Special Issue: Numerical Methods for Engineering Quantum Computers

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 6, 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

1

will also lead to improved algorithms for utilizing Quantum Computers.

1 Guest Editors

- Mark Sussman, Florida State University `sussman@math.fsu.edu`

- Lin Lin, University of California, Berkeley `linlin@math.berkeley.edu`

- Shi Jin, Shanghai Jiao Tong University `shijin-m@sjtu.edu.cn`

- Stefanie Guenther, Lawrence Livermore National Laboratory `guenther5@llnl.gov`

- Anders Petersson, Lawrence Livermore National Laboratory `petersson1@llnl.gov`

- Philip Lotshaw, Oak Ridge National Laboratory `lotshawpc@ornl.gov`

2 Full scope of the special issue

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

3 Special Issue Keywords

Computational Quantum Physics, Quantum Computer, control of Quantum Systems, Schrodinger equation, inverse problems in Quantum Mechanics, Quantum error correction, Designing Fault Tolerant Quantum Computers, Hybrid Quantum/Classical algorithms, Benchmarking Quantum circuits, Computational Quantum Electrodynamics.

4 Rationale for special issue and recommended contibuters

As quoted from Shalf[60], "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: [50][48][49].

In Figure 3 of the article by Shalf[60], 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[60], this special issue will address the "Numerical Methods for Engineering Quantum Computers" aspects associated with the emerging "quantum computing" paradigm. As outlined by Gamble[19], 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"[12] (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.

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 "Numerical Methods for Engineering Quantum Computers."

- Callison and Chancellor[12] "Hybrid quantum-classical algorithms in the noisy intermediate-scale quantum era and beyond"

- Muqeet et al[51] "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[64] "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[32], "Quantum Simulation for Quantum Dynamics with Artificial Boundary Conditions"

- S. Jin, N. Liu, and Y. Yu[34], "Quantum Circuits for the heat equation with physical boundary conditions via Schrodingerisation"

- S. Jin, H. Liu, S. Osher, R. Tsai[33], "Computing multivalued physical observables for the semiclassical limit of the Schrödinger equation"

- Jiequn Han and Linfeng Zhang and Weinan E[25] "Solving many-electron Schrödinger equation using deep neural networks"

- Bernien et al[10] "Probing many-body dynamics on a 51-atom quantum simulator"

- Zhang et al[67] "Observation of a many-body dynamical phase transition with a 53-qubit quantum simulator"

- Cerezo et al[13] "Variational quantum algorithms"

- Anshu et al[2] "Sample-efficient learning of interacting quantum systems"

- Toshiaki Kanai, Dafei Jin, and Wei Guo[35] "Single-Electron Qubits Based on Quantum Ring States on Solid Neon Surface"

- Hermann et al[28] "Deep-neural-network solution of the electronic Schrödinger equation"

- Ilin and Arad[30] "Dissipative variational quantum algorithms for Gibbs state preparation"

- Somma et al[62] "Shadow Hamiltonian Simulation"

- Lotshaw et al[46] "Exactly solvable model of light-scattering errors in quantum simulations with metastable trapped-ion qubits"

- Lotshaw et al[45] "Modeling noise in global Mølmer-Sørensen interactions applied to quantum approximate optimization"

- Lotshaw et al[47] "Simulations of frustrated Ising Hamiltonians using quantum approximate optimization"

- Friesen et al[18] "Practical design and simulation of silicon-based quantum-dot qubits"

- Kai Jiang et al[31] "High-accuracy numerical methods and convergence analysis for Schrödinger equation with incommensurate potentials"

- Lin and Lu[40] "A mathematical introduction to electronic structure theory"

- Nielsen and Chuang[53] "Quantum computation and quantum information"

- Ding and Lin[17] "Simultaneous estimation of multiple eigenvalues with short-depth quantum circuit on early fault-tolerant quantum computers"

- Ding et al[16] "Random coordinate descent: A simple alternative for optimizing parameterized quantum circuits"

- Liu and Lin[44] "Dense outputs from quantum simulations"

- Lin, Saad, and Yang[41] "Approximating spectral densities of large matrices"

- Kubischta and Teixeira[37] "Family of quantum codes with exotic transversal gates"

- Chen et al[14] "Quantum-Classical-Quantum Workflow in Quantum-HPC Middleware with GPU Acceleration"

- Biamonte et al[11] "Quantum machine learning"

- Benedetti et al[9] "Parameterized quantum circuits as machine learning models"

- Jin-Guo Liu et al[43] "Variational quantum eigensolver with fewer qubits"

- Saurabh et al[57] "A conceptual architecture for a quantum-hpc middleware"

