University of South Carolina
NSF REU in Quantum Information Science
Research Projects

Twelve projects have been assembled to support the REU site participants. While each summer will involve only a subset of these projects to accommodate REU participants, this larger library of research topics will ensure that selected participants can be paired with projects that best match their research interests. The collaborative projects below include detailed research descriptions and the associated learning outcomes. Together, these projects exemplify the REU site theme of "Quantum Computing Workforce Development."

Contents

Project Title: Planning for Robust Quantum Compilation of SAT Problems

Project Mentors:

Biplav Srivastava — MCEC, Computer Science & Engineering
External: Minh Binh Do — NASA Ames

Project Summary: Compilation of quantum algorithms on upcoming quantum processors is an important problem with new challenges as processor architectures mature and more complex programming tasks are considered. Artificial Intelligence (AI) Planning, with its focus on sequential decision making, provides a promising avenue to tackle such compilation problems. Previous works have tackled graph coloring extensively using temporal planning [DWO+20, BDB+18]. In this project, we will consider new formulations for robust planning that model runtime uncertainty along with problem goals, including conditional and epistemic, but without requiring probability estimations. We will also consider satisfiability (SAT) problems since they are already known for their generality in expressing practical problems.

Learning Outcomes: Anticipated outcome will establish an understanding of uncertainty in the context of program compilation for SAT problems and large quantum processors where there is more scope for failure. The project will also contribute to the AI planning community by providing a challenging domain where novel integration of learning (neural) and symbolic (search) techniques may provide effective solutions. We will foster external collaborations to provide our students state-of-the-art tools and methods.

Project Title: Quantum-Inspired Probabilistic Machine Learning System
Project Mentor: Ramtin Zand, Computer Science and Engineering Department

Project Summary: Quantum machine learning (QML) has shown promise in providing a quantum advantage to several learning subroutines and models. Although there are various formulations to implement QMLs, many are being realized by variational quantum circuits (VQC). The VQCs function similarly to automatic differentiation techniques, such as what are commonly applied in neural network learning. Parametrized quantum gates are variationally updated such that the final measurement of the circuit delivers the desired result. These algorithms enable a quantum advantage for several problems including combinatorial optimization, however, the likeness to machine learning (ML) methods makes their application to such systems natural. The QMLs can achieve better performance and convergence rates than classical methods in many cases. However, a pertinent question arises: Can we achieve similar results to variational QML by incorporating stochasticity inspired by its architecture into classical ML models? If this were the case, then perhaps some of these advantages could be achieved by emerging probabilistic computers, such as intrinsically stochastic neuromorphic systems, without the need for quantum hardware. The project focuses on addressing the aforementioned research question.

Learning Outcomes: The anticipated learning outcomes of the proposed project for the student include: understanding the fundamentals of quantum machine learning algorithms; learning how to use QML libraries like PennyLane and ML frameworks such as PyTorch and TensorFlow; understanding the basics of probabilistic ML systems from both hardware and algorithm perspectives; improving soft skills such as communication, teamwork, and critical thinking.

Project Title: Ripple carry addition and quantum addition on near term quantum computer
Project Mentor: Peng Fu, Assistant Professor, Department of Computer Science and Engineering

Project Summary: This project studies how the existing methods of addition perform on a near-term quantum computer. We will implement the following three algorithms: ripple-carry addition based on Cuccaro et al. [CDKM04], quantum addition by Draper [Dra00], and measurement-assisted addition by Gidney [Gid18]. These algorithms will be implemented in a quantum programming language called Qiskit, which allows us to run programs on both a simulator and quantum computer. By comparing the error rate and run time of each method, the project will give empirical evidence of which method is more suitable for a near term quantum computer.

Learning Outcomes: Student will be able to learn about the basics of quantum computing, unitary operations and measurements. By learning about different methods of implementing addition, they will further gain knowledge on quantum circuits, programming reversible circuits and the quantum Fourier transform. By implementing these algorithms, they will not only obtain programming experience, but also experience working on a simulator and near-term quantum computer, with a good understanding of the limitations and trade-offs of different methods.

