Introduction

I think I can safely say that nobody understands quantum mechanics.

Feynman (1965)

I have been impressed by numerous instances of mathematical theories that are really about particular algorithms; these theories are typically formulated in mathematical terms that are much more cumbersome and less natural than the equivalent formulation today's computer scientists would use.

Knuth (1974)

This book is an introduction to quantum computing from the perspective of a classical programmer. All major concepts and algorithms are explained with code, based on the insight that much of the complicated-looking math typically found in quantum computing books may look quite simple in code. For many programmers, reading code is faster than reading complex mathematical derivations. Coding also allows experimentation, which helps build intuition and understanding of the fundamental mechanisms of quantum computing. I believe that this approach will make it efficient and fun to get started.

Contrary to other learning resources, we will not use available software frameworks in this book, such as the well-developed Qiskit toolkit from IBM or Google's Cirq. The goal is to learn about quantum computing without being burdened by the complexities of these frameworks. Instead, we build our own infrastructure from the ground up, based initially on Python's `numpy` library. It turns out that, to learn the fundamentals, only a few hundred lines of code are required. This initial code is slow but easy to debug and experiment with, making it an excellent learning vehicle.

We also improve this infrastructure, accelerate it with C++, and detail an elegant sparse representation. We introduce basic compiler concepts that allow for the transpilation of our circuits to platforms like Qiskit, Cirq, and others. This enables the use of these systems' advanced features, such as scale-out performance and advanced error models.

Typically, an introduction to quantum computing is preceded by a sizable reintroduction of complex linear algebra. We will not follow this pattern here. Many programmers have a solid foundation in linear algebra, but others lack the background or interest in this topic. It is my goal to produce an attractive learning resource for both groups without getting too deep into linear algebra. Hence, I only assume basic

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familiarity with complex numbers, vectors, and matrices. Some core concepts are reviewed in Chapter 1. These basics will be sufficient for most of the book.

Nevertheless, this second edition of the book goes deeper into the mathematical foundation and adds a dedicated section on more advanced topics. Although those will only be needed for a few algorithms, the book would not be complete without them. I hope that this format will be helpful to the linear algebra-challenged and not be too shallow for the cognoscenti.

The book is organized into 16 chapters plus an appendix. To get started, it is recommended to read the first three chapters on the fundamentals of quantum computing and the code base that we use throughout the book. Chapters 4 and 5 are the bridge to the remaining chapters on various classes of algorithms, which can be read in almost any order. The book closes with a discussion of quantum programming languages, compilation techniques, and other aspects of productivity in Chapter 16. Some of the later chapters may reuse insights from earlier chapters, but the references and extensive index will allow you to find any missing information.

Chapter 1 The Mathematical Minimum This brief chapter discusses the minimum mathematical background required to fully understand the derivations in this text. Basic familiarity with matrices and vectors is assumed. The chapter reviews key properties of complex numbers, the Dirac notation with inner and outer products, the Kronecker product, unitary and Hermitian matrices, eigenvalues and eigenvectors, the matrix trace, and how to construct the Hermitian adjoint of matrix-vector expressions.

Chapter 2 Quantum Computing Fundamentals This chapter introduces the fundamental concepts and rules of quantum computing. In parallel, it develops an initial, easy-to-understand Python code base for building and simulating small-scale quantum circuits and algorithms. The chapter details single qubits, superposition, quantum states with many qubits and operators, including a sizable set of important single-qubit gates and controlled gates. The Bloch sphere and the quantum circuit notation are introduced. Entanglement follows, that fascinating "spooky action at a distance," as Einstein called it. The chapter then discusses maximally entangled Bell states, the no-cloning and no-deleting theorems, local and global phases, and uncomputation. The quantum postulates are discussed briefly in preparation for the discussion on measurements.

Chapter 3 Simulation Infrastructure This chapter builds a more complete software framework, including a high-performance simulator. It discusses transpilation, a powerful compiler-based technique that allows seamless porting of circuits to other frameworks. The methodology further enables implementing of key features found in quantum programming languages, such as automatic uncomputation or conditional blocks. The chapter also introduces an elegant sparse representation.

