ECE 792-066 / CSC 791-025
Quantum Algorithms for Physical Sciences

Instructor: Yuan Liu (q_yuanliu@ncsu.edu)

Time and Location: Monday and Wednesday 3-4:15 pm, 1229 EB2

Course is hosted on Moodle. Recorded course lectures can be accessed on Panopto.

Office hours: Wednesdays, 4:15-5:15 pm, 2064 EB2, also available on Zoom

Objective or Description: This course will introduce advanced topics of modern quantum algorithms and their applications in physical sciences including quantum chemistry, many-body physics, and classical mechanics. The goal is to help students develop intuition and skills to design new quantum algorithms for novel applications in the future. Both near-term and fault-tolerant quantum algorithms will be discussed although the course will focus more on fault-tolerant algorithms with provable speedups. A brief discussion on quantum algorithms based on continuous-variable systems (such as bosonic modes instead of qubits) will be presented toward the end of the course. As a special topic course, contents of the course will be drawn from recent literature. By the end of the course, students will develop a broad picture of the landscape of quantum algorithms research and how they can be used to solve important problems in physical sciences. Student will also learn how to quantify and analyze quantum algorithm complexity. Light hands-on numerical programming exercises will be given to ensure best understanding of the course materials.

Prerequisites: Linear algebra and general background in quantum mechanics is required. Introductory courses on quantum computing (for example CSC 591-001/ECE 592-081, ECE 592-100), but not required.

Textbook and references: Course materials will be compiled from different sources including recent literature. Written lecture notes will be uploaded to Moodle after each lecture.

Useful textbooks:

- For a textbook on quantum information science, see *Quantum Computation and Quantum Information* by Nielsen and Chuang. Another source on the topic is *Classical and Quantum Computation* by Kitaev, Shen, and Vyalyi.
- For an introduction to quantum chemistry, see *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory* by Szabo and Ostlund.
- For an introduction to quantum mechanics, see *Introduction to Quantum Mechanics* by Griffiths and Schroeter.
- For an introduction to many-body physics, see *Introduction to Many-Body Physics* by Coleman.

Useful lecture notes:

- Lecture notes on "*Quantum Algorithms for Scientific Computation*" by Lin (UC Berkeley).

Topics:

- Introduction (week 1 and 2)
  - Overview of quantum mechanics and computation (week 1, 1/8)
    - Basics of quantum mechanics and quantum algorithms
    - Assessment of quantum algorithm performance: qubit count, gate depth, sampling complexity
    - Heuristics and provable speedups
  - Overview of Physical Sciences Simulation (week 1-2, 1/10, 1/17)

    - Static versus dynamics problems: state prep., Hamiltonian simulation, classical differential equations
    - Quantum chemistry: electronic structure, fermion to qubit mapping
    - Many-body physics: Heisenberg spin model, Hubbard model
    - Classical PDEs: heat transport/convection, fluid dynamics

- Heuristic Quantum Algorithms (week 3-4)
  - Variational algorithms (week 3, 1/22, 1/24)
  - QAOA and Quantum Machine Learning (week 4, 1/29, 1/31)

- Quantum Algorithms with Provable Speedups (Week 5-8)
  - Grover's algorithms and amplitude amplification (week 5, 2/5, 2/7)
  - Quantum Phase Estimation (week 6, 2/12)
  - Solving linear system of equations (week 6, 2/14)
  - Quantum Signal Processing (QSP) and Quantum Singular Value Transform (QSVT) (week 7, 2/19, 2/21)
  - Trotter and Product Formula (week 8, 2/26)
  - Linear Combination of Unitaries (week 8, 2/28)

- Week 9: no lecture on 3/4, midterm on 3/6, final project proposal due 3/8
- Week 10, 3/11-15, spring break, no classes

- Applications to physical sciences (Week 11-12)
  - State Preparation: ground states, excited states, thermal states (week 11, 3/18, 3/20)
  - Hamiltonian simulation (week 12, 3/25, 3/27)
  - Solving Partial Differential Equations: heat transport equation, fluid dynamics, biology (optional)

- Hybrid discrete-continuous-variable quantum algorithms (Week 13-15)
  - Introduction to continuous-variable systems and their physical realization (week 13, 4/1)
  - Notion of universal control and universal computation on hybrid CV-DV systems (week 13, 4/3)
  - Generalization of DV quantum algorithms to CV, QSP, Trotter, LCU (week 14, 4/8, 4/10)
  - Examples and Applications of Hybrid CV-DV algorithms (week 15):
    - DV-CV state transfer (4/15)
    - Quantum Fourier transform from a continuous oracle (4/17)
    - Bosonic Hamiltonian simulation (optional)

- Final project Due and Presentations (Week 16, 4/22)

Grading: bi-weekly homework (40%), one in-class midterm (20%), take-home final project and in-class presentation (30%), attendance and participation (10%).