# Review article: Numerical Methods for Engineering Quantum Computers

Liu, Shu
Mathematics, Florida State University

Georgiadou, Antigoni
Oak Ridge National Laboratory

Kubischta, Eric
Mathematics, Florida State University

Melton, Daniel
Mathematics, Florida State University

Guenther, Stefanie
Lawrence Livermore National Laboratory

Jin, Shi
Mathematics, Shanghai Jiao Tong University

Lin, Lin
Mathematics, U.C. Berkeley

Lotshaw, Philip
Oak Ridge National Laboratory

Petersson, Anders
Lawrence Livermore National Laboratory

Sussman, Mark
Mathematics, Florida State University

May 5, 2025

ABSTRACT: The main techniques in physically storing information in a "Quantum superposition state" and inducing "entanglement" amongst pairs of "Qubits" are (a) trapped ions, (b) superconducting circuits (e.g. Unimon Qubit), (c) Nitrogen-vacancy centers in diamond, and (d) Photonic Qubits. Each of these vehicles for quantum information technology have their advantages and disadvantages. Important properties to consider are (i) resiliance to noise, (ii) ability to communicate "quantum" information over long distances,

(iii) decoherence time, (iv) operating temperature, (v) scalability of multi Qubit entanglement, and (vi) being amenable to strategic control. Right now, Quantum computers are in the "Noisy Intermediate-Scale Quantum" (NISQ) era. In an effort to constantly improve the design of quantum computers, scientists and engineers answer questions regarding the aforementioned Qubit technology either experimentally or computationally. In this special issue, it is the computational methods which are reported on. It is the objective of this Special Issue to serve as a complete reference on the subject matter of "Numerical Methods for Engineering Quantum Computers" for use by students and established researchers. As a side benefit, it is expected that understanding the mathematical models and computational algorithms used to engineer Quantum Computers will also lead to improved algorithms for utilizing Quantum Computers.

As quoted from Shalf[8], "Moore's Law [1] is a techno-economic model that has enabled the IT industry to double the performance and functionality of digital electronics roughly every 2 years within a fixed cost, power and area. This expectation has led to a relatively stable ecosystem (e.g. electronic design automation tools, compilers, simulators and emulators) built around general-purpose processor technologies, such as the $\times$86, ARM and Power instruction set architectures. However, within a decade, the technological underpinnings for the process that Gordon Moore described will come to an end, as lithography gets down to atomic scale. At that point, it will be feasible to create lithographically produced devices with dimensions nearing atomic scale, where a dozen or fewer silicon atoms are present across critical device features, and will therefore represent a practical limit for implementing logic gates for digital computing [2]. Indeed, the ITRS (International Technology Roadmap for Semiconductors), which has tracked the historical improvements over the past 30 years, has projected no improvements beyond 2021, as shown in figure 1, and subsequently disbanded, having no further purpose. The classical technological driver that has underpinned Moore's Law for the past 50 years is failing [3] and is anticipated to flatten by 2025, as shown in figure 2. Evolving technology in the absence of Moore's Law will require an investment now in computer architecture and the basic sciences (including materials science), to study candidate replacement materials and alternative device physics to foster continued technology scaling." References one through three in the above quote correspond to the following references respectively: [5][3][4].

In Figure 3 of the article by Shalf[8], a roadmap is provided for possible paths forward when the density of circuits on classical computers exceeds a critical value. There are three categories: (a) roadmap for the next ten years, (b) 20 years, and (c) "Decades beyond exascale," "New Models of Computation." For category (c), some of the prospective technology listed is: (i) approximate computing, (ii) adiabatic reversible, (iii) Analog, (iv) Neuromorhic, and (v) quantum.

Of the "new models of computation" listed in Shalf's article[8], this special issue will address the "Numerical Methods for Engineering Quantum Computers" aspects associated with the emerging "quantum computing" paradigm. As outlined by Gamble[2], the development of reliable quantum computers will have

a tranformative effect on computer technology. That being said, right now we are in the "Noisy Intermediate-Scale Quantum"[1] (NISQ) era. The purpose of this special issue is to bring to the forefront the current research being done, from the computational perspective, in order to move beyond the NISQ era.

