Quantum Computing for Biomedical Computational and Data Sciences: A Joint DOE-NIH Roundtable Report

Report on the 2-day roundtable held on March 17 and March 27, 2023

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1. Executive Summary

1.1 Background and Objectives

The overlap of quantum computing and biomedical research, while less explored, presents significant near-term opportunities. The Department of Energy (DOE) and the National Institutes of Health (NIH) are interested in exploiting the DOE community's capabilities and expertise in quantum computing to potentially advance biomedical research, targeting fundamental studies of biological and molecular structures, understanding of human health as well as mental and physical disorders and diseases, and deriving insights from clinical data. NIH's approach to quantum computing is guided by its Strategic Plan for Data Science, emphasizing the importance of findable, accessible, interoperable, and reusable (FAIR) data assets, security and privacy of data, and efficient computing and storage. DOE's Office of Science (SC), and more specifically the Advanced Scientific Computing Research (ASCR) program, supports quantum information science (QIS) research, contributing to a unique portfolio of quantum computing and communications expertise.

This roundtable was assembled to consider the opportunities and challenges in the near-, medium-, and long-term at the intersection of quantum computing, data science, and biomedical research and how these could be addressed through inter-agency collaboration and multi-disciplinary partnerships.

1.2 Key Outcomes and Research Directions

Experts in quantum computing and biomedical research gathered in a roundtable to highlight significant opportunities and challenges in these intersecting domains. Presentations and discussions led to the identification of potential biomedical applications of quantum computing, assessing current research status, and considering technical and practical aspects. This section summarizes the promising research directions and strategies to tackle identified challenges, guiding future collaborations between DOE and NIH to foster groundbreaking quantum solutions for biomedical research.

1.2.1 Biomedical Use-Cases for Quantum Applicability and Impact

The roundtable discussions identified potential biomedical use-cases for quantum computing in the near-term, i.e., although many of the quantum challenges are medium- and long-term, there could be initial applicability and impact in the next 5 years (near-term). Notably, three fields stood out due to their preliminary work and anticipated impact: *medical imaging and diagnostics*, *biological sequence analysis and processing*, and *drug discovery*. There was recognition of the complexity and diversity within these fields, including the variety of algorithms employed depending on the data type and research question. Crucially, steps where classical computation restricts problem size [1], and could hence benefit from a quantum advantage [2], must be highlighted.

Medical Imaging and Diagnostics. This field could greatly benefit from quantum algorithms as traditional methods for image analysis (e.g., segmentation), reconstruction (e.g., iterative methods), and registration (e.g, feature/intensity/distance-based methods) are computationally demanding, and the need for improved diagnostic accuracy is paramount. Quantum algorithms, including quantum Fourier transform [3], quantum phase estimation, quantum optimization methods [4], quantum machine learning (QML) [5], and quantum image processing techniques [6], can be adapted to enhance medical imaging applications. The demand for quicker, more accurate, and efficient diagnostics is high, and specific applications, such as image denoising and filtering applied to smaller scale classical and quantum input, may be feasible with near-term quantum hardware due to their modest qubit requirements, especially the initial study and development of proof-of-principle demonstrations.

Biological Sequence Data Analysis. The process of extracting meaningful biological insights from raw DNA/RNA sequencing data involves tasks such as identifying genes, detecting mutations, and understanding gene expression patterns. There is a great need for faster sequence alignment and search, enhanced phylogenetic analysis, and multi-omics data integration. This field has potential for short-term impact by the use of quantum algorithms, including the ones based on distance metrics such as Edit distance [7] and Hamming distance [8], and quantum random walks [9], which could be directly applied to sequence search and sequence matching. Moreover, there is an extremely high-demand for efficient analysis in this field, making the need for more efficient algorithms urgent.

Drug Discovery and Design. Computer-aided drug design (CADD) is used in the drug discovery process to identify and develop a potential lead. This process is computationally challenging given the combinatorial nature of the problem and the extensive simulation timescales that may be necessary. Methods based on quantum simulation and optimization [10], QML [11, 12], and hybrid quantum-classical algorithms [13] are the most promising near-term approaches in this area. For example, the work proposed in [13] used a hybrid quantum-classical workflow combining classical docking and molecular dynamics with quantum machine learning to find ligands binding to proteins.