- Uvarov et al[65] "Machine learning phase transitions with a quantum processor"

- Khait et al[36] "Variational quantum eigensolvers in the era of distributed quantum computers"

- Huang et al[29] "Predicting many properties of a quantum system from very few measurements"

- Cong et al[15] "Quantum convolutional neural networks"

- Parekh et al[55] "Quantum algorithms and simulation for parallel and distributed quantum computing"

- Vallero et al[66] "State of practice: evaluating GPU performance of state vector and tensor network methods"

- Nguyen et al[52] "Tensor network quantum virtual machine for simulating quantum circuits at exascale"

- Liu et al[42] "Training classical neural networks by quantum machine learning"

- Bayraktar et al[7] "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 [27], "Efficient Optimal Control of Open Quantum Systems"

- Alexander Nusseler et al [54], "Efficient simulation of open quantum systems coupled to a fermionic bath"

- Selsto and Kvaal [59], "Absorbing boundary conditions for dynamical many-body quantum systems"

- Sawaya et al[58], "HamLib: A Library of Hamiltonians for Benchmarking Quantum Algorithms and Hardware"

- Symeon Grivopoulos[22], "Optimal control of quantum systems"

- Theisen and Stamm[63], "A Scalable Two-Level Domain Decomposition Eigensolver for Periodic Schrödinger Eigenstates in Anisotropically Expanding Domains"

- Guenther, Petersson, and DuBois[24], "Quandary: An open-source C++ package for high-performance optimal control of open quantum systems"

- Guenther and Petersson[23], "A practical approach to determine minimal quantum gate durations using amplitude-bounded quantum controls"

- Lidar[39], "Lecture notes on the theory of open quantum systems"

- Hangleiter et al[26], "Robustly learning the Hamiltonian dynamics of a superconducting quantum processor"

- Beer et al[8], "Training deep quantum neural networks"

- Lalanne et al[38], "Light Interaction with Photonic and Plasmonic Resonances"

- Shukrinov et al[61], "Modeling of LC-shunted intrinsic Josephson junctions in high-Tc superconductors"

- Georgadou et al[21] Hele-Shaw simulation on quantum computer.

- Rupert Klein[56] WaveTrain: A Python package for numerical quantum mechanics of chain-like systems based on tensor trains

- `psiquantum.com` [6] "Fusion based quantum computation," Bartolucci et al

- Roy Goodman et al[20], "QGLAB: A MATLAB PACKAGE FOR COMPUTATIONS ON QUANTUM GRAPHS"

- Campolattaro, Alfonso A "Generalized Maxwell equations and quantum mechanics. I. Dirac equation for the free electron"

- Brannick et al, "Least-Squares Finite Element Methods for Quantum Electrodynamics"

- Roth and Chew, "Macroscopic Circuit Quantum Electrodynamics: A New Look Toward Developing Full-Wave Numerical Models"

- Devoret et al, "Quantum fluctuations in electrical circuits"

- Adriazola and Roszak, "Nonconvex optimization strategy for computing convex-roof entanglement"

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 November 2025.
Editorial acceptance deadline: 30 May 2026

References

[1] ANDRADE, B., DAVOUDI, Z., GRASS, T., HAFEZI, M., PAGANO, G., AND SEIF, A. Engineering an effective three-spin hamiltonian in trapped-ion systems for applications in quantum simulation. *Quantum Science and Technology 7*, 3 (apr 2022), 034001.

[2] ANSHU, A., ARUNACHALAM, S., KUWAHARA, T., AND SOLEIMANIFAR, M. Sample-efficient learning of interacting quantum systems. *Nature Physics 17*, 8 (2021), 931–935.

[3] ANTHONY-PETERSEN, R., BIEKERT, A., BUNKER, R., CHANG, C. L., CHANG, Y.-Y., CHAPLINSKY, L., FASCIONE, E., FINK, C. W., GARCIA-SCIVERES, M., GERMOND, R., ET AL. A stress-induced source of phonon bursts and quasiparticle poisoning. *Nature Communications 15*, 1 (2024), 6444.

[4] BAO, W., CHANG, Z., AND ZHAO, X. Computing ground states of bose-einstein condensation by normalized deep neural network. *Journal of Computational Physics 520* (2025), 113486.

[5] BAO, W., JIN, S., AND MARKOWICH, P. A. On time-splitting spectral approximations for the schrödinger equation in the semiclassical regime. *Journal of Computational Physics 175*, 2 (2002), 487–524.

