git, HPC

EDUCATION

08/2019 - present	**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**

INDUSTRY EXPERIENCE

5/2024 – 8/2024   **Modeling Product Engineer Intern**   **ASML, Silicon Valley, CA**

- Optimized optical simulations for geometrical corner rounding, achieving a **5% reduction in runtime**, **10% reduction in memory usage**, and **70% reduction in rounding time**. These enhancements were integrated into ASML's latest software release and adopted by customers.
- Led electromagnetic simulations and optimized the Transition Cross Coefficient (TCC), reducing runtime by **9%** and memory usage by **34%**. These improvements were incorporated into ASML's latest software release for a major customer.
- Developed a **Python library** along with **ETL data pipelines** for data cleaning, analysis, and pattern recognition, improving the interpretability of large-scale simulation results.
- Collaborated with **cross-functional teams** to enhance the efficiency of computational lithography models.

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Python  /  C/C++  /  Bash
```

EXPERIENCE

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

- Engineered numerical methods for large-scale data simulations, improving predictive accuracy and enabling data-driven engineering decisions.
- Architected and optimized a deep learning model in **PyTorch** that outperformed Density Functional Theory in speed, accelerating semiconductor fabrication simulations and material discovery workflows.
- Implemented **CNN** models in **PyTorch** using 3D atomic voxel data to predict semiconductor deposition morphology, cutting modeling costs and matching the accuracy of traditional simulations.
- Constructed a graph convolutional neural network (GCNN) in **Flux.jl** for rapid data retrieval, integrated into a production-grade simulation tool to accelerate material growth predictions.
- Designed and built end-to-end **ETL** and **ML pipelines**, automating data preprocessing, feature engineering, and model training to enhance operational efficiency.
- Developed **three custom Python libraries** adopted by university engineering teams for modeling fabrication systems, simulating electrochemical processes, and visualizing 3D simulation data in 2D.
- **Engineered** voltage control **algorithms** for electrochemical systems and integrated them into simulation platforms to generate high-quality data for predictive modeling.
- Optimized HPC simulations and conducted **end-to-end data analysis**, **gathering**, **cleaning**, and **interpreting** data, to demonstrate the superior performance of non-metallic cations over metallic ones in CO_2 reduction reactions.
- Designed **algorithms** for CO_2 reduction **analysis**, enabling rapid energy barrier estimation and identifying novel, low-energy reaction pathways.
- **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 organizing and storing large datasets, improving data accessibility and enabling faster result validation across team members.

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

10/2017 – 7/2019
NKUA Funded   **Research Assistant**   **National and Kapodistrian University of Athens**

- Designed simulations and developed a **Machine Learning** approach for identifying dark matter particles.
- Taught **modeling** and applications of **Machine Learning**, focusing on **feature engineering techniques**.

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Python  /  C/C++  /  Bash                                      GitHub
```

TECHNICAL SKILLS

- **Libraries & Frameworks:** TensorFlow, PyTorch, Scikit-Learn, XGBoost, Pandas, NumPy, SciPy, StatsModels, Spark, Hadoop.

- Strong knowledge of **data structures**, designing and implementing efficient solutions for complex data challenges.

- Proficient in High-Performance Computing (HPC), specializing in Slurm for job scheduling, resource allocation, and optimization.

- Expertise in **algorithm design** and linear programming

- Experienced in **parallel programming** and **GPU acceleration**,

- Proficient in **Git**, organizing code repositories for collaborative ML projects, with **CI/CD** experience.

MANAGEMENT SKILLS

- **Supervising and independently completing projects**, consistently meeting budget and deadline goals with high-quality execution.

- Proficient in **conceptualizing, planning, and executing** end-to-end data science initiatives to solve critical business challenges.

- Thriving in **diverse teams**, **fostering collaboration** and energizing **collective success**.

- Exceptional **communication and presentation skills**, bridging knowledge gaps and **ensuring clarity**.

- Excelled in **problem solving** and **analytical thinking** in dynamic evolving environments.

- **Excels in both written and verbal communication**, proficiently acquires knowledge and imparts insights with clarity.

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