1.2.2 Cross-Cutting Supporting Research Topics - Current State of the Field and What is Needed

This section presents the roundtable's view on advancing quantum computing for biomedical applications summarizing the most crucial and relevant cross-cutting topics supporting this research endeavor.

Data Preprocessing, Encoding/Decoding, and Input/Output Data. Quantum data encoding methods to represent classical data in quantum states exist [14, 15, 16, 17, 18, 8] but their use in biomedical sciences is in early exploration stages. Data preprocessing and encoding for biomedical sciences require efficient and robust techniques to translate complex, high-dimensional data into quantum states while preserving relevant information. Advances needed include efficient encoding schemes that reduce qubit usage, gate complexity, and circuit depth. Additional considerations include the use of not only classical input but also quantum input, which would be quantum data directly obtained from quantum sensors. Despite the "Big Data" aspect, some problems involve small data sets, posing unique challenges like limited statistical power, data quality, and a low signal to noise ratio, which often leads to greater uncertainty.

Quantum Algorithms. *Quantum optimization* algorithms have the potential for solving problems more efficiently than their classical counterparts. These include, e.g., Quantum Approximate Optimization Algorithms (QAOA) [19], optimization algorithms based on Grover's search [20], quantum data fitting, quantum semidefinite programming, quantum annealing [20], and adiabatic quantum computing [21]. Initial research could focus on tailoring existing algorithms to address specific biomedical challenges, developing noise-resilient algorithms, and exploring hybrid approaches. *QML* leverages the unique capabilities of quantum computing to develop and enhance machine learning algorithms to provide speedups and novel approaches to data analysis problems. There are already well-established QML algorithms such as quantum support vector machine (QSVM) [22], variational quantum classifier (QVC) [23], quantum (convolutional) neural networks (Q(C)NNs) [24], and quantum transfer learning [25]. Also, some existing applications to biomedical sciences have been explored for breast cancer detection [26, 27], molecular docking process [28], and medical imaging [29]. However, much more progress is needed to unveil the potential of QML for biomedical applications. Potential initial steps include adapting QML algorithms to accommodate specific characteristics of biomedical data, novel ways for data preprocessing and feature extraction, feature learning, and geometric quantum machine learning [30]. Finally, *mathematical foundations* are essential to the development of quantum algorithms, e.g., efficient quantum techniques for performing linear algebraic operations, such as matrix inversion, eigendecomposition, and singular value decomposition. Block encodings [31, 32], for example, serve as a crucial tool for representing and manipulating matrices in quantum algorithms. These types of techniques form the basis for many quantum algorithms, including QML and optimization. The applicability of these techniques to biomedical sciences lies in the potential to enable more efficient processing of large-scale data, often encountered in genomics, medical imaging, and drug discovery. Potential research directions could include adapting quantum-numerical linear algebra techniques [33, 34, 35] and block encodings to accommodate the specific characteristics, structure, and volume of biomedical data, for example.

Addressing noise. Quantum computing and quantum algorithms can be affected by various sources of errors and inaccuracies which can corrupt quantum states and operations. Such errors influence the reliability and performance of quantum computations, which are crucial for data-sensitive applications. Consequently, a specific area of research in QIS focuses on developing error mitigation techniques and noise-resilient quantum algorithms to tackle the impact of noise. Particularly for near-term applications, dealing with noise associated with noisy intermediate-scale quantum (NISQ) devices is a pressing need. The development of specific error mitigation techniques, noise-robust algorithms, and noise learning techniques are examples of potential first steps in this area. Also, studying the relationship between inductive bias and quantum error may play a key role, i.e., the choice of inductive bias can impact the resilience of the quantum algorithm to noise and error, potentially affecting the algorithm's performance and its ability to generalize well.

