

Yaoguang (Ray) Zhai

Ph.D. Candidate

Computer Science and Engineering
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Research Interests

- Sample driven and Monte-Carlo based **search** and **optimization** algorithms on **nonlinear and black-box optimization**
- Modeling and optimization applications for large and complex systems encompassing **molecular dynamics simulations, SMT solvers, and chip designs**.
- High-performance computing** simulations on supercomputer clusters and cloud.

Education

2018 - Present **Ph.D. in Computer Science and Engineering**
University of California, San Diego

2016 - 2018 **Master in Computational Science and Engineering**
University of California, San Diego

2006 - 2008 **Master in Sustainable Energy Engineering**
Royal Institute of Technology
Stockholm, Sweden

SKILL

C++	Python	AWS
Linux	OPENMP	CUDA
Matlab	SQL	FORTRAN

Experience

Jun. 2022 – Sep. 2022, Jun.2023 – Present **Amazon**, Applied Scientist

- Utilizing **C++** on **AWS** for development and adhered to **high-level industrial coding standards**, ensuring robust and maintainable code through stringent review.
- Engineering the **optimization** for the nonlinear automated reasoning solver, significantly enhancing its problem-solving capabilities and efficiency.

Sep. 2018 – Present **University of California, San Diego**, Researcher

- Researching and developing sample-driven and Monte-Carlo based search and optimization algorithms for **nonlinear and black-box** problems.
- Applying cutting-edge optimization algorithms to various complex systems spanning areas such as **molecular dynamics modeling, SMT solving, and chip design**.
- Enhancing processing efficiency for real-world computational problems by leveraging expertise in **Python, C++, and Bash** in **high-performance computing** environment.

Jun. 2020 – Sep. 2020 **Lawrence Livermore National Laboratory**, Data Scientist

- Directed **Gaussian process models for protein design**, facilitating improved interpretation of complex biological data.
- Integrated **active learning** algorithms to boost model performance and accelerating the design process.

Jun. 2019 – Sep. 2019 **Interpreta**, Data Scientist

- Leveraged **Python and SQL** to dissect and analyze complex data sets related to public healthcare, deriving valuable insights for strategic decision-making.
- Conducted a **time series classification model** to identify and adjust customer risk based on healthcare information, significantly enhancing predictive accuracy and risk management strategies.

Jun. 2017 – Jun. 2019 **San Diego Supercomputer Center**, Researcher

- Trained a sophisticated Deep Neural Network (DNN) model for the complex system using **Tensorflow** and **Pytorch**, significantly enhancing the accuracy of estimations.
- Implemented parallel computing capabilities via **OpenMP and CUDA/CUDNN**, resulting in significantly improved computational efficiency.
- Improved the performance of complex scientific **FORTRAN** code through optimization.

Jun. 2018 – Sep. 2018 **Veritone Inc.**, Data Scientist

- Led enhancements to single-channel audio speaker recognition accuracy with **Python**.
- Established processes and tools for benchmarking audio/media transcriptions.

Dec. 2008 – Sep. 2016 **Siemens, Sweden**, Mechanical Engineer

- Developed **Matlab** scripts for autonomous and parametric exploration, enhancing process efficiency and accuracy.

Publications

Zhai, Y., Qin, Z., Gao, S., Sample-and-Bound for Non-Convex Optimization, under submission 2023

Zhai, Y., Caruso, A., Bore, S.L. et al., A "short blanket" dilemma for a state-of-the-art neural network potential for water: Reproducing experimental properties or the physics of the underlying many-body interactions? *Journal of Chemical Physics* 2023

Zhai, Y., Gao, S., Monte Carlo Tree Descent for Black-Box Optimization, *Advances in Neural Information Processing Systems*, 2022

Zhai, Y., Caruso, A., Gao, S. et al. Active learning of many-body configuration space: Application to the Cs water MB-nrg potential energy function as a case study, *Journal of Chemical Physics*, 2019

Zhai, Y., Goetz, A., Parallel Implementation of Machine Learning Based Many-Body Potentials on CPU and GPU, *ACM/IEEE Supercomputing Conference*, 2018

Zhai, Y., Bladh, R., Dyverfeldt, G. et al. Mistuned aeroelastic stability assessment of an industrial compressor blade, *Journal of Turbomachinery*, 2012