PHYS 513 Applications of quantum computing

Units: 4

Term—Day—Time: Two 100 minutes classes per week

Location: DMC 207

Instructor: Prof. Rosa Di Felice and Prof. Aiichiro Nakano
Office: SSC 215D (RDF), VHE 610 (AN)
Office Hours: upon appointment
Contact Info: difelice@usc.edu, anakano@usc.edu

Course Description

This class will give a one-semester graduate-level training on available quantum computing hardware and the respective functional principles, available software and algorithms. We will focus on gate-model IBM and adiabatic D-Wave devices and their applications mostly in chemistry and materials sciences. Students are welcome to deepen applications in other fields for the final project.
The students will have the opportunity to program quantum computers and run sample problems. Some classes will include hands-on tutorials, using own laptops. Information for obtaining credentials on quantum computers will be given in class.

Learning Objectives

Quantum hardware that is now available to users on the cloud include adiabatic quantum optimizers and gate-logic devices. The different principles of operation will be introduced at a practical level, for the purpose of computer programming rather than theoretical foundations/development.

After the first introductory week, the course will split in two parts, separately on gate-logic quantum computers and adiabatic quantum computers.

Gate-logic quantum computing. The existing IBM devices will be characterized, in terms of qubit types and qubit connectivity. Then we will consider one- and two-qubit gates. Existing software will be illustrated. Then we will consider classes of problems that may be solved on and take advantage from these quantum devices and we will teach the basics on quantum chemistry and quantum dynamics, at the level to prepare the students for programming these classes of problems on the existing hardware exploiting the available software, as well as future-generation hardware and software.
A section of the course will be devoted to quantum dynamics on quantum computers, taught by Prof. Nakano.

Adiabatic quantum computing. After reviewing the quantum adiabatic theorem, the D-Wave available devices will be outlined. We will describe what means programming on D-Wave and review available software. Then we will consider classes of problems that may be solved on and take advantage of adiabatic quantum optimizers. We will teach the basics on optimization problems focusing on multiple linear regression, implementation of quantum chemistry on D-Wave and mapping of graphs and networks onto quadratic unconstrained binary optimization (QUBO) forms.

Other. Different hardware and software packages: In-Quanto by Quantinuum, PennyLane by Xanadu, CUDA-Q by NVIDIA.

Eventually, the students will be able to program and run at least a couple of the above problem types on the available quantum hardware.

Recommended preparation: introductory quantum mechanics and quantum computing.

Co-requirement: EE 520 (or PHYS 558A).

Course Notes

This course will comprise lectures, homework, a midterm exam and a student research project. The course will ordinarily be taken for a letter grade. Documents, including lecture notes, homework assignments, and additional readings, will be distributed online via the course Brightspace site.

Technological Proficiency and Hardware/Software Required

Prior knowledge of python, Jupiter and notebooks is an advantage, or proficiency with these tools will have to be acquired during the course.
Student projects and tutorials will involve programming.
Familiarity with a variety of operating systems, including Linux, will greatly help.

Required Readings and Supplementary Materials

Lecture notes and research papers or other handouts, available via Brightspace.
For quantum chemistry: "Introduction to computational chemistry", by Frank Jensen (Third edition); "Molecular Electronic-Structure Theory", by Trygve Helgaker, Poul Jørgensen, Jeppe Olsen (Wiley).

Description and Assessment of Assignments

The coursework will include 6 homework assignments, a midterm assignment and a student final project. The assignments will draw on the material learned in class. Topics are specified in the weekly breakdown.

Description of Student Project

The project will be based on programming and running on a noisy intermediate-stage quantum (NISQ) computing machine. Codes available on GitHub, QISKIT or other similar platforms can be used as starting points.
It can be one of: (1) reproducing a published research paper; (2) a piece of original research; (3) a review-type project. The latter will only reach a maximum of 75% of the available final grade.

The subject of the project will be agreed on between the student and the course instructor(s); the instructor(s) will suggest suitable sources for the selected topic, and will meet with each student in the second half of the semester to give guidance on the project. The students will have access over the cloud to NISQ machines from IBM and D-Wave, and potentially other devices.
Project deliverables will include a written report and an oral presentation in class. Of the 50% it contributes to the final grade (37.5% for option 3), the report and oral presentation are worth half and half, respectively. The report is expected to be about 4-6 pages (preprint style), including figures and references (at least 1 figure, at least 5 references). The presentation is expected to be 20-30 minutes.
Typical project topics: ground-state energy estimation of small molecules on quantum devices and classical simulators with the variational quantum eigensolver and other quantum or hybrid algorithms; programming simple circuits; analyzing qubit coherence; optimization problems on materials or biological data, error correction strategies; natural language processing; quantum machine learning and neural networks.