Privacy preserving. Given challenges in data sharing and computation on protected or proprietary data, there is tremendous interest in privacy-preserving quantum machine learning. Proof-of-principle demonstrations were discussed which could ensure confidentiality and accurate learning on NISQ technology. These involve hybrid quantum-classical models trained to preserve privacy using differentially private optimization algorithms that can curtail information leakage from training data, with improved model accuracy and faster convergence [36]. These efforts are key for providing the groundwork for secure QML infrastructure and support distributed QML training which can better utilize available NISQ devices [37]. More recent work has combined quantum Federated Learning (QFL) and Quantum Differential Privacy (QDP) to achieve comprehensive protection against both data leakage (QFL) and model inversion attacks (QDP) [38] .

Quantum hardware, simulators, software packages. Existing NISQ devices have a limited amount of qubits and high error rates, restricting their ability to perform large-scale computations. Alongside NISQ devices, quantum simulation tools have been developed to design, test, and optimize quantum algorithms on classical computers, offering insights into quantum computing capabilities and potential applications. There is an enormous potential for the combined use of NISQ devices, simulators executed in supercomputers, and software packages to make impactful progress in quantum for biomedical data processing. However, specific advancements are needed including expanding the range of available quantum software packages focused on this scientific field and the development of benchmarks. Given the rapid advancement in quantum hardware technology, initial proof-of-concept algorithms have the potential to scale rapidly to solve large-scale problems in the future.

Workforce development, accessibility, ethics, and governance. Much of the focus to date in quantum-related training and workforce development has been on QIS, such as DOE efforts and others. However, there are distinct skills and training considerations for applied quantum biological data science. These include interdisciplinary training, emphasis on team science and critical evaluation of application of quantum approaches in the context of the biological domain. Access will also be critical to facilitate uptake of these approaches and application to relevant data science problems both with respect to access to technology (e.g., cloud, simulators) and cognitive accessibility (e.g., user-friendly software and toolkits that are integrated into domain specific workflows). The Roundtable also discussed the disruptive potential of quantum if existing information technology, data, and governance capabilities are not expanded upon. In fact, ethics and governance issues around Artificial Intelligence (AI) will be naturally carried out to quantum-based algorithms.

1.2.3 Examples of Promising Research Areas

The topics and themes presented above and discussed during the Roundtable may result in several key research directions related to quantum for biomedical data analysis. The table below presents a few illustrative examples of research areas that aim to inspire new collaborations to advance the state of the field and foster a deeper understanding of the potential applications and limitations of quantum computing in biomedical research.

Category	Research Area	Description
Medical Imaging and Diagnostics	Quantum-enhanced medical imaging analysis	Developing novel quantum algorithms to improve denoising, segmentation, and registration of MRI and CT scans
Biological Sequence Data Analysis	Quantum algorithms for genome analysis	Designing quantum algorithms to accelerate genomic data analysis at scale, allowing population level characterization and efficient meta-analysis
Drug Discovery and Design	Quantum simulation for drug discovery	Leveraging quantum devices and simulators to perform quantum molecular simulations for drug discovery and protein folding prediction
Data Preprocessing, Encoding, and Input Data	Quantum data encoding for biomedical applications	Investigating efficient quantum data encodings and preprocessing techniques for complex biomedical data types
Quantum Machine Learning	Quantum machine learning for precision medicine	Developing quantum machine learning algorithms to guide therapeutic selection and patient stratification for precision medicine and diagnostics
Privacy Preserving	Privacy-preserving quantum algorithms	Developing privacy-preserving quantum algorithms to protect sensitive biomedical data during processing and analysis
Accessibility & Workforce Development	Quantum education for biomedical scientists	Developing educational resources, training programs, and multidisciplinary collaborations to build a quantum-ready workforce in in the biomedical field and develop accessible, integrated quantum workflows

1.2.4 List of Roundtable Participants

Roel Van Beeumen (LBNL)
E. Wes Bethel (SFSU)
Marco Cerezo (LANL)
Benjamin Cordier (OHSU)
Fida Dankar (NYU)
Prashant Emani (Yale)
Mark Gerstein (Yale)
Kathleen Hamilton (ORNL)
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Jeffrey Larson (ANL)
Carlos O. Marrero (PNNL)
Murphy Niu (University of Maryland)
Antonio G. Peña (UCSD)
Carlo Pierpaoli (NIH)
Gregory Quiroz (JHU)
Gaoyuan Wang (Yale)
Shinjae Yoo (BNL)

