Yifan Shen

Homepage: yifanshensz.github.io

Employment

Apple Inc., Seattle, Washington
· Deep Learning Software Engineer   January 2023 –
Meta Platforms Inc., New York, New York
· Software Engineer Machine Learning Intern   May 2022 – August 2022

Education

Johns Hopkins University, Baltimore, Maryland
· Ph. D. in Quantum Chemistry   August 2018 – December 2022
· M. A. in Quantum Chemistry   August 2018 – August 2022
Zhejiang University, Hangzhou, Zhejiang, China
· B. S. in Chemistry, minor in Physics, Qiushi honors program   September 2014 – July 2018

Skills

Machine learning, parallel supercomputing, quantum modeling
· Machine learning framework: PyTorch, TensorFlow, JAX, Core ML
· Programming language: C++, Python, Fortran, Bash
· Parallel programming language: OpenMP, MPI
· Supercomputing library: Math Kernel Library, LAPACK, BLAS

Awards

· National Science Foundation, CHE-1663692
· National Science Foundation, CHE-1954723
· National Science Foundation, CBET-1603851
· National Natural Science Foundation of China, 21703202

Peer Reviews

· Journal of Chemical Information and Modeling, 2 times
· Molecular Physics, 4 times
· International Journal of Quantum Chemistry, 1 time

Publications

6. **Y. Shen**, D. R. Yarkony. Unified Description of the Jahn–Teller Effect in Molecules with Only C_s Symmetry: Cyclohexoxy in Its Full 48-Dimensional Internal Coordinates. Journal of Physical Chemistry A, 2022

5. **Y. Shen**, D. R. Yarkony. Compact Bases for Vibronic Coupling in Spectral Simulations: The Photoelectron Spectrum of Cyclopentoxide in the Full 39 Internal Modes. Journal of Physical

<u>Chemistry Letters</u>, 2020

4. **Y. Shen**, D. R. Yarkony. Construction of Quasi-diabatic Hamiltonians That Accurately Represent *ab Initio* Determined Adiabatic Electronic States Coupled by Conical Intersections for Systems on the Order of 15 Atoms: Application to Cyclopentoxide Photoelectron Detachment in the Full 39 Degrees of Freedom. <u>Journal of Physical Chemistry A</u>, 2020

3. **Y. Shen**, L. Wang. Semiclassical Moyal dynamics. <u>Journal of Chemical Physics</u>, 2018

2. K. Shi, **Y. Shen**, E. E. Santiso, K. E. Gubbins. Microscopic Pressure Tensor in Cylindrical Geometry: Pressure of Water in a Carbon Nanotube. <u>Journal of Chemical Theory and Computation</u>, 2020

1. K. Shi, K. Gu, **Y. Shen**, D. Srivastava, E. E. Santiso, K. E. Gubbins. High-density Equation of State for a 2-Dimensional Lennard-Jones Solid. <u>Journal of Chemical Physics</u>, 2018

Projects

Nested Tensors
· A new PyTorch feature to batch heterogeneous-length data, important for sequential models
· Define nested tensor as an implicit batch of variable-length data tensors
· Define nested tensor operation as batched operation on underlying data tensors
· Define nested tensor memory layout as contiguous buffer with offsets, sizes, and strides
· Expand operation support to enable multi-head attention inference and training
· PyTorch nested tensor tutorial <u>https://pytorch.org/tutorials/prototype/nestedtensor</u>

A Machine-Learning Model for Quantum Chemistry
· Previously, quantum simulation has to trade accuracy for efficiency
· Machine learning provides the potential to carry out fast and accurate quantum simulation
· Design a special neural network architecture to go beyond Born-Oppenheimer approximation
· Define a general and flexible loss function to guide machine to learn
· Apply regularization to deal with overfitting: no unphysical prediction out of training set
· Use OpenMP (multi-threaded parallel programming) to boost training performance
· Open-source code <u>fortran-library</u>: mathematical & chemical routines with c++ & python API
· Open-source code <u>foptim</u>: fortran nonlinear optimization library with c++ API

A Machine-Learning Pipeline from Training Models to Predicting Spectra on Supercomputers
· Use parallel supercomputing to obtain the training set for machine to learn
· Implement an efficient Lanczos solver to diagonalize the large-scale sparse Hamiltonian matrix
· Apply binary search / hash map to efficiently construct matrix elements
· Use OpenMP (multi-threaded parallel programming) to boost solver performance
· Open-source code <u>torch-chemistry</u>: chemistry kernel library based on PyTorch
· Open-source code <u>cpp-library</u>: argument parser & basic templates & operator overloads etc.
· Open-source code <u>vibronics</u>: vibronic spectrum simulation package

Simulate High-Pressure Effects in Nano Materials
· The pressure can go as high as 5,000 standard atmospheres in nano materials
· However, previously there was no theory to compute the pressure for the mesoscopic world
· Modify the Irving-Kirkwood theory to compute the micro-dimension pressure tensor element

· Modify the Harasima theory to compute the macro-dimension pressure tensor element
· Combine the micro and the macro elements to produce the whole mesoscopic pressure
· Open-source code <u>mc</u>: Monte Carlo simulation package for canonical ensembles

Semiclassical Moyal Dynamics
· Quantum dynamics is accurate but slow; classical dynamics is fast but inaccurate
· Semiclassical dynamics provides a way to control the balance between accuracy and efficiency
· Rewrite the Heisenberg equations of motion with the quantum phase-space formulation
· Moyal bracket gives the hierarchical equations connecting low- and high-order expectations
· Construct phase-space distribution from low-order expectations by machine learning
· Estimate high-order expectations from the machine-learning phase-space distribution
· Open-source code <u>onedimdvr</u>: numerically solve the time-dependent Schrödinger equation
· Open-source code <u>mcsmd</u>: multi-centred semiclassical Moyal dynamics