Special Issue: Numerical Methods for Engineering Quantum Computers

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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. 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.

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2 Full scope of the special issue

Computational Quantum Physics: Numerical Algorithms for the optimal control of Qubit(s), computing ground states and sensitivity thereof due to perturbations in the Hamiltonian, hybrid classical and quantum algorithms, numerical methods for the unsteady/steady Schrodinger equation, nonlinear Schrodinger equation, inverse problems for the Hamiltonian, Error Correction Algorithms, Quantum circuits for benchmarking quantum computers.

3 Special Issue Keywords

Computational Quantum Physics, Quantum Computer, control of Quantum Systems, Schrodinger equation, inverse problems in Quantum Mechanics, Quantum error correction, Hybrid Quantum/Classical algorithms, Benchmarking Quantum circuits

4 Rationale for special issue and recommended contibuters

As quoted from Shalf[51], "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: [42][40][41].

In Figure 3 of the article by Shalf[51], 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[51], this special issue will address the "Numerical Methods for Engineering Quantum Computers" aspects associated with the emerging "quantum computing" paradigm. As outlined by Gamble[16], the development of reliable quantum computers will have a tranformative effect on computer technology.

At the present, the research activity associated with "Numerical Methods for Engineering Quantum Computers" is spread out over many journals: IEEE Journals, "Quantum Information Processing," "Quantum Science and Technology," "Quantum," "ACM Transactions on Quantum Computing," "SIAM review," "Journal of Computational Physics," "Journal of Scientific Computing," "Physical Review A," "Journal of Chemical Physics," "Journal of Physics: Condensed Matter," "Physical Review A," "Physical Review Letters," "Physical Review Research," "Nature," "Nature Communications," "Nature Physics," "Nature Photonics," "Nature Chemistry," "PRX Quantum," "AVS Quantum Science," "Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences."

It is the intention of this special issue to have information pertaining to "Numerical Methods for Engineering Quantum Computers" in one accessble issue.

The following is a list of authors and the articles they have previously published which motivate inviting them to contribute to the proposed special issue on "The numerical analysis of Quantum Computer Design."

- Muqeet et al[43] "A Machine Learning-Based Error Mitigation Approach for Reliable Software Development on IBM's Quantum Computers"
- Anthony-Petersen et al[3] "A stress-induced source of phonon bursts and quasiparticle poisoning"
- Tuysuz et al[54] "Learning to generate high-dimensional distributions with low-dimensional quantum Boltzmann machines"

- W. Bao, Z. Chang, X. Zhao[4], "Computing ground states of Bose-Einstein condensation by normalized deep neural network"
- W. Bao, S. Jin, and P. Markowich[5] "On Time-Splitting Spectral Approximations for the Schrödinger Equation in the Semiclassical Regime"
- S. Jin, X. Li, N. Liu, and Y. Yu[27], "Quantum Simulation for Quantum Dynamics with Artificial Boundary Conditions"
- S. Jin, N. Liu, and Y. Yu[29], "Quantum Circuits for the heat equation with physical boundary conditions via Schrodingerisation"
- S. Jin, H. Liu, S. Osher, R. Tsai[28], "Computing multivalued physical observables for the semiclassical limit of the Schrödinger equation"
- Jiequn Han and Linfeng Zhang and Weinan E[20] "Solving many-electron Schrödinger equation using deep neural networks"
- Bernien et al[8] "Probing many-body dynamics on a 51-atom quantum simulator"
- Zhang et al[57] "Observation of a many-body dynamical phase transition with a 53-qubit quantum simulator"
- Cerezo et al[10] "Variational quantum algorithms"
- Anshu et al[2] "Sample-efficient learning of interacting quantum systems"
- Toshiaki Kanai, Dafei Jin, and Wei Guo[30] "Single-Electron Qubits Based on Quantum Ring States on Solid Neon Surface"
- Hermann et al[23] "Deep-neural-network solution of the electronic Schrödinger equation"
- Ilin and Arad[25] "Dissipative variational quantum algorithms for Gibbs state preparation"
- Somma et al[52] "Shadow Hamiltonian Simulation"
- Lotshaw et al[38] "Exactly solvable model of light-scattering errors in quantum simulations with metastable trapped-ion qubits"
- Lotshaw et al[37] "Modeling noise in global Mølmer-Sørensen interactions applied to quantum approximate optimization"
- Lotshaw et al[39] "Simulations of frustrated Ising Hamiltonians using quantum approximate optimization"
- Friesen et al[15] "Practical design and simulation of silicon-based quantum-dot qubits"