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Shannon McWeeney (OHSU)
Talita Perciano (LBNL)

2. Introduction

2.1 The Role of Quantum Computing in Biomedical Computational and Data Sciences

Biomedical data science integrates principles and techniques from computer science, statistics, mathematics, biology and medicine to extract meaningful insights and knowledge in order to advance our understanding of diseases, developing new treatments, and improving healthcare delivery. It facilitates evidence-based medicine, precision medicine, and the integration of data-driven approaches into healthcare systems, ultimately leading to better patient care and outcomes. Computing is an indispensable component of biomedical data science needed to process, analyze, and interpret increasingly larger and more heterogenous datasets, enabling data-driven insights and accelerating research. However, classical computing is facing increasing challenges with regard to scale and complexity. Quantum computing provides a cutting-edge computational paradigm that leverages the principles of quantum mechanics and could hold significant promise for biomedical data science by addressing these issues.

2.2 DOE and NIH Collaboration: Aims and Scope

Despite the recent advances in quantum computing and its applications in many scientific fields, the intersection of quantum computing, and biomedical research remains a less explored research area. The development of quantum competencies, experience with utilizing prototype quantum computing systems, and the identification of relevant quantum applications and algorithms in the biomedical sciences are realistic near-term goals that will better position and benefit the biomedical research community in quantum computing capabilities. Both NIH and DOE are interested in exploiting the DOE community's capabilities and expertise in quantum computing to advance biomedical research and support the NIH objectives, which include, for example, fundamental studies of biological and molecular structures; improving understanding of human health as well as mental and physical disorders and diseases; and deriving insights from clinical data and healthcare. In addition to the NIH's mission in biomedical and behavioral research, NIH's interests in quantum computing are also guided by the NIH Strategic Plan for Data Science with strategic priorities in, for example, metadata for FAIR data reuse and data interoperability; privacy and integrity for controlled access data; and computational and storage efficiency. This roundtable was assembled to consider the opportunities and challenges in the near-, medium-, and long-term at the intersection of quantum computing, data science, and biomedical research and how these could be addressed through multi-disciplinary partnerships. DOE's Office of Science supports a diverse portfolio of quantum information science (QIS) research, and the DOE community has built up a unique suite of capabilities and expertise in this area. Office of Science's Advanced Scientific Computing Research (ASCR) program invests in a QIS portfolio focused on quantum computing and communications research including quantum algorithms, mathematical methods, and quantum computer science

2.3 Roundtable Participants and Structure

Two co-chairs were selected by NIH (ODSS) and DOE (ASCR) respectively and worked closely with them to recruit roundtable participants and develop the roundtable agenda. All participants were provide pre-work with regard to key questions to consider.

- What are some of the most pressing challenges in biomedical data science computationally?
- What are the most promising application areas that we should focus on initially?
- What are the key opportunities and challenges on the development of quantum algorithms associated with the identified application areas?
- What would be the main priority basic research topics in quantum algorithms?
- What would be needed for a successful NIH-DOE collaboration to have real engagement on both sides?
- Identify in terms of biomedical use-cases or classes of applications that can only be addressed via interdisciplinary teams of biomedical and QIS experts
- What biomedical communities/groups are best brought together with quantum computing experts?

- What potential benefits and research goals may be expected for the biomedical and computational science communities?
- What part of a biomedical researcher's workflow could quantum computing best facilitate?

A pre-roundtable discussion was then held to review scope, provide background, and focus on identification of the relevant biomedical applications/use-cases (including their potential "parallelism" and "quantum-ism") as well as current bottlenecks in data analysis workflow that could benefit from quantum (steps, operations, etc). The formal roundtable discussion comprised of short talks and discussions based on these use cases and pre-work.