Grading Breakdown

Course Element	% of Grade (final options 1 and 2)	% of Grade (final option 3)
Problem Sets (6)	18%	18%
Midterm Exam	32%	32%
Student Project (paper and presentation)	50%	37.5%
TOTAL	100% -- max A	87.5% -- max B+

Assignment Submission Policy

Problem sets will be submitted through Brightspace on the assigned date. Late homework will not be accepted. After the midterm exam, students will choose their project topics; the presentations will be scheduled for the last week of class, and the project reports will be due on the date of the scheduled final exam (Tuesday, May 13, 2025, 1pm).

Grading Timeline

Strong effort will be made to grade and return homework a week after it is received. Homework solutions will be posted on Brightspace.

Statement for observance of religious holidays

USC's policy grants students excused absences from class to observe religious holidays: http://orl.usc.edu/life/calendar/absences/. In this case, please contact your instructor in advance to agree on alternative course requirements.

Course Schedule: A Weekly Breakdown (approximate)

		Topics	Readings	Deliverables
Week 1	**1/13-1/17, 2025**	Fundamentals of gate-logic quantum computation and adiabatic quantum computation; differences between the two paradigms, and their equivalence.	TBA	
Week 2	**1/20-1/24, 2025**	Hardware in IBM. Principles of superconducting qubits (transmons). Topology and connectivity if IBM cloud devices. Quantum logic gates on single and multiple qubits. Circuit depth.	TBA	HW1 due (basics)
Week 3	**1/27-1/31, 2025**	Software on the IBM quantum platform: QISKIT, its modules and plugins. Evolution of QISKIT.	IBM software manuals, additional lecture notes and research/review papers	
Week 4	**2/3-2/7, 2025**	Characterization of classes of problems that may be solved advantageously using quantum logic circuits: quantum chemistry, quantum dynamics, machine learning.	Extracts from books will be distributed via Blackboard	HW2 due (use of QISKIT to program simple circuits)
Week 5	**2/10-2/14, 2025**	Quantum chemistry. The many-body problem for the electronic structure. Methods to solve the electronic structure of solids and molecules: HF, DFT, configuration interaction, active space, coupled cluster, DFMRG, benchmarks. The molecular Hamiltonian.	Textbooks, research/review papers TBA	
Week 6	**2/17-2/21, 2025**	The phase estimation algorithm for ground-state energy estimation. Hybrid solution of the electronic structure problem (ground-state energy): the variational quantum eigensolver (VQE) algorithm, imaginary time evolution (ITE) and other methods. Finding the ground-state energy of the molecular Hamiltonian in second and first quantization.	Research/review papers, IBM manuals	HW3 due (computational electronic structure problems with available classical software packages)
Week 7	**2/24-2/28, 2025**	Preparation of the initial state for VQE: new algorithmic approaches. Going beyond VQE for excited state properties of materials (electron energy spectrum, excitons, photoluminescence, etc.): active space downsizing, environment, circuit optimization, other.	Research/review papers, lecture notes, textbook	
Week 8	**3/3-3/7, 2025**	Quantum dynamics: quantum many-body dynamics on NISQ computers, quantum compiler optimization.	Lecture notes, research/review papers	
Week 9	**3/10-3/14, 2025**	Quantum dynamics: quantum-circuit simulators: Schroedinger vs. Feynman solvers.	Lecture notes, research papers	HW4 (quanum dynamics)
Spring break 3/16-3/23, 2025				
Week 10	**3/24-3/28, 2025**	**Midterm exam**: quantum chemistry and quantum dynamics.	Lecture notes, research/review papers	Choice of student project

		Constant-depth circuits for Hamiltonian dynamics: spin chains.		
Week 11	**3/31-4/4, 2025**	Beyonf IBM gate-model devices and software packages: Quantinuum, Xanadu, Google, NVIDIA CUDA-Q.	Lecture notes and research/review papers	
Week 12	**4/7-4/11, 2023**	The adiabatic theorem of quantum mechanics and its implementation on D-Wave devices. The D-Wave hardware: superconducting qubits, magnetic field coupling, Chimera and Pegasus graphs. Minor embedding.	D-Wave manuals, research/review papers	HW5 due (gate-model quantum software)
Week 13	**4/14-4/18, 2023**	Programming D-Wave: the Ising Hamiltonian. Limitations of connectivity and "gauge". Different hardware generations.	Lecture notes, book chapters TBA	
Week 14	**4/21-4/25, 2023**	Multiple linear regression on D-Wave. Quantum chemistry on D-Wave. Graphs and networks on D-Wave. Connection to materials science.	Lecture notes and research/review papers	HW6 due (D-Wave)
Week 15	**4/28-5/2, 2023**	Presentation of student projects.		Final projects: oral presentations in class.
FINAL	**5/7/2023**	Tuesday, May 13, 2025, 11am-1pm. Written report on final project.		Project reports due by 1pm on 5/13/2025

