Fall 2022

CHEM 567/PHYS 581/ECE 595

Advanced Topics: Quantum Computing for Quantum Chemistry

Tues./Thurs. 5:00-6:15 PM, PAÍS 1160

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"... because nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy..."

— Richard P. Feynman, Nobel Laureate in Physics, "Simulating Physics on Computers" (1982)

This 3-credit seminar course is for students and researchers interested in exploring methods for performing quantum chemistry calculations on emerging quantum computing platforms. Quantum chemistry is widely regarded as a potential "killer app" for demonstrating the practical utility of quantum computers, with applications to drug discovery, energy technologies, and novel materials design. The key question we will explore is: can the dense encoding of quantum chemical problems enabled by quantum computing architectures overcome the exponential scaling bottlenecks of quantum chemistry on traditional (classical) computers? This will be a highly interdisciplinary course at the nexus of computing, physics, chemistry, engineering, and mathematics. For this reason, the course is designed to be self-contained: no prior knowledge of quantum computing, quantum chemistry, or scientific programming is required.

The first part of the course will cover the theory and practice of quantum mechanics and electronic structure as implemented on contemporary parallel supercomputers, including Hartree-Fock theory and state-of-the-art methods for treating electron correlation (configuration interaction, perturbation theory, coupled cluster theory, and density functional theory). The second part of the course will introduce the circuit model of quantum computing, and concepts of entanglement, computational complexity, scaling, and quantum advantage. Methods for mapping quantum chemical problems onto quantum computers, including orbital to qubit mappings, quantum gates for encoding quantum chemical energy operators, first vs. second quantization, and the variational quantum eqigensolver will be discussed. Computational labs over the course of the semester will provide practical experience with concepts covered in the lectures. In the final part of the course, students will present and lead a class discussion on a related paper from the contemporary literature; together with class participation, this will contribute to the majority of the course grade. The philosophy of the course will be one of collaborative exploration of theoretical and computational challenges in this exciting new field.

Prerequisites: There are no formal prerequisites or textbooks for the course. Lecture notes and references will be provided. Knowledge of elementary calculus and familiarity with basic matrix algebra is required, although a brief mathematical review will be provided at the start of the course. Some background in quantum mechanics at the level of undergraduate physical chemistry, and experience with a high-level programming language (C, C++, Fortran 90; Matlab, Python) is helpful but not required. Please email the instructor with any questions about the course or suggested background. *Recommended references:* CJ Cramer, *Essentials of Computational Chemistry*; MA Nielsen and IL Chuang, *Quantum Computation and Quantum Information.*