2.3.1 Participants

Seventeen panelists along with the two co-chairs contributed to this report. Thy are:

Roel Van Beeumen PhD is a research scientist in the Computational Research Division at Lawrence Berkeley National Laboratory Lab. His research interests range from numerical linear algebra and numerical software to quantum computing and quantum algorithms.

E. Wes Bethel PhD is an Associate Professor in the Computer Science Department at San Francisco State University, and a Research Affiliate at Lawrence Berkeley National Laboratory. His technical interests include high performance scientific computing, scientific visualization and computer graphics, image analysis and computer vision, scientific machine learning, quantum computing, scientific data science, and their collective application to challenging scientific data understanding problems. ACM Distinguished Scientist

Marco Cerezo PhD is a staff scientist at Los Alamos National Laboratory. HIs research interests include Quantum Machine Learning, Quantum Information, Quantum Computing and Quantum Algorithms, for near-term quantum devices and for simulation o quantum systems.

Benjamin Cordier, PhD is a senior computational biologist at the OHSU Knight Cancer Institute. HIs research interests include quantum machine learning applications across biology and medicine, cancer genomics, novel approaches to democratize access to data and accelerate the creation of FAIR (Findable, Accessible, Interoperable, and Reusable) and ethically sourced data sets for AI/ML.

Fida Dankar PhD is a visiting Associate Professor of Computer Science at NYUAD. Her general research interests include Machine learning and data privacy. Currently, her research focuses on the development of multidisciplinary approaches for the private and secure mining of biomedical data (distributed and central) that draws upon methods from cryptography, statistics, machine learning, federated learning, and synthetic data generation.

Prashant Emani PhD is Associate Research Scientist at Yale University; His reach interests include human health genomics, bioinformatics and machine learning.

Mark Gerstein PhD is the Albert L Williams Professor of Biomedical Informatics and Professor of Molecular Biophysics & Biochemistry, of Computer Science, and of Statistics & Data Science at Yale University. His research is focused on biomedical data science, and he is particularly interested in machine learning, macromolecular simulation, human genome annotation & disease genomics, and genomic privacy.

Kathleen Hamilton PhD is a research staff member in the Quantum Computational Science Group at Oak Ridge National Laboratory. Her research is focused on developing algorithms for next-generation processors including: neuromorphic computing and adiabatic quantum annealing.

Mustafa Irfanoglu PhD is a staff scientist at the National Institutes of Health. His research interests are in the application of image processing, computer vision and machine learning techniques to medical imaging data, with focus on MRI.

Jeffrey Larson PhD is a computational mathematician at Argonne National Laboratory. His research centers on optimization algorithms and their application to challenging problems ranging over quantum computing/sensing, particle acclerator design/control, and vehicle platooning/routing.

Carlos Ortiz Marrero PhD is a data scientist at the U.S. Department of Energy's Pacific Northwest National Laboratory (PNNL) As the PI for the Computing Optimal States via Quantum Neural Networks project, he is working on problems related to Quantum Computing and Machine Learning for the Mathematics for Artificial Reasoning in Science (MARS) initiative. His project is focusing on the study and development of quantum algorithms for near-term hardware. The goal is to showcase how quantum neural networks provide an interpretable search space for domain-aware learning problems.

Shannon McWeeney PhD (co-chair) is a professor and vice chair and the Chief Data Officer for the OHSU Knight Cancer Institute. Her research is the intersection of computer science, biostatistics and genetics to develop computational approaches to solve research bottlenecks and novel ways to visualize and interpret information in order to identify clinically relevant signatures for patient stratification and treatment.

Murphy Niu PhD is an Assistant Professor of Computer science at the joint Center for Quantum Information and Computer Science (QuICS) at the University of Maryland. Her research is focused on intelligent quantum control optimization and metrology, quantum machine learning, quantum algorithm design and near-term quantum error correction.

Antonio G. Peña PhD is a computational biologist at UC San Diego. His research is focused on approaches to facilitate the meta-analysis of the largest microbiome studies to date.