Chapter 4 Quantum Tools and Techniques This chapter details the mathematical tools and techniques required by some of the advanced algorithms. Beginners may choose to skip this section and refer back to it as needed. The chapter discusses the spectral theorem, density matrices, the partial trace, Schmidt decomposition, state purification, and various operator decompositions.

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Chapter 5 Beyond Classical This chapter serves as a bridge from the introductory material to the sections on quantum algorithms. We start by implementing a classical circuit using quantum gates and show that quantum computers are at least as capable as classical computers. Then we discuss the term "beyond classical," which is now the preferred term to describe a computation that can be run efficiently on a quantum computer but would be intractable to run on a classical computer. For this, we discuss Google's seminal quantum supremacy paper in detail.

Chapter 6 Algorithms Exploiting Entanglement This chapter presents the first real algorithm – a quantum "Hello World" program, a simple random number generator. The chapter then details quantum teleportation, superdense coding, entanglement swapping, and the CHSH game. This game is a simplified version of the Bell inequalities, which established that classical theories assuming hidden states cannot explain quantum entanglement.

Chapter 7 State Similarity Tests This chapter discusses the terms overlap and similarity between quantum states and introduces the important swap test, as well as the Hadamard test, and the inversion test. The mathematical derivations in this chapter are still very detailed.

Chapter 8 Black-Box Algorithms The algorithms presented in this chapter were the first to establish a query complexity advantage for quantum algorithms. The list includes the Bernstein–Vazirani algorithm, Deutsch's algorithm, and Deutsch–Jozsa algorithm. Quantum oracles and their construction are introduced.

Chapter 9 State Preparation Quantum algorithms operate on inputs encoded as quantum states. Preparing these input states can be quite complicated. The chapter discusses the trivial basis and amplitude encoding schemes, as well as Hamiltonian encoding. It also discusses smaller circuits for two- and three-qubit states. Then, this chapter presents two of the most complex algorithms in this book, the general state preparation algorithms from Möttönen, and the Solovay–Kitaev algorithm for gate approximation. Beginners may decide to skip these two algorithms on a first read.

Chapter 10 Algorithms Using Amplitude Amplification This chapter discusses the fundamental Grover's algorithm, which enables searching over a domain of N elements with $\mathcal{O}\left(\sqrt{N}\right)$ complexity. Several derivative algorithms and applications are being discussed, including amplitude amplification, amplitude estimation, quantum counting, Boolean satisfiability, graph coloring, and quantum mean, median, and minimum finding.

Chapter 11 Algorithms Using Quantum Fourier Transform The quantum Fourier transform is another fundamental quantum algorithm. The chapter begins with a simple phase-kick circuit and expands to quantum phase estimation before detailing the quantum Fourier transform itself. A short section on arithmetic in the quantum domain introduces techniques that are used in a final elaborate section on Shor's famous algorithm for number factorization.

Chapter 12 Quantum Walk Algorithms A quantum walk algorithm is the quantum analog to a classical random walk with potential applications in search problems, graph problems, quantum simulation, and even machine learning. In

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this section, we describe the basic principles of this class of algorithms on a simple one-dimensional topology.

Chapter 13 Optimization Algorithms This chapter details several optimization algorithms. The variational quantum eigensolver is presented, which allows finding a minimum eigenvalue for a given Hamiltonian. This chapter also includes extensive notes on performing measurements in arbitrary bases. After a brief introduction to the quantum approximate optimization algorithm, the chapter further discusses the quantum maximum cut algorithm and the quantum subset sum algorithm in great detail.

Chapter 14 Quantum Machine Learning Quantum machine learning is an exciting field that explores the intersection of quantum computing and machine learning. It aims to leverage the principles of quantum computing to enhance machine learning algorithms and potentially revolutionize how we analyze data and solve complex problems. This chapter begins with a simple algorithm for computing the Euclidean distance between vectors. We discuss the quantum principal component analysis and, finally, detail the complex but beautiful HHL algorithm for solving systems of linear equations.

Chapter 15 Quantum Error Correction This chapter discusses quantum noise and techniques for quantum error correction, which is necessary for quantum computing. It discusses bit-flip errors, phase-flip errors, and their combinations. The formalism of quantum operations is introduced, along with the operator-sum representation and the Kraus operators. With this in mind, the chapter discusses the depolarization channel and imprecise gates, as well as (briefly) amplitude and phase damping. For error correction, repetition codes are introduced to motivate Shor's 9-qubit error correction technique.

