

Nicholas Ho

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Education **Arizona State University**, Tempe, Arizona, USA August 2019-Present
Computer Science and Mathematics Graduation: May 2023
GPA: overall 4.0/4.0; CS-only 4.0/4.0; Math-only 4.0/4.0

Publications - Accepted **Nicholas Ho**, John Kevin Cava, John Vant, Ankita Shukla, Jacob Miratsky, Pavan Turaga, Ross Maciejewski, Abhishek Singharoy. *Learning Free Energy Pathways through Reinforcement Learning of Adaptive Steered Molecular Dynamics* Machine Learning In Structural Biology (MLSB) Workshop at the 36th Conference on Neural Information Processing Systems (5 Pages)

John Kevin Cava, John Vant, **Nicholas Ho**, Ankita Shukla, Pavan Turaga, Ross Maciejewski, Abhishek Singharoy. *Towards Conditional Generation of Minimal Action Potential Pathways for Molecular Dynamics* ELLIS ML4Molecules Workshop, October 2021, (5 Pages).

Wei Du, Gaoyang Li, **Nicholas Ho**, Landon Jenkins, Drew Hockaday, Jiankang Tan, Huansheng Cao *CyanoPATH: a knowledgebase of genome-scale functional repertoire for toxic cyanobacterial blooms* Briefings in Bioinformatics, Volume 22, Issue 4, July 2021, (12 Pages).

Research Experience **Harvard Medical School Department of Biomedical Informatics** with Dr.Marinka Zitnik, June 2022-Present

Accepted as a visiting research fellow at Harvard Medical through a highly competitive application process. Working with Masters Student Yepeng Huang.

- Currently developing a multimodal machine learning architecture to *learn from complex biological systems to predict side effects for drugs*. More specifically, a modal capable of training on missing modalities and making high quality predictions on a single modality.

ASU Structural Systems Biology Lab in the Biodesign Institute with Dr.Abhishek Singharoy Feb 2020 - Present

Worked as an undergraduate researcher in the Singharoy Lab. Lead research for my honors thesis to utilize deep ML methods with statistical mechanical methodologies.

- Lead the research of *sampling transition paths for rare events* by designing a novel framework which uses reinforcement learning, Jarzynski equality and steered molecular dynamics.
- Worked with two other PhD students to develop the Conditional Generative Adversarial Network to generate low-free energy pathways for rare events. I designed a novel objective function that allowed potential energy to be directly minimized.
- Deployed molecular dynamic simulations to study conformational changes on Hexokinase 1 that influence binding mechanisms with the mitochondria to combat neurodegenerative diseases.
- Rewrote and accelerated the differentiable molecular dynamics engine TorchMD for faster differentiable simulations on biomolecules. *Up to 20 times CPU speedup*.

Carnegie Mellon Statistics and Data Science with Dr. Konstantinos Pelechris, Summer 2021 Accepted as a visiting research fellow through a highly competitive application process.

- Created a novel methodology for using stochastic simulators to model soccer dynamics based on ball movement. Our method had comparable results to models trained directly on scores.

ASU Cao Lab in the Biodesign Institute with Dr. Huangsheng Cao Sept 2019 - May 2021 Worked under Professor Huangsheng Cao as a undergraduate researcher.

- Contributed heavily to *CyanoPATH* by designing databases that tracked cellular processes for 120 cyanobacteria species and set up front-end dashboards to visualize these processes. Used PFAM's Hidden Markov Model, JavaScript, SQL databases, shell and Python. Work published in Briefings in Bioinformatics.
- Conducted data engineering and analysis on genomes assembled from a metagenome in order to study the strain level variance within microbiome communities.

ASU Garcia-Pichel Lab in the Biodesign Institute with Dr. Ferran Garcia Pichel May 2020 - May 2021

Worked under professor Ferran Garcia Pichel as an undergraduate researcher.

- Developed CaVE, a Qiime2 Python plugin to get the relative volume and cell count based on predicted ribosomal counts.