# 1 preiliminaries

In order to appreciate the complexities associated with designing a quantum computer, it is suggested that one first gain some intuition on electricity and magnetism.

The phenomena of electromagnetism and light is a very complex field, in of itself. One could choose as a starting point Maxwell's equations which are,

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0} \quad \text{(Gauss's Law for Electricity)} \tag{1}$$

$$\nabla \cdot \mathbf{B} = 0 \quad \text{(Gauss's Law for Magnetism)} \tag{2}$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \quad \text{(Faraday's Law of Induction)} \tag{3}$$

$$\nabla \times \mathbf{B} = \mu_0 \left( \mathbf{J} + \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} \right) \quad \text{(Ampere-Maxwell's Law)} \tag{4}$$

Also, there is the Lorentz force law:

$$\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$$

A good textbook that describes these fundamentals is by Purcell and Morin third edition[6].

Maxwell's equations, and relativity though are not sufficient to describe the quantum nature of matter and light. Matter and Light, when considering small enough scales, have a dual particle and wave property to them. Also Matter and light posess discrete "quantum," energy levels. For a good reference, see the following quantum mechanics textbook[7].

The mathematical model that describes the dynamics of matter and light, including "quantum" properties and the dual particle wave property is Schrodinger's equation:

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \hat{H} \Psi(\mathbf{r}, t)$$

where: i is the imaginary unit $\hbar$ is the reduced Planck constant $\frac{\partial}{\partial t}$ is the partial derivative with respect to time $\Psi(\mathbf{r}, t)$ is the wave function $\hat{H}$ is the Hamiltonian operator $\mathbf{r}$ is the position vector $t$ is time The time-independent Schrödinger equation can be written as:

$$\hat{H}\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

where:

$$\hat{H}$$

is the Hamiltonian operator

$$\psi(\mathbf{r})$$

is the time-independent wave function

$$E$$

is the energy of the system.

If relativistic effects must be considered then the following relativistic wave equation models have been developed:

- Klein Gordon equation (spin zero particles) (flat space time)

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2 + \frac{m^2c^2}{\hbar^2}\right)\phi(x,t) = 0 \tag{5}$$

- Klein Gordon equation (spin zero particles) (in terms of the four-dimensional derivative operator (d'Alembertian))

$$\Box\phi(x) + \frac{m^2c^2}{\hbar^2}\phi(x) = 0 \tag{6}$$

$$\Box = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2 \tag{7}$$

- Dirac equation (spin one half particles)

$$\left(\beta mc^2 + c\left(\sum_{n=1}^{3}\alpha_n p_n\right)\right)\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t} \tag{8}$$

$$i\hbar\gamma^\mu\partial_\mu\psi - mc\psi = 0 \tag{9}$$

$$(i\partial\!\!\!/ - m)\psi = 0 \tag{10}$$

Finally, in some scenarios, the most appropriate mathematical models correspond to the nonlinear Schrodinger equation:

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\nabla^2\psi + V(\psi)\psi$$

# References


[1] Callison, A., and Chancellor, N. Hybrid quantum-classical algorithms in the noisy intermediate-scale quantum era and beyond. *Physical Review A 106*, 1 (2022), 010101.

[2] Gamble, S. Quantum computing: What it is, why we want it, and how we're trying to get it. In *Frontiers of Engineering: Reports on Leading-Edge Engineering from the 2018 Symposium* (2019), National Academies Press, pp. 5–8.

[3] Mack, C. The multiple lives of moore's law. *IEEE Spectrum 52*, 4 (2015), 31–31.

[4] Markov, I. L. Limits on fundamental limits to computation. *Nature 512*, 7513 (2014), 147–154.

[5] Moore, G. Cramming more components onto integrated circuits (1965).

[6] Purcell, E., and Morin, D. Electricity and magnetism third edition, 2013.

[7] Sakurai, J. J., and Napolitano, J. *Modern quantum mechanics*. Cambridge University Press, 2020.

[8] Shalf, J. The future of computing beyond moore's law. *Philosophical Transactions of the Royal Society A 378*, 2166 (2020), 20190061.