Yifan Shen

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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 – August 2023
· 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 Review

· Journal of Chemical Information and Modeling Manuscript ci-2021-002773
· Journal of Chemical Information and Modeling Manuscript ci-2021-00563d
· Current Chinese Science Manuscript BMS-CCS-2022-32

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

Chemistry Letters, 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. Journal of Physical Chemistry A, 2020

3. **Y. Shen**, L. Wang. Semiclassical Moyal dynamics. Journal of Chemical Physics, 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. Journal of Chemical Theory and Computation, 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. Journal of Chemical Physics, 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 https://pytorch.org/tutorials/prototype/nestedtensor

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 fortran-library: mathematical & chemical routines with c++ & python API
· Open-source code foptim: 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 torch-chemistry: chemistry kernel library based on PyTorch
· Open-source code cpp-library: argument parser & basic templates & operator overloads etc.
· Open-source code vibronics: 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 mc: 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 onedimdvr: numerically solve the time-dependent Schrödinger equation
· Open-source code mcsmd: multi-centred semiclassical Moyal dynamics