IMPORTANT DATES

- Beginning of classes – Monday, January 13, 2025
- Martin Luther King Day (University holiday) – Monday, January 20, 2025
- Last day to add classes – Friday, January 31, 2025
- Last day to drop without a "W" and receive a refund – Friday, January 31, 2025
- Last day to change to pass/no pass – Friday, January 31, 2025
- President's Day (University holiday) – Monday, February 17, 2025
- Last day to withdraw without a mark of "W" on the transcript or change pass/no pass to letter grade – Friday, February 28, 2025
- Spring recess (University holiday) – March 16-23, 2025
- Midterm exam – Tuesday March 25, 2025
- Last day to drop with a mark of "W" – Friday, April 11, 2025
- Last day of class – Friday, May 2, 2025

- Study days – May 3-6, 2025
- Final Exam – Tuesday, May 13, 2025, 11am-1pm

Statement on Academic Conduct and Support Systems

Academic Conduct:

Plagiarism – presenting someone else's ideas as your own, either verbatim or recast in your own words – is a serious academic offense with serious consequences. Please familiarize yourself with the discussion of plagiarism in SCampus in Part B, Section 11, "Behavior Violating University Standards" policy.usc.edu/scampus-part-b. Other forms of academic dishonesty are equally unacceptable. See additional information in SCampus and university policies on scientific misconduct, https://policy.usc.edu/research-and-scholarship-misconduct/.

Support Systems:

Counseling and Mental Health - (213) 740-9355 – 24/7 on call
studenthealth.usc.edu/counseling
Free and confidential mental health treatment for students, including short-term psychotherapy, group counseling, stress fitness workshops, and crisis intervention.

National Suicide Prevention Lifeline – 988 Lifeline – 24/7 on call
https://988lifeline.org

Relationship and Sexual Violence Prevention and Services (RSVP) - (213) 740-9355(WELL), press "0" after hours – 24/7 on call
https://sites.usc.edu/clientservices/
Free and confidential therapy services, workshops, and training for situations related to gender-based harm.

Office of Equity and Diversity (OED)- (213) 740-5086 | Title IX – (213) 821-8298
equity.usc.edu
Information about how to get help or help someone affected by harassment or discrimination, rights of protected classes, reporting options, and additional resources for students, faculty, staff, visitors, and applicants. The university prohibits discrimination or harassment based on the following *protected characteristics*: race, color, national origin, ancestry, religion, sex, gender, gender identity, gender expression, sexual orientation, age, physical disability, medical condition, mental disability, marital status, pregnancy, veteran status, genetic information, and any other characteristic which may be specified in applicable laws and governmental regulations. The university also prohibits sexual assault, non-consensual sexual contact, sexual misconduct, intimate partner violence, stalking, malicious dissuasion, retaliation, and violation of interim measures.

Reporting Incidents of Bias or Harassment - (213) 740-5086 or (213) 821-8298
usc-advocate.symplicity.com/care_report
Avenue to report incidents of bias, hate crimes, and microaggressions to the Office of Equity and Diversity |Title IX for appropriate investigation, supportive measures, and response.

The Office of Disability Services and Programs - (213) 740-0776
dsp.usc.edu

Support and accommodations for students with disabilities. Services include assistance in providing readers/notetakers/interpreters, special accommodations for test taking needs, assistance with architectural barriers, assistive technology, and support for individual needs.

USC Support and Advocacy - (213) 821-4710
uscsa.usc.edu
Assists students and families in resolving complex personal, financial, and academic issues adversely affecting their success as a student.

Diversity at USC - (213) 740-2101
diversity.usc.edu
Information on events, programs and training, the Provost's Diversity and Inclusion Council, Diversity Liaisons for each academic school, chronology, participation, and various resources for students.

USC Emergency - UPC: (213) 740-4321, HSC: (323) 442-1000 – 24/7 on call
dps.usc.edu
Emergency assistance and avenue to report a crime. Latest updates regarding safety, including ways in which instruction will be continued if an officially declared emergency makes travel to campus infeasible.

USC Department of Public Safety - UPC: (213) 740-6000, HSC: (323) 442-120 – 24/7 on call
dps.usc.edu
Non-emergency assistance or information.