

Advancing Quantum-Classical Hybrid Workflows:
Algorithm Selection, Circuit Generation, and
Optimization for NISQ Processors

Yikai Mao

A thesis for the degree of Ph.D. in Engineering
Under the supervision of **Prof. Masaaki Kondo**

Graduate School of Science and Technology
Keio University

August 2025

Thesis Abstract

No. _____

Registration Number	☒ “KOU” ☐ “OTSU” No. _____ *Office use only	Name	Mao, Yikai
Thesis Title Advancing Quantum-Classical Hybrid Workflows: Algorithm Selection, Circuit Generation, and Optimization for NISQ Processors			
<u>Thesis Summary</u> Quantum computing represents a novel computing paradigm with the potential to revolutionize problem-solving in science and technology. This thesis introduces a comprehensive quantum-hybrid computing workflow encompassing three core components: algorithm selection, circuit automation, and circuit optimization. To enable effective algorithm selection, a survey of 15 realistic quantum algorithms is conducted, and they are systematically organized based on their computing theory, circuit structure, and targeted applications. This structured approach not only aids in selecting suitable algorithms but also defines the necessary circuit generation parameters, providing a strong foundation for subsequent workflow steps. For circuit automation, the Q-gen quantum circuit generator is presented as an intuitive and powerful tool for creating practical quantum circuits. Q-gen supports researchers and developers of varying expertise levels by offering tailored generation parameters for 15 quantum algorithms. Its capabilities are demonstrated through the creation of a large quantum circuit dataset, revealing extensive coverage of circuit properties such as size, depth, and gate counts. This automation framework accelerates progress in current Noisy Intermediate-Scale Quantum (NISQ) applications and provides a seamless integration pathway for future quantum computing workflows. To address circuit optimization challenges, the Q-fid system is introduced for accurately predicting the fidelity of quantum circuits executed on NISQ processors. Recognizing the sensitivity of NISQ processors to external noise, Q-fid leverages LSTM neural networks to learn the noise characteristics of qubits and quantum gate interactions without relying on explicit hardware calibration data. The system employs a novel text-based modeling method for quantum circuits and uses the d-R² metric for intuitive fidelity evaluation. Comparative analysis with mapomatic confirms Q-fid's effectiveness in characterizing qubits, gates, and circuit structures. Together, these advancements contribute significantly to the development of the quantum-classical computing workflow.			