Talita Perciano PhD (Co-chair) is a Research Scientist at Lawrence Berkeley National Laboratory. She conducts research in the areas of quantum algorithms, quantum image processing and machine learning, scientific machine learning, image analysis and high-performance computing motivated by the incredible challenges around scientific data generated by computational models, simulations, and experiments.

Carlo Pierpaoli MD, PhD is a Senior Investigator in the Laboratory on Quantitative Medical Imaging at NIH. His rsearch is aimed at extracting accurate and reproducible biomarkers from data acquired with non-invasive imaging techniques, primarily Magnetic Resonance Imaging.

Gregory Quiroz PhD is a staff scientist at the Johns Hopkins University Applied Physics Laboratory. His current research interests include quantum characterization and control, applications of quantum control to quantum algorithm design, and quantum sensing.

Gaoyuan Wang PhD is a bioinformaticist at Yale University. Her current research interests lie in understanding biological systems via large-scale datasets using interdisciplinary approaches. She primarily works on the development and application of tools that provide insights on biological data. She is also interested in the ethical implication of the rapidly growing field of health technology, in particular issues related to privacy.

Shinjae Yoo PhD is a computational scientist in the Computer Science and Math of Computational Science Initiative at Brookhaven National Laboratory. His research interests include quantum machine learning, scalable scientific machine learning, and foundation models.

3. Roundtable Perspective on Current State of Quantum Computing and Biomedical Research

3.1 Discussed Quantum Computing Technologies and Advancements

The theoretical promise of quantum computers is highly enticing, as they hold the potential to revolutionize computing by exploiting the laws of quantum mechanics. Unlike classical computers, quantum computers can use superposition, entanglement, and interference to perform certain computations exponentially faster. This is the reason why quantum computers are the only known form of computation expected to violate the strong Church-Turing thesis, which states that all computing devices are equivalent up to polynomial-factor overheads [39].

The violation of the strong Church-Turing thesis directly implies the possibility of quantum advantages. This has led to significant interest in the application of quantum computing methods to numerous problems in scientific computing. For instance, quantum algorithms have been developed to increase the computational efficiency of solving linear systems of equations, differential equations, optimization problems, and decomposing matrices [40, 41, 42, 43, 44, 45]. If quantum advantages can be established in practice, these methods have the potential to unlock new insights and possibilities that are not available through classical computing.

However, the full realization of quantum advantages in these methods remains an open challenge, as the development of practical quantum hardware is still in its early stages. Nevertheless, these routines underlie many problems across numerous applied science domains including biomedical research. Of course, to be most beneficial, such approaches must be tailored to integrate domain context and account for the specific issues arising when dealing with biomedical applications.

Existing NISQ hardware platforms are limited by two key constraints. First among them is coherence time, which measures the time duration that a device is able to maintain a coherent quantum state. In practice, this constraint is largely captured by device error rates, which can be decomposed into (input) state preparation and measurement (SPAM) error, gate error (both phase and bit-flip errors), and emergent device error (such as cross-talk between qubits and interactions between the qubits and their environment). Together, these errors limit the number of gates that can be executed by a quantum algorithm. The second constraint relates to the number of qubits (currently on the order of 200 to 400) and the connectivity map between them. These two characteristics of a NISQ device directly imply both i) representational constraints on the size of soluble problem instances and ii) qubit routing overheads [46] (e.g. when a quantum algorithm assumes all-to-all connectivity, practical implementations may require additional quantum gates or qubit shuttling to emulate full connectivity), respectively.

Recent advancements in quantum software and hardware have allowed for the development of methods to mitigate these key constraints. For example, methods to improve the signal-to-noise ratio of quantum circuit outputs, such as error mitigation [47, 48, 49] and postselection [50, 51], now being used to implement computations of increasing complexity. Similarly, methods to deconstruct the components of quantum simulation, optimization, and machine learning problems and map them to quantum circuits that can be executed in parallel [52, 53, 54, 55, 56] offer a path towards quantum computations beyond the scale of individual NISQ devices while retaining much of the potential for practical advantages. These examples represent a small sample of the many methods in development to expand the real-world capabilities of NISQ devices. Finally, while fully error corrected devices are still not available, early-stage demonstration of error protected qubits are becoming more common (e.g. see [57, 58, 59]). These observations also point at the possibility of utilizing hybrid devices composed of some error corrected qubit coupled to non-error corrected ones.