- Kai Jiang et al[26] “High-accuracy numerical methods and convergence analysis for Schrödinger equation with incommensurate potentials”
- Lin and Lu[32] “A mathematical introduction to electronic structure theory”
- Nielsen and Chuang[45] “Quantum computation and quantum information”
- Ding and Lin[14] “Simultaneous estimation of multiple eigenvalues with short-depth quantum circuit on early fault-tolerant quantum computers”
- Ding et al[13] “Random coordinate descent: A simple alternative for optimizing parameterized quantum circuits”
- Liu and Lin[36] “Dense outputs from quantum simulations”
- Lin, Saad, and Yang[33] “Approximating spectral densities of large matrices”
- Chen et al[11] “Quantum-Classical-Quantum Workflow in Quantum-HPC Middleware with GPU Acceleration”
- Biamonte et al[9] “Quantum machine learning”
- Benedetti et al[7] “Parameterized quantum circuits as machine learning models”
- Jin-Guo Liu et al[35] ”Variational quantum eigensolver with fewer qubits”
- Saurabh et al[48] “A conceptual architecture for a quantum-hpc middleware”
- Uvarov et al[55] “Machine learning phase transitions with a quantum processor”
- Khait et al[31] ”Variational quantum eigensolvers in the era of distributed quantum computers”
- Huang et al[24] “Predicting many properties of a quantum system from very few measurements”
- Cong et al[12] “Quantum convolutional neural networks”
- Parekh et al[47] “Quantum algorithms and simulation for parallel and distributed quantum computing”
- Vallero et al[56] “State of practice: evaluating GPU performance of state vector and tensor network methods”
- Nguyen et al[44] “Tensor network quantum virtual machine for simulating quantum circuits at exascale”

- Liu et al[34] “Training classical neural networks by quantum machine learning”
- Bayraktar et al[6] “cuQuantum SDK: A High-Performance Library for Accelerating Quantum Science”
- Andrade et al[1] “Engineering an effective three-spin Hamiltonian in trapped-ion systems for applications in quantum simulation”
- Wenhao He et al [22], “Efficient Optimal Control of Open Quantum Systems”
- Alexander Nusseler et al [46], “Efficient simulation of open quantum systems coupled to a fermionic bath”
- Selsto and Kvaal [50], “Absorbing boundary conditions for dynamical many-body quantum systems”
- Sawaya et al[49], “HamLib: A Library of Hamiltonians for Benchmarking Quantum Algorithms and Hardware”
- Symeon Grivopoulos[17], “Optimal control of quantum systems”
- Theisen and Stamm[53], ”A Scalable Two-Level Domain Decomposition Eigensolver for Periodic Schrödinger Eigenstates in Anisotropically Expanding Domains”
- Guenther, Petersson, and DuBois[19], “Quandary: An open-source C++ package for high-performance optimal control of open quantum systems”
- Guenther and Petersson[18], “A practical approach to determine minimal quantum gate durations using amplitude-bounded quantum controls”
- Hangleiter et al[21], “Robustly learning the Hamiltonian dynamics of a superconducting quantum processor”

The following is a template for inviting researchers to contribute to the special issue:

Dear first and last name,

In response to the growing interest in Quantum Computing, and the constant effort to design ever more resilient systems, we plan to publish a Special Issue on “Numerical Methods for Engineering Quantum Computers” in the Journal of Computational Physics (JCP). This Special Issue will span a broad range of related topics from numerical methods for determining ground states, numerical methods for solving the unsteady or nonlinear Schrodinger Equation, Density Functional Theory, Computer Aided Design of Quantum Algorithms in order to optimize the “decoherence time,” Hybrid classical quantum algorithms, and optimal design and control of qubits. Our special issue will serve as a complete reference on the subject matter for use by students and established researchers.

Given your expertise in the related field, we extend a personal invitation to you to contribute a paper to this Special Issue on a topic of your choice. If agreeable, please send us a reply by Email with a tentative title by 22 November, 2024. Please copy Ms Yuan Li (yuan.li@elsevier.com) who is copied on this Email and happy to answer any questions you may have. Please see below details about the submission portal and other relevant information.

We look forward to hearing from you.

Our kindest regards,

Mark Sussman, guest editor 2, guest editor 3, . . .

Journal:
Journal of Computational Physics (ISSN: , CiteScore: , Impact Factor:)

Special Issue: "Numerical Methods for Engineering Quantum Computers"
Website:
Guest Editors: (e.g. 3 or more)
All submissions will be peer-reviewed.
Important dates:
Submission Website:
select the article type of " VSI: Numerical Methods for Engineering Quantum Computers "
Submission portal closes: 30 April 2025.
Publication date (estimate): 30 October 2025.

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