

# 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 Relaxation 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

Performed all lectures, office hours, homework grading, exams proctoring and laboratory supervision in CHEM 1107 and 1108.

## 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

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### Jorge Morales, PhD

Associate Professor

Department of Chemistry and Biochemistry

Texas Tech University

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Email: jorge.morales@ttu.edu

### Thomas Gibson, PhD

Associate Professor

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member of my dissertation committee