Dong Zhou

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Summary

Physicist and programmer, passionate about method development and innovation. 30+ papers with 2k+ citations, Erdös number ≤ 5 , 1k+ stars on GitHub. Past experience includes crystal structure prediction, medical imaging, quantum computing, and spectro-microscopy.

SKILLS

Python, Go, C, Bash, AWS/GCloud Computational physics/mathematics, Image processing, Machine learning

EXPERIENCE

• Senior Developer I then II, Schrödinger Inc.

2016-2024

Invented a divide-and-conquer algorithm for molecular crystal structure prediction. Implemented prototype for products (crystal packing search as optimization with Python; speedup with Cython, analytical gradients for geometric operations, and two-stage convergence; workflow automation with GNU Make). Maintained atom mapping module (subgraph isomorphism) for free energy perturbation (FEP). Implemented atom mapping schemes for lambda dynamics, fragment linking, and linker enumeration FEP (Python). Implemented analysis library for molecular dynamics trajectories (Python, C⁺⁺). Maintained scientific computing web services for FEP+ (aws/gcloud, Go, Python, PostgreSQL, gRPC, Docker, Polymer.js).

- Postdoc in radiology, Weill Medical College of Cornell University 2012–2016 Invented a novel method (LBV) for background magnetic field removal using full multigrid solver. Solved ill-posed inverse problems using Bayesian inference such as magnetic susceptibility and susceptibility tensor imaging, magnetic quadrupole imaging, 3D phase unwrapping (Matlab, C/C++). Developed probes for transcranial magnetic stimulation both in simulation (COMSOL multiphysics) and on hardware (electronics, 3D printing).
- Postdoc in physics, Yale University 2011–2012

 Developed state preparation scheme using quantum bath engineering, and adiabatic phase based two-qubit CNOT gate scheme on circuit QED hardware (3D transmon). Simulated these schemes using Python package QuTip.
- Research assistant, University of Wisconsin-Madison 2007–2011 Solved open quantum systems dynamics in the presence of classical stochastic noises both analytically and numerically (Matlab). Developed schemes for quantum gate, quantum control, and entanglement preparation for quantum dot systems. Developed algorithm for graph isomorphism problem using continuous-time quantum random walk. Performed experiments and data analyses for biological and geological samples such as nacre, pyrite, etc (machining, X-ray diffraction, X-ray absorption near edge spectroscopy and microscopy using synchrotron radiation @ SRC and LLNL). Implemented GUI program for spectra analysis (KaleidaGraph).

EDUCATION

| • Ph.D in physics, University of Wisconsin-Madison (GPA 4.0, 71 credits) | 2006 – 2011 |
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| • Graduate study in physics, University of Georgia-Athens (GPA 4.0, 49 credits) | 2004-2006 |

• B.S. from Honored Mixed Class, Zhejiang University (GPA 3.8, 196 credits) 2000–2004