Presentations	<p><i>Novel Drug Drug Interaction Side Effect Prediction</i>, Harvard Summer Institute of Biomedical Informatics (2022).</p> <p><i>An Interpretable Method of Learning Stochastic Game Dynamics</i> [Co-presented]. Carnegie Mellon Sports Analytics Conference, (2021) and Ohio State University Sports Analytics Conference (2021).</p> <p><i>Towards autoregressive generation of steered MD simulations</i> [Co-presented]. NAMD Developer Workshop at Urbana Champaign (2021).</p> <p><i>Concordia International IOT Environmental Sensors and Data Analysis</i> at the International Conference on Big Data and Education, (ICBDE 2018).</p>
Significant Course Projects	<p>APM541 Grad. Stochastic Processes and Biology with Dr. Nicolas Lanchier Fall 2021</p> <ul style="list-style-type: none"> • My final project was <i>Particle System Dynamics for Compromised Social Networks</i> where I extended and implemented the infinite graph contact process for Facebook graphs to simulate and visualize the stability of compromised accounts. Code available on github. <p>MBB495 Microbiology Research with Dr. Abhishek Singharoy Spring 2022</p> <ul style="list-style-type: none"> • Studied statistical mechanics and various tools in molecular dynamics to enhance sampling of conformational states and obtain free energy estimates. <p>PHY598 Grad. Data Driven Inference for Life Sciences with Dr. Steve Presse Spring 2021</p> <ul style="list-style-type: none"> • Bayesian data analysis for several problems in life sciences, I implemented various data inference algos from scratch such as Gaussian processes and Viterbi for Hidden Markov Models. <p>CSE485 Senior Capstone Project with Dr. Ross Maciejewski Fall 2021 -Spring 2022</p> <ul style="list-style-type: none"> • Lead project developer, developed a data visualization dashboard for CSRankings of universities.
Industry Experience	<p>iMetabolic Biopharma Corporation March 2021 - May 2021 Research Intern</p> <ul style="list-style-type: none"> • Helped consolidate a database of literature for machine learning enhanced drug design <p>Western Tool and Supply June 2019 - July 2019, June 2020 - July 2020 Summer Software Developer Intern</p> <ul style="list-style-type: none"> • Successfully integrated and programmed Bluetooth LE into the IOT interfaced storage system. <p>IOT Environmental Sensors for Concordia Intl' School Shanghai Jan 2018 - May 2019</p> <ul style="list-style-type: none"> • Built, programmed, and deployed 30 microcontroller sensors that streamed air quality data.
Awards	<p>2022 Wojcik Family Research Fellowship – \$4,500</p> <p>2022 ON Semiconductor Engineering Scholarship – \$2,338</p> <p>2022 Barrett Honors Thesis Funding – \$2,000</p> <p>2019-2023 President's Award - New American University – \$7,750 each semester</p>
Community Involvement	<p>Mathematical Organization for Rehumanizing Education (MORE), <i>Member</i> 2022-Now</p> <p>Machine Learning Club, <i>Eboard Member, Technical Advisor</i> 2022-Now</p> <p>Arizona State University Fulton Student Council <i>Student Volunteer</i> August 2019 - 2020</p>
Skills / Experience	<p>Proficient with Python, C/C++, MatLab, Bash, R, JavaScript, PHP, SQL, Perl, PyTorch, TensorFlow, JAX, Pandas, Numpy.</p> <p>Other Skills Violin, Cooking, Yo-Yoing (very good)[video link]</p>
References	<p>Dr. Marinka Zitnik Assistant Professor at Harvard Department of Biomedical Informatics, Email: Marinka@hms.harvard.edu</p> <p>Dr. Abba Gumel Endowed E-Nnovate Chair in Mathematics in University of Maryland, Email: agumel@umd.edu</p> <p>Dr. Abhishek Singharoy Assistant Professor at ASU School of Molecular Sciences Email: asinghar@asu.edu</p> <p>Dr. Ross Maciejewski Professor at ASU in the School of Computing and Augmented Intelligence, Email: rmacieje@asu.edu</p>