Project Title: Crystal structure prediction using quantum computing
Project Mentor: Jianjun Hu — CEC, Computer Science & Engineering

Project Summary: This project aims to apply a computational framework to speed up Crystal Structure Prediction (CSP) by transforming the search for stable atomic arrangements into an exact mathematical optimization problem compatible with quantum hardware. By discretizing the continuous potential energy surface into a periodic lattice and encoding atomic interactions—specifically electrostatic and repulsive forces—as a Quadratic Unconstrained Binary Optimization (QUBO) model, the methodology allows for the guaranteed identification of the global energy minimum using Integer Programming and quantum annealers. This approach overcomes the lack of certainty in traditional heuristic methods by identifying the optimal discrete configuration, which reliably relaxes into the correct experimental structure via a single local minimization. Ultimately, the project aims to leverage the specific capabilities of quantum annealing to bypass the combinatorial explosion inherent in complex inorganic materials, providing absolute energetic optimality guarantees and a verified ground truth for materials discovery.

Learning Outcomes: The student will gain specialized expertise in quantum-enabled optimization by learning to map the combinatorial challenges of crystal structure prediction onto quantum annealers. They will master the formulation of Quadratic Unconstrained Binary Optimization (QUBO) models, specifically learning to translate hard physical constraints—such as stoichiometry and atomic exclusivity—into energy penalty terms suitable for Ising machines. Through hands-on work with D-Wave hardware, the student will navigate the practicalities of Noisy Intermediate-Scale Quantum (NISQ) computing, developing hybrid quantum-classical workflows that leverage quantum strategies to overcome combinatorial barriers in materials discovery.

Project Title: Benchmarks for quantum circuit error-mitigation techniques
Project Mentor: Stephen Fenner — Computer Science & Engineering Dept., University of South Carolina

Project Summary: The project will devise new benchmark quantum circuits to test recent error-mitigation techniques, running them on noisy simulators as well as real quantum hardware. It will concentrate on QuTracer, a recently-proposed error mitigation technique that uses measurements on different subsets of the qubits and combines the results via Bayesian reconstruction to improve the fidelity of the circuit [LLG+24]. Besides subset tracing, QuTracer incorporates Pauli check sandwiching and various circuit optimizations. Previously used benchmarks include the inverse quantum Fourier transform, the Bernstein-Vazirani algorithm, and variational quantum eigensolvers, among others. Our new proposed benchmarks include Toffoli gate implementation with CNOT and 1-qubit gates, as well as multiqubit teleportation circuits.

Learning Outcomes: Participants will gain an in-depth knowledge of quantum circuit behavior, both ideally and with the noise limitations of current NISQ devices. They will gain hands-on experience with quantum simulators and actual quantum hardware, as well as learning the importance of quantum error mitigation and some specific techniques it involves.

Project Title: Exploring Causality in Quantum Computing Systems
Project Mentor: Pooyan Jamshidi, Computer Science & Engineering, University of South Carolina

Project Summary: This undergraduate research project aims to integrate quantum computing with information theory, causal structure learning, and counterfactual inference to advance machine learning methodologies. Causal structure learning focuses on identifying and understanding the relationships between variables, while counterfactual inference involves predicting the outcome of hypothetical scenarios. By applying principles from information theory and leveraging quantum computing capabilities, this project seeks to develop efficient and accurate algorithms for discovering causal structures and performing counterfactual analysis in complex datasets.

The project will be conducted over a nine-week summer period, involving a combination of theoretical exploration and practical implementation. Specific tasks include reviewing relevant literature, designing quantum algorithms for causal discovery and counterfactual inference, implementing these algorithms on quantum simulators, and testing them on example datasets. The primary goal is to create a functional prototype that demonstrates the advantages of quantum-enhanced methods in these areas.

Learning Outcomes: Students will gain foundational knowledge in quantum computing, information theory, causal structure learning, and counterfactual inference. They will develop and implement quantum algorithms, gaining hands-on experience with quantum simulators and potentially real quantum processors. Additionally, students will enhance their skills in data analysis, statistical methods, and algorithm development. By the end of the program, participants will be equipped with valuable interdisciplinary skills, preparing them for advanced study or careers in quantum information science and machine learning.

Project Title: Software Testing and Debugging for Quantum Computing Systems
Project Mentor: Pooyan Jamshidi, Computer Science & Engineering

Project Summary: This undergraduate research project aims to develop effective software testing and debugging techniques specifically designed for quantum systems. As quantum computing advances, the complexity and scale of quantum software increase, highlighting the need for robust testing and debugging methodologies. Traditional software testing approaches are often insufficient due to the unique characteristics of quantum computation, such as superposition, entanglement, and quantum noise.

The project will be conducted over a nine-week summer period and will involve both theoretical and practical components. Key tasks include a comprehensive review of existing quantum software testing methods, the design of novel testing and debugging algorithms, the implementation of these algorithms on quantum simulators, and validation through testing on various quantum programs. The goal is to create a suite of tools that can identify and rectify errors in quantum software, thereby improving reliability and performance.

