# Nicholas Ho

https://nickdst.github.io/ nichola2 [at] asu.edu +1 971-998-8162

## 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 May 2020 - Present
Worked as a Research Associate 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 Pelechrinis, 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 Bioinformatician.

- 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 Assistant Research Bioinformatician.

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

Presentations

*Novel Drug Drug Interaction Side Effect Prediction*, Harvard Summer Institute of Biomedical Informatics (2022).

*An Interpretable Method of Learning Stochastic Game Dynamics* [Co-presented]. Carnegie Mellon Sports Analytics Conference, (2021) and Ohio State University Sports Analytics Conference (2021).

*Towards autoregressive generation of steered MD simulations* [Co-presented]. NAMD Developer Workshop at Urbana Champaign (2021).

*Concordia International IOT Environmental Sensors and Data Analysis* at the International Conference on Big Data and Education, (ICBDE 2018).

Significant Course Projects

**APM541 Grad. Stochastic Processes and Biology** with Dr. Nicolas Lanchier Fall 2021
- My final project was *Particle System Dynamics for Compromised Social Networks* 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.

**MBB495 Undergrad. Research Microbiology** with Dr. Abhishek Singharoy Spring 2022
- Studied statistical mechanics and various tools in molecular dynamics to enhance sampling of conformational states.

**PHY598 Grad. Data Driven Inference for Life Sciences** with Dr. Steve Presse Spring 2021
- For several problems in life sciences, I implemented various data inference algos from scratch such as Gaussian processes and Viterbi for Hidden Markov Models.

**CSE485 Capstone Project** with Dr. Ross Maciejewski Fall 2021 -Spring 2022
- Lead project developer, developed an improved data visualization dashboard for CSRankings of universities.

Industry Experience

**Western Tool and Supply** June 2019 - July 2019, June 2020 - July 2020
Summer Software Developer Intern
- Successfully integrated and programmed Bluetooth LE between microcontrollers and Google Chrome into their IOT interfaced storage system.

**IOT Environmental Sensors for Concordia Intl' School Shanghai** Jan 2018 - May 2019
- Built, programmed, and deployed 30 microcontroller sensors from scratch capable of streaming air quality data to model student health.

Awards

2022 Wojcik Family Research Fellowship – $4,500
2022 ON Semiconductor Engineering Scholarship – $2,338
2022 Barrett Honors Thesis Funding – $2,000
2019-2023 President's Award - New American University – $7,750 each semester

Community Involvement

Mathematical Organization for Rehumanizing Education (MORE), *Member* 2022-Now
Machine Learning Club, *Eboard Member, Technical Advisor* 2022-Now
Arizona State University Fulton Student Council *Student Volunteer* August 2019 - 2020

Skills / Experience

**Proficient with** Python, C/C++, MatLab, Bash, R, JavaScript, PHP, SQL, Perl, PyTorch, TensorFlow, JAX, Pandas, Numpy.

**Other Skills** Violin, Cooking, (very good) Yo-Yoing [**video link**]

References

**Dr. Marinka Zitnik**
Assistant Professor at Harvard Department of Biomedical Informatics, **Email:** Marinka@hms.harvard.edu

**Dr. Abba Gumel**
Endowed E-Nnovate Chair in Mathematics in University of Maryland, **Email:** agumel@umd.edu

**Dr. Abhishek Singharoy**
Assistant Professor at ASU School of Molecular Sciences **Email:** asinghar@asu.edu

**Dr. Ross Maciejewski**
Professor at ASU in the School of Computing and Augmented Intelligence, **Email:** rmacieje@asu.edu