[6] BARTOLUCCI, S., BIRCHALL, P., BOMBIN, H., CABLE, H., DAWSON, C., GIMENO-SEGOVIA, M., JOHNSTON, E., KIELING, K., NICKERSON, N., PANT, M., ET AL. Fusion-based quantum computation. *Nature Communications 14*, 1 (2023), 912.

[7] BAYRAKTAR, H., CHARARA, A., CLARK, D., COHEN, S., COSTA, T., FANG, Y.-L. L., GAO, Y., GUAN, J., GUNNELS, J., HAIDAR, A., HEHN, A., HOHNERBACH, M., JONES, M., LUBOWE, T., LYAKH, D., MORINO, S., SPRINGER, P., STANWYCK, S., TERENTYEV, I., VARADHAN, S., WONG, J., AND YAMAGUCHI, T. cuquantum sdk: A high-performance library for accelerating quantum science. In *2023 IEEE International Conference on Quantum Computing and Engineering (QCE)* (2023), vol. 01, pp. 1050–1061.

[8] BEER, K., BONDARENKO, D., FARRELLY, T., OSBORNE, T. J., SALZMANN, R., SCHEIERMANN, D., AND WOLF, R. Training deep quantum neural networks. *Nature communications 11*, 1 (2020), 808.

[9] BENEDETTI, M., LLOYD, E., SACK, S., AND FIORENTINI, M. Parameterized quantum circuits as machine learning models. *Quantum Science and Technology 4*, 4 (nov 2019), 043001.

[10] BERNIEN, H., SCHWARTZ, S., KEESLING, A., LEVINE, H., OMRAN, A., PICHLER, H., CHOI, S., ZIBROV, A. S., ENDRES, M., GREINER, M., ET AL. Probing many-body dynamics on a 51-atom quantum simulator. *Nature 551*, 7682 (2017), 579–584.

[11] BIAMONTE, J., WITTEK, P., PANCOTTI, N., REBENTROST, P., WIEBE, N., AND LLOYD, S. Quantum machine learning. *Nature 549*, 7671 (2017), 195–202.

[12] 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.

[13] CEREZO, M., ARRASMITH, A., BABBUSH, R., BENJAMIN, S. C., ENDO, S., FUJII, K., MCCLEAN, J. R., MITARAI, K., YUAN, X., CINCIO, L., ET AL. Variational quantum algorithms. *Nature Reviews Physics 3*, 9 (2021), 625–644.

[14] CHEN, K.-C., LI, X., XU, X., WANG, Y.-Y., AND LIU, C.-Y. Quantum-classical-quantum workflow in quantum-hpc middleware with gpu acceleration. In *2024 International Conference on Quantum Communications, Networking, and Computing (QCNC)* (2024), pp. 304–311.

[15] CONG, I., CHOI, S., AND LUKIN, M. D. Quantum convolutional neural networks. *Nature Physics 15*, 12 (2019), 1273–1278.

[16] DING, Z., KO, T., YAO, J., LIN, L., AND LI, X. Random coordinate descent: A simple alternative for optimizing parameterized quantum circuits. *Physical Review Research 6*, 3 (2024), 033029.

[17] DING, Z., AND LIN, L. Simultaneous estimation of multiple eigenvalues with short-depth quantum circuit on early fault-tolerant quantum computers. *Quantum 7* (2023), 1136.

[18] FRIESEN, M., RUGHEIMER, P., SAVAGE, D. E., LAGALLY, M. G., VAN DER WEIDE, D. W., JOYNT, R., AND ERIKSSON, M. A. Practical design and simulation of silicon-based quantum-dot qubits. *Phys. Rev. B 67* (Mar 2003), 121301.

[19] 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.

[20] GOODMAN, R. H., CONTE, G., AND MARZUOLA, J. L. Qglab: A matlab package for computations on quantum graphs. *SIAM Journal on Scientific Computing 47*, 2 (2025), B428–B453.

[21] GOPALAKRISHNAN MEENA, M., GOTTIPARTHI, K. C., LIETZ, J. G., GEORGIADOU, A., AND COELLO PÉREZ, E. A. Solving the hele–shaw flow using the harrow–hassidim–lloyd algorithm on superconducting devices: A study of efficiency and challenges. *Physics of Fluids 36*, 10 (2024).

[22] GRIVOPOULOS, S. *Optimal control of quantum systems*. University of California, Santa Barbara, 2005.

[23] GÜNTHER, S., AND PETERSSON, N. A. A practical approach to determine minimal quantum gate durations using amplitude-bounded quantum controls. *AVS Quantum Science 5*, 4 (2023).