Learning Outcomes: Students will gain a thorough understanding of quantum computing principles and the challenges associated with quantum software development. They will learn to design and implement testing and debugging algorithms tailored for quantum systems, gaining hands-on experience with quantum simulators and potentially real quantum processors. Additionally, students will enhance their skills in software engineering, algorithm development, and problem-solving within the context of quantum information science. By the end of the program, participants will be equipped with specialized knowledge and practical skills, preparing them for advanced study or careers in quantum computing and software engineering.

Project Title: Monotonicity of quantum entropies in quantum information theory
Project Mentor: Haonan Zhang — Department of Mathematics, University of South Carolina

Project Summary: The study of quantum entropies is of fundamental importance in quantum information theory. One cornerstone of quantum information is the monotonicity of quantum relative entropy under quantum channels, also known as the data processing inequality. Due to noncommutativity, the relative entropy, as well as the Rényi relative entropies, has a number of different quantum variants, and they have operational meanings in various problems. Recent years has seen great progress in studying monotonicity of these quantum entropy quantities. The proposed project focus on the study of monotonicity of α-z Rényi relative entropies under more general positive linear maps with the goal of proving the monotonicity for the largest family of positive linear maps. Our collaborative work integrates the newly-developed variational formulas for α-z Rényi relative entropies and the characterization of some operator inequalities, such as Schwarz inequality, in terms of trace inequalities.

Learning Outcomes: Anticipated outcome will establish an understanding of quantum entropies in quantum information theory. In particular, the students will learn the quantum relative entropy and its variants such as α-z Rényi relative entropies, quantum channels and their structures, the monotonicity of quantum relative entropies under quantum channels and more general positive maps. Along the way, the students will also learn how to apply the methods of complex interpolation and variational formulas in analyzing these monotonicity problems and the closely related concavity/convexity results such as Lieb's concavity theorem.

Project Title: Compiling Quantum Algorithms with Deep Reinforcement Learning and Heuristic Search

Project Mentors:

Forest Agostinelli — MCEC, Computer Science & Engineering
Stephen Fenner — MCEC, Computer Science & Engineering
Peng Fu — MCEC, Computer Science & Engineering

Project Summary: The efficient compilation of quantum algorithms from elementary quantum gates is crucial to taking quantum computing from theory to practice. However, how to compile quantum algorithms in an optimal or near-optimal manner in a reasonable amount of time is still an open problem. Furthermore, since there is still research on which gates sets should be used for compilation, including that of topological compilation, algorithms used for one gate set may not transfer over to another. We propose to develop an artificial intelligence (AI) algorithm that learns to compile quantum algorithms using a given gate set. As a result, quantum computing practitioners need only define their gate set and the algorithm to use the given gate set for compilation will be discovered by the AI algorithm. This approach will have a significant impact on both putting quantum computing algorithms into practice as well as the discovery of novel gate sets to improve the efficiency of quantum algorithms.

Learning Outcomes: The student will gain knowledge of quantum gate sets and how they can be combined to create algorithms for quantum computing. The student will get hands-on experience using the DeepCubeA system, developed by mentor Agostinelli, to train an AI agent to compile quantum algorithms. Since the DeepCubeA system is capable of solving a broader class of problems, called pathfinding problems, the student will also obtain a high-level theoretical understanding of classes of problems in AI.

Project Title: Creation of educational quantum puzzles
Project Mentor: George Androulakis, Mathematics Department, USC

Project Summary: An attractive introduction of undergraduate students into quantum information science can be done using quantum games. There are several quantum games that already exist, such as: Bas|ket⟩ball; Quantum TiqTaqToe; Quantum Chess. (See the Additional Documents section for webpages describing these games.)

We propose to create a list of puzzles for the existing quantum games. These puzzles will be used in outreach talks that the mentor will be presenting to undergraduates, as well as in a textbook that the mentor currently writes on quantum information. Usually the quantum games are played on a computer which either connects to a quantum computer or to a simulation program in order to perform quantum measurements, or in order to run a quantum circuit. We propose to create the puzzles on paper where all possibilities can be manually examined for the results of the quantum measurements. Currently there exist many (classical) chess puzzles, that include "best next move," or "mate in 2," or "mate in 3," etc. We propose to create similar puzzles for Quantum Chess.

