Chaowen Guo

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https://github.com/chaowenGUO

(806) 789-5718

Education

Texas Tech University

2010-Present

Ph.D.: Theoretical and Computational Chemistry, GPA 4.00/4.00 (many A+ grades)

Dissertation: Quantum Reactive Scattering Quantities in Molecular Physics: New computational approaches based on quantum trajectories

Advisor: Bill Poirier

University of Science and Technology of China

2005-2009

B.Sc.: Biochemistry and Molecular Biology

Thesis: The NMR Relexation Study of PDZ Domain of GOPC Protein Complexed with Frizzled-8 and Production of V-set of Nectin-2 Protein

Advisor: Shi Yunyu

Research Experience

Research Assistant (Texas Tech University, Dr. L. William Poirier)

2010-Present

- Developed quantum hydrodynamic trajectory simulation algorithms, with similar computational cost as a classical algorithm, to calculate chemical reactive scattering quantities.
- Implemented novel microcanonical statistical simulation called "phase space approximation", to incorporate quantum structural effects into the quantum simulations described above.
- Programmed hybrid MPI-multithread code, and operated supercomputer clusters, to analyze performance of the above technique vs. the traditional exact quantum dynamics approach (discrete variable representation).
- Analyzed 2D and 3D data visualization to validate the accuracy of the novel approach.

Teaching Experience (Texas Tech University)

- Quantum Chemistry (graduate course CHEM 5343) with Dr. Jorge A. Morales
  Led discussion sections and graded homework.

  Spring 2015

- Experimental Principles of Chemistry II (CHEM 1107)

  Summer 2015

- Experimental Principles of Chemistry I (CHEM 1108)

  Summer 2015
  Fall 2013

Presentations

- *Quantum and Classical Trajectory Simulations with Phase Space Approximation Sampling*, Quantum Trajectories: Foundations and future, Oral Presentation, Telluride Science Research Center, Telluride, CO, July 15-19, 2013.
- *Quantum and Classical Trajectory Simulations with PSA Sampling*, Research Exam Seminar, Department of Chemistry, Texas Tech University, August, 2012.
- *ATP synthase, a rotary molecular motor*, Literature Seminar, Department of Chemistry, Texas Tech University, April, 2012.

Conferences

Quantum Trajectories: Foundations and future, Telluride Science Research Center, Telluride, CO, July 15-19, 2013

Awards and Honors

- Open Science Grid School Travel Fellowship, University of Wisconsin, Madison, 2014
- Provost Fellowship, Texas Tech University, 2010
- Nominated for Chateaubriand Fellowship

Skills

Computer Techniques

- **Programming Language:** Java14, C++17/C, Python3(jupyter), javascript(es6), Fortran, Cuda(gpgpu), HTML, CSS
- **Operating System:** Unix/Linux, Windows

- **Library:** MPI(Message Passing Interface with Multithread), Boost, MKL(Intel Math Kernel Library), BLAS, LAPACK, SCALAPACK, DAAL(Intel Data Analytics Acceleration Library), sklearn
- **Database:** Postgresql, pandas
- **Data Visualization:** matplotlib

Numerical Analysis and Simulation

- Proficient in developing numerical solutions to systems of ordinary differential equations and partial differential equations
- Ability to solve problems involving large matrices, both dense and sparse, including both linear solves and eigenproblems, especially those requiring multi-node supercomputer clusters

Language

English; Mandarin Chinese; Cantonese

References

- Bill Poirier, PhD
- Professor and Graduate Advisor
- Department of Chemistry and Biochemistry
- Texas Tech University
- 1204 Boston Avenue, Lubbock, TX 79409-1061
- Phone: 806-834-3099
- Email: bill.poirier@ttu.edu

- Jorge Morales, PhD
- Associate Professor
- Department of Chemistry and Biochemistry
- Texas Tech University
- 1204 Boston Avenue, Lubbock, TX 79409-1061
- Phone: 806-834-3094
- Email: jorge.morales@ttu.edu

- Thomas Gibson, PhD
- Associate Professor
- Department of Physics and Astronomy
- Texas Tech University
- Box 41051, Lubbock, TX 79409-1051
- Phone: 806-834-1561
- Email: Thomas.Gibson@ttu.edu
- member of my dissertation committee