PHYS 513 Applications of quantum computing

Units: 4

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

Location: CPA 207

Instructor: Prof. Rosa Di Felice and Prof. Aiichiro Nakano

Office: SSC 215D (RDF), VHE 610 (AN)

Office Hours: upon appointment

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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.
Moreover, 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 an operational level, for the purpose of computer programming rather than theoretical development.

After the first introductory week, the course will split in two parts, separately on gate-logic quantum computers and adiabatic quantum computers. The final week will be used either for describing other quantum computers that are expected to be released in the near future, or to deepen one of the applications.

Gate-logic quantum computing. The existing 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, quantum dynamics and machine learning, at the level to prepare the students for programming these classes of problems on the existing hardware exploiting the available software and future-generation hardware and software.
A section of the course will be devoted to quantum dynamics on quantum computers.

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.

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.

Co-requirement: EE 520.

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 Blackboard 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 Blackboard.
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 4 homework assignments and a student 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 one of: (1) a programming project on a NISQ machine; (2) a piece of original research. 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. For the NISQ programming option, and the research option (if appropriate), 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, the report is worth 25% and the presentation 25%. The report is expected to be between 2 and 5 pages (preprint style), including figures and references (at least 1 figure). The presentation is expected to be 20-30 minutes.
Typical project topics: electronic structure calculations of small molecules on quantum devices and classical simulators with the variational quantum eigensolver; programming simple circuits; analyzing qubit coherence; optimization problems on materials or biological data, error correction strategies.

Grading Breakdown

Course Element	% of Grade
Problem Sets (4)	20%
Midterm Exam	30%
Student Project (paper and presentation)	50%
TOTAL	100%

Assignment Submission Policy

Problem sets will be submitted through Blackboard 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 last day of class.

Grading Timeline

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

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	**1/9-1-13, 2023**	Fundamentals of gate-logic quantum computation and adiabatic quantum computation; differences between the two paradigms, and equivalence.	TBA	
Week 2	**1/16-1/20, 2023**	Hardware in IBM and Rigetti devices, including connectivity. Quantum logic gates on single and multiple qubits. Circuit depth.	TBA	
Week 3	**1/23-1/27, 2023**	Software on IBM and Rigetti quantum platforms: QISKIT, Forest.	IBM and Rigetti software manuals, additional lecture notes	
Week 4	**1/30-2/3, 2023**	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	HW1 due (use of QISKIT – and Forest – to program simple circuits)
Week 5	**2/6-2/10, 2023**	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.	Textbook, research papers TBA	
Week 6	**2/13-2/17, 2023**	The phase estimation algorithm. Hybrid solution of the electronic structure: the variational quantum eigensolver (VQE) algorithm in OpenFermion and QISKIT.	Research papers, IBM and Rigetti manuals	HW2 due (computational electronic structure problems with available classical software packages)
Week 7	**2/20-2/24, 2023**	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.)	Research papers, lecture notes, textbook	
Week 8	**2/27-3/3, 2023**	Quantum dynamics: quantum many-body dynamics on NISQ computers, quantum compiler optimization.	Lecture notes, research papers	
Week 9	**3/6-3/10, 2023**	Quantum dynamics: quantum-circuit simulators: Schroedinger vs. Feynman solvers.	Lecture notes, research papers	
Spring break 3/12-3/19, 2022				
Week 10	**3/20-3/24, 2023**	**Midterm exam**: quantum chemistry and quantum dynamics. The adiabatic theorem of quantum mechanics and its implementation on D-Wave devices.	Lecture notes, research papers	Choice of student project
Week 11	**3/27-3/31, 2023**	The D-Wave hardware: superconducting qubits, magnetic field coupling, Chimera and Pegasus graphs. Minor embedding.	D-Wave manuals, research papers	HW3 due (quantum dynamics)

Week 12	**4/3-4/7, 2023**	Programming D-Wave: the Ising Hamiltonian. Limitations of connectivity and "gauge". Different hardware generations.	Lecture notes, book chapters TBA	
Week 13	**4/10-4/14, 2023**	Multiple linear regression on D-Wave. Quantum chemistry on D-Wave.	Lecture notes	
Week 14	**4/17-4/21, 2023**	Graphs and networks on D-Wave. Connection to materials science.	Lecture notes	HW4 due (D-Wave)
Week 15	**4/24-4/28, 2023**	Presentation of student projects.		Projects due
FINAL	**5/9/2023**	Tuesday, May 9, 2023, 11am-1pm. Written report on final project.		Project reports due by 1pm on 5/9/2023

IMPORTANT DATES

- Beginning of classes – Monday, January 9, 2023
- Martin Luther King Day (University holiday) – Monday, January 16, 2023
- Last day to add classes – Friday, January 27, 2023
- Last day to drop without a "W" and receive a refund – Friday, January 27, 2023
- Last day to change to pass/no pass – Friday, January 27, 2023
- President's Day (University holiday) – Monday, February 20, 2023
- Last day to withdraw without a mark of "W" on the transcript or change pass/no pass to letter grade – Friday, February 24, 2023
- Spring recess (University holiday) – March 12-19, 2023
- Midterm exam – Tuesday March 21, 2023
- Last day to drop with a mark of "W" – Friday, April 7, 2023
- Last day of class – Friday, April 28, 2023
- Study days – April 29-May 2, 2023
- Final Exam – Tuesday, May 9, 2023, 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, policy.usc.edu/scientific-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 - 1 (800) 273-8255 – 24/7 on call
suicidepreventionlifeline.org
Free and confidential emotional support to people in suicidal crisis or emotional distress 24 hours a day, 7 days a week.

Relationship and Sexual Violence Prevention and Services (RSVP) - (213) 740-9355(WELL), press "0" after hours – 24/7 on call
studenthealth.usc.edu/sexual-assault
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, titleix.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.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.