[24] GÜNTHER, S., PETERSSON, N. A., AND DUBOIS, J. L. Quandary: An open-source c++ package for high-performance optimal control of open quantum systems. In *2021 IEEE/ACM Second International Workshop on Quantum Computing Software (QCS)* (2021), pp. 88–98.

[25] HAN, J., ZHANG, L., AND E, W. Solving many-electron schrödinger equation using deep neural networks. *Journal of Computational Physics 399* (2019), 108929.

[26] HANGLEITER, D., ROTH, I., FUKSA, J., EISERT, J., AND ROUSHAN, P. Robustly learning the hamiltonian dynamics of a superconducting quantum processor. *Nature Communications 15*, 1 (2024), 9595.

[27] HE, W., LI, T., LI, X., LI, Z., WANG, C., AND WANG, K. Efficient optimal control of open quantum systems, 2024.

[28] HERMANN, J., SCHÄTZLE, Z., AND NOÉ, F. Deep-neural-network solution of the electronic schrödinger equation. *Nature Chemistry 12*, 10 (2020), 891–897.

[29] HUANG, H.-Y., KUENG, R., AND PRESKILL, J. Predicting many properties of a quantum system from very few measurements. *Nature Physics 16*, 10 (2020), 1050–1057.

[30] ILIN, Y., AND ARAD, I. Dissipative variational quantum algorithms for gibbs state preparation, 2024.

[31] JIANG, K., LI, S., AND ZHANG, J. High-accuracy numerical methods and convergence analysis for schrödinger equation with incommensurate potentials. *Journal of Scientific Computing 101*, 1 (2024), 18.

[32] JIN, S., LI, X., LIU, N., AND YU, Y. Quantum simulation for quantum dynamics with artificial boundary conditions. *SIAM Journal on Scientific Computing 46*, 4 (2024), B403–B421.

[33] JIN, S., LIU, H., OSHER, S., AND TSAI, Y.-H. R. Computing multivalued physical observables for the semiclassical limit of the schrödinger equation. *Journal of Computational Physics 205*, 1 (2005), 222–241.

[34] JIN, S., LIU, N., AND YU, Y. Quantum circuits for the heat equation with physical boundary conditions via schrodingerisation. *arXiv preprint arXiv:2407.15895* (2024).

[35] KANAI, T., JIN, D., AND GUO, W. Single-electron qubits based on quantum ring states on solid neon surface. *Phys. Rev. Lett. 132* (Jun 2024), 250603.

[36] KHAIT, I., THAM, E., SEGAL, D., AND BRODUTCH, A. Variational quantum eigensolvers in the era of distributed quantum computers. *Physical Review A 108*, 5 (2023), L050401.

[37] KUBISCHTA, E., AND TEIXEIRA, I. Family of quantum codes with exotic transversal gates. *Physical Review Letters 131*, 24 (2023), 240601.

[38] LALANNE, P., YAN, W., VYNCK, K., SAUVAN, C., AND HUGONIN, J.-P. Light interaction with photonic and plasmonic resonances. *Laser & Photonics Reviews 12*, 5 (2018), 1700113.

[39] LIDAR, D. A. Lecture notes on the theory of open quantum systems. *arXiv preprint arXiv:1902.00967* (2019).

[40] Lin, L., and Lu, J. *A mathematical introduction to electronic structure theory*. SIAM, 2019.

[41] Lin, L., Saad, Y., and Yang, C. Approximating spectral densities of large matrices. *SIAM review 58*, 1 (2016), 34–65.

[42] Liu, C.-Y., Kuo, E.-J., Lin, C.-H. A., Chen, S., Young, J. G., Chang, Y.-J., and Hsieh, M.-H. Training classical neural networks by quantum machine learning. *arXiv preprint arXiv:2402.16465* (2024).

[43] Liu, J.-G., Zhang, Y.-H., Wan, Y., and Wang, L. Variational quantum eigensolver with fewer qubits. *Phys. Rev. Res. 1* (Sep 2019), 023025.

[44] Liu, J.-P., and Lin, L. Dense outputs from quantum simulations. *Journal of Computational Physics 514* (2024), 113213.

[45] Lotshaw, P. C., Battles, K. D., Gard, B., Buchs, G., Humble, T. S., and Herold, C. D. Modeling noise in global mølmer-sørensen interactions applied to quantum approximate optimization. *Phys. Rev. A 107* (Jun 2023), 062406.

[46] Lotshaw, P. C., Sawyer, B. C., Herold, C. D., and Buchs, G. Exactly solvable model of light-scattering errors in quantum simulations with metastable trapped-ion qubits. *Phys. Rev. A 110* (Sep 2024), L030803.