Given the limitations of current quantum hardware, it is important to think about how these would impact the performance of algorithms aimed at biomedical applications. Specifically, embedding high-resolution images into quantum states will likely require a large number of qubits, and perhaps prohibitively deep circuits. Developing algorithms aware of the limitations imposed by near-term devices will be crucial.

3.2 Discussed Existing Quantum Algorithms

A wide variety of quantum algorithms have been developed targeting a range of applications and scopes. Many foundational algorithms, such as Grover's algorithm [20], the quantum Fourier transform [60], and the quantum walk [61] realize quantum computational primitives; in these cases, unstructured search, mapping from the time to frequency domain, and graph sampling and property estimation, respectively. Similarly, generalizations of these algorithms have expanded the set of primitives that can be realized in a quantum computation. For example, amplitude amplification and estimation [62] provides a means of implementing more general quantum search algorithms and quantum counting. By implementing computational primitives, these quantum algorithms provide key operations that are relevant to larger quantum algorithms and subroutines. For example, Grover's algorithm is leveraged by many quantum algorithms targeting NP-hard optimization problems; the quantum Fourier transform and its inverse are exploited for matrix inversion (a key subroutine in many machine learning algorithms) and phase estimation for quantum simulation; quantum walks provide a means for computing graph properties such as st-connectivity and bipartiteness.

Other quantum algorithms provide larger subroutines for algorithms targeting specific application areas, such as machine learning, optimization, and quantum simulation. For machine learning and optimization, examples include variants of the quantum linear systems algorithm (QLSA) [44], quantum singular value decomposition (QSVD) [63], quantum backtracking [64], and a quantum dynamic programming method augmented by the amplitude amplification and estimation framework [65], among many others. Especially relevant to quantum simulation is phase estimation [66], which provides a key subroutine for estimating the energy of molecular ground states (among other quantities of quantum mechanical systems) via the estimation of the eigenvalues of Hamiltonian operators. For both quantum primitives and subroutines, the Quantum Algorithm Zoo provides an extensive catalog of quantum algorithms, their bounds, and their formal applications [67].

Recently, device constraints have inspired the development of a wide variety of heuristic approaches for optimization, machine learning, and quantum simulation with the requisite flexibility to accommodate NISQ hardware. Among these heuristic methods targeting optimization problems are the quantum approximate optimization algorithm (QAOA) [19] (and its generalization to the quantum alternating operator ansatz [68]) and quantum unconstrained binary optimization (QUBO) [69], the latter of which is principally deployed by quantum annealers to target NP-hard combinatorial optimization problems. Another class of methods, known as variational quantum algorithms (VQAs) [70] for their use of the variational principle [71], are commonly applied for machine learning and simulation tasks. Within quantum simulation, the variational quantum eigensolver (VQE) [72] has been used to target a wide variety of problems, including estimations of electronic ground state [73], molecular binding [74] and dissociation [75], and chemical reactions [76]. More generally, variational quantum machine learning algorithms, including a wide variety of quantum neural networks (QNNs) [77, 78, 79, 80, 81] and quantum kernel methods [82, 23], have been applied to a wide variety of supervised, unsupervised, generative, and reinforcement learning tasks. While substantial focus has been placed on quantum methods for supervised learning in the context of medical diagnostics, there is growing interest in the use of generative methods to explore the chemical space of small molecules [11], which may have relevance to drug discovery.

3.3 What are the applications that are amenable for the shift from Classical to Quantum?

Within the scope of biomedical research, practical quantum advantages represent the key motivation for shifting from classical to quantum methods. Past work has defined a quantum advantage as any quantum computation that improves upon the state-of-the-art classical computation given a specific evidence context [2]. Crucially, this definition requires the identification of i) a specific problem (or problem instance), ii) a quantum and classical algorithm pair, iