Yaoguang (Ray) Zhai

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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, USA

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

2002 - 2006 **Bachelor in Engineering Mechanics**
Zhejiang University, China

SKILL

C++	Python	AWS
Linux	OPENMP	CUDA
Matlab	SQL	FORTRAN

Experience

Jun. 2022 – Sep. 2022, Jun.2023 – Dec.2023 **Amazon**, Applied Scientist Intern
- Engineered **optimization** modulo for the nonlinear automated reasoning solver in **C++**, enhancing its efficiency by 80 times.
- Designed and implemented a proof system to ensure soundness; developed the proof checker using **Rust** and deployed it on **AWS**.

Sep. 2018 – Present **University of California, San Diego**, Graduate Researcher
- Researching and developing **machine learning** model with **MCTS** (Monte-Carlo Tree Search) optimization algorithms for nonlinear and black-box problems.
- 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 Intern
- 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 Intern
- Leveraged **Python and SQL** to dissect and analyze complex data sets related to public healthcare, deriving valuable insights for strategic decision-making.
- Established 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**, Graduate 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 Intern
- 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**, Research and Development Engineer
- Developed **Matlab**, **Python** and **FORTRAN** codes for autonomous and parametric exploration, deployed into production phase to improve process efficiency and accuracy.

Publications

Zhai, Y., Qin, Z., Gao, S., Sample-and-Bound for Non-Convex Optimization, *AAAI (AAAI Conference on Artificial Intelligence)* 2024

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, *NeurIPS (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