Learning Outcomes: The students will learn basic notions of quantum information science, such as quantum measurement, entanglement, superposition, quantum gates and circuits, in a fun environment via creating quantum puzzles.

Project Title: Research in quantum information pedagogy
Project Mentor(s): George Androulakis, Mathematics Department, USC

Project Summary: The mentor is currently writing a textbook on quantum information. The creation of the textbook was initiated in Spring 2024 when the mentor was teaching the graduate class MATH/CSCE/PHYS 764 "Quantum Information." An important part of the process of writing a textbook is to test its use in real classroom environments, where the students will be reading the chapters and solving the exercises. In this project the students will be taught certain chapters of the mentioned textbook and they will be asked to work on the included homework.

Learning Outcomes: The students will learn important parts of the theory of quantum information and all the mathematical foundations that are necessary.

Project Title: Quantum protocols for position verification and related tasks
Project Mentor(s): Csilla Farkas, Stephen Fenner

Project Summary: As mobile devices proliferate, confirming an entity's position in space is crucial to secure communication in the presence of spoofers. Despite an early no-go theorem [BCF+11], quantum communication protocols now exist to verify an object's position with high accuracy under reasonable security models, at least in principle. QPV is only one of a number of related communication schemes, including summoning a quantum state at a given location, preventing forgery of quantum money, improved quantum key distribution protocols, secure distributed quantum computation, etc. These protocols all have two things in common: (1) they harness quintessentially quantum properties such as superposition and entanglement, and (2) they use absolute limits on the speed of information signaling dictated by the theory of relativity. There are many variations on any of these schemes that undergraduates can explore, such as tweaks to the security model, resources of the actors (both quantum and classical), and various restrictions on spatial configurations. We plan to investigate combinations of these and construct simulations of them.

Learning Outcomes: Students will learn how to apply principles of quantum communication channels, including quantum cryptography, teleportation, and entanglement distribution. They will also learn about the interplay between quantum information and relativity, which requires geometrical reasoning.

Project Title: The use of quantum computing in drug discovery
Project Mentor(s): Homayoun Valafar

Project Summary: Quantum computing has the potential to significantly advance intelligent drug design by enabling more accurate simulation of molecular interactions at the quantum mechanical level. Many biochemical processes such as protein–ligand binding, reaction energetics, and conformational changes are fundamentally governed by quantum phenomena that are computationally expensive to model using classical methods. Quantum algorithms, particularly for electronic structure calculations and optimization problems, may allow researchers to evaluate candidate compounds with greater precision and efficiency. When combined with artificial intelligence and machine learning, quantum computing could accelerate the identification, screening, and refinement of drug candidates, ultimately reducing development time and cost while improving predictive accuracy in molecular discovery.

References

[BCF$^+$11] Harry Buhrman, Nishanth Chandran, Serge Fehr, Ran Gelles, Vipul Goyal, Rafail Ostrovsky, and Christian Schaffner. Position-based quantum cryptography: Impossibility and constructions. In *Advances in Cryptology – CRYPTO 2011*, pages 429–446. Springer Verlag, 2011.

[BDB$^+$18] Kyle E. C. Booth, Minh Do, J. Christopher Beck, Eleanor Rieffel, Davide Venturelli, and Jeremy Frank. Comparing and integrating constraint programming and temporal planning for quantum circuit compilation, 2018, arXiv:1803.06775. https://arxiv.org/abs/1803.06775.

[CDKM04] Steven A Cuccaro, Thomas G Draper, Samuel A Kutin, and David Petrie Moulton. A new quantum ripple-carry addition circuit. *arXiv preprint quant-ph/0410184*, 2004.

[Dra00] Thomas G Draper. Addition on a quantum computer. *arXiv preprint quant-ph/0008033*, 2000.

[DWO$^+$20] Minh Do, Zhihui Wang, Bryan O'Gorman, Davide Venturelli, Eleanor Rieffel, and Jeremy Frank. Planning for compilation of a quantum algorithm for graph coloring, 2020, arXiv:2002.10917. https://arxiv.org/abs/2002.10917.

[Gid18] Craig Gidney. Halving the cost of quantum addition. *Quantum*, 2:74, 2018.

[LLG$^+$24] Peiyi Li, Ji Liu, Alvin Gonzales, Zain Hamid Saleem, Huiyang Zhou, and Paul Hovland. QuTracer: Mitigating quantum gate and measurement errors by tracing subsets of qubits, 2024, arXiv:2404.19712. https://arxiv.org/abs/2404.19712.