Chapter 16 Quantum Languages, Compilers, and Tools We have introduced a compact infrastructure for exploration and experimentation, at the level of individual gates. Higher levels of abstraction are needed to scale to larger programs. The chapter discusses several quantum programming languages, including their specific tooling, such as hierarchical program representations or entanglement analysis. General challenges for compilation are discussed as well as compiler optimization techniques.

Appendix The appendix contains a detailed description of the sparse simulation infrastructure.

Notes on the 2nd Edition

This second edition is a substantial rewrite and edit of the first edition. No page has been left untouched.

- The book is now organized into 16 chapters, compared to the 8 chapters before. Much of the material from the first edition had to be compacted to make space for the new material.
- The didactic flow has been substantially improved. Several sections have been rearranged to provide a better learning experience.

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- Many graphical elements have been modified to be more clear and visually appealing. Pointers to the code are now clearly marked (with hyperlinks in the online editions).
- More attention is now given to the mathematical foundation. This is based on reader feedback. For some, even the limited math of the first edition was already too much, while for many others the math was too shallow. The additional focus on the math may not help the first group, but will make the second group much happier.

A lot of new content has been added:

- Chapter 2 adds content on the W state, the U_3 gate, and how it can be used to make other gates, a section on the No-Deleting Theorem, and a short exercise section on the practice of tensor expressions.
- Chapter 3 condenses the previous sections on various pieces of software infrastructure and acceleration into a single section.
- Chapter 4 is a new chapter on mathematical tools and techniques. It includes discussions of the spectral theorem, density matrices, the Schmidt decomposition and state purification, maximal entanglement, and several operator decompositions, such as the Pauli, *ZYZ*, and *XYX* decompositions. The previous section on the partial trace has been moved here as well.
- Chapter 6 on algorithms using entanglement adds the entanglement swapping algorithm and a discussion of the CHSH game.
- Chapter 7 is a new chapter on similarity tests and adds the Hadamard test, the inversion test, and a new multi-qubit swap test, to the previous swap test.
- Chapter 9 is a new chapter on state preparation. It discusses the basis, amplitude, and Hamiltonian encoding, adds material on effective initialization of 2-qubit and 3-qubit states, and an elaborate section on Möttönen's algorithm for general state preparation. The material on Solovay–Kitaev's algorithm has been moved here as well.
- Chapter 10 is an extended chapter on algorithms using quantum amplitude amplification. It has previous sections on Grover's algorithm, amplitude amplification, and quantum counting, and it adds new sections on amplitude estimation, Boolean satisfiability, graph coloring, quantum mean, median, and minimum finding.
- Chapter 11 on the quantum Fourier transform and Shor's algorithm is a rewrite and restructuring of prior material with more emphasis on detailed mathematical derivations. The section on arithmetic now adds multiplication in the Fourier domain.
- Chapter 14 on quantum machine learning algorithms is new and includes a discussion of the Euclidean distance, the principal component analysis, and a very detailed discussion of the HHL algorithm for solving systems of linear equations.

A significant number of problems and inaccuracies in the first edition were corrected during the writing of this second edition. It is my sincere hope that I fixed more problems from the first edition than I introduced in this second edition. Naturally, the

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inevitable remaining errors are solely my own responsibility, and I apologize for all of them.

Source Code

Much of the content of this book is explained with both math and code. However, to avoid turning this book into a giant code listing, we abbreviate less interesting or repetitive code with constructs such as `[...]`. Scaffolding code, such as Python `import` statements or #`include` directives for C++, as well as many redundant comments, are typically omitted.

To run the code, as a minimal setup, a working Python interpreter is required with the Python packages `absl`, `numpy`, and `scipy`. Without the C++ acceleration described later in the book, some of the algorithms will continue to work but run rather slowly. The complete sources are hosted under a permissive Apache license on GitHub, along with instructions on how to download, build, and run:

`www.github.com/qcc4cp/qcc`

I will maintain the errata on this site as well. Contributions, comments, and suggestions are always welcome. The code typesetting may have introduced errors, but the source of truth is the working code in the online repository. The code may also have evolved beyond what is published here.

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