[47] Lotshaw, P. C., Xu, H., Khalid, B., Buchs, G., Humble, T. S., and Banerjee, A. Simulations of frustrated ising hamiltonians using quantum approximate optimization. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences 381*, 2241 (2023), 20210414.

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

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

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

[51] Muqeet, A., Ali, S., Yue, T., and Arcaini, P. A machine learning-based error mitigation approach for reliable software development on ibm's quantum computers. In *Companion Proceedings of the 32nd ACM International Conference on the Foundations of Software Engineering* (2024), pp. 80–91.

[52] Nguyen, T., Lyakh, D., Dumitrescu, E., Clark, D., Larkin, J., and McCaskey, A. Tensor network quantum virtual machine for simulating quantum circuits at exascale. *ACM Transactions on Quantum Computing 4*, 1 (2022), 1–21.

[53] NIELSEN, M. A., AND CHUANG, I. L. *Quantum computation and quantum information*. Cambridge university press, 2010.

[54] NÜSSELER, A., DHAND, I., HUELGA, S. F., AND PLENIO, M. B. Efficient simulation of open quantum systems coupled to a fermionic bath. *Phys. Rev. B 101* (Apr 2020), 155134.

[55] PAREKH, R., RICCIARDI, A., DARWISH, A., AND DIADAMO, S. Quantum algorithms and simulation for parallel and distributed quantum computing. In *2021 IEEE/ACM Second International Workshop on Quantum Computing Software (QCS)* (2021), IEEE, pp. 9–19.

[56] RIEDEL, J., GELSS, P., KLEIN, R., AND SCHMIDT, B. Wavetrain: A python package for numerical quantum mechanics of chain-like systems based on tensor trains. *The Journal of Chemical Physics 158*, 16 (2023).

[57] SAURABH, N., JHA, S., AND LUCKOW, A. A conceptual architecture for a quantum-hpc middleware. In *2023 IEEE International Conference on Quantum Software (QSW)* (2023), IEEE, pp. 116–127.

[58] SAWAYA, N. P., MARTI-DAFCIK, D., HO, Y., TABOR, D. P., BERNAL NEIRA, D. E., MAGANN, A. B., PREMARATNE, S., DUBEY, P., MATSUURA, A., BISHOP, N., DE JONG, W. A., BENJAMIN, S., PAREKH, O. D., TUBMAN, N. M., KLYMKO, K., AND CAMPS, D. Hamlib: A library of hamiltonians for benchmarking quantum algorithms and hardware. In *2023 IEEE International Conference on Quantum Computing and Engineering (QCE)* (2023), vol. 02, pp. 389–390.

[59] SELSTØ, S., AND KVAAL, S. Absorbing boundary conditions for dynamical many-body quantum systems. *Journal of Physics B: Atomic, Molecular and Optical Physics 43*, 6 (mar 2010), 065004.

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

[61] SHUKRINOV, Y. M., RAHMONOV, I., KULIKOV, K., BOTHA, A., PLECENIK, A., SEIDEL, P., AND NAWROCKI, W. Modeling of lc-shunted intrinsic josephson junctions in high-tc superconductors. *Superconductor Science and Technology 30*, 2 (2016), 024006.

[62] SOMMA, R. D., KING, R., KOTHARI, R., O'BRIEN, T., AND BABBUSH, R. Shadow hamiltonian simulation, 2024.

[63] THEISEN, L., AND STAMM, B. A scalable two-level domain decomposition eigensolver for periodic schrödinger eigenstates in anisotropically expanding domains. *SIAM Journal on Scientific Computing 46*, 5 (2024), A3067–A3093.

[64] TÜYSÜZ, C., DEMIDIK, M., COOPMANS, L., RINALDI, E., CROFT, V., HADDAD, Y., ROSENKRANZ, M., AND JANSEN, K. Learning to generate high-dimensional distributions with low-dimensional quantum boltzmann machines. *arXiv preprint arXiv:2410.16363* (2024).

[65] UVAROV, A., KARDASHIN, A., AND BIAMONTE, J. D. Machine learning phase transitions with a quantum processor. *Physical Review A 102*, 1 (2020), 012415.

[66] VALLERO, M., VELLA, F., AND RECH, P. State of practice: evaluating gpu performance of state vector and tensor network methods. *arXiv preprint arXiv:2401.06188* (2024).

[67] ZHANG, J., PAGANO, G., HESS, P. W., KYPRIANIDIS, A., BECKER, P., KAPLAN, H., GORSHKOV, A. V., GONG, Z.-X., AND MONROE, C. Observation of a many-body dynamical phase transition with a 53-qubit quantum simulator. *Nature 551*, 7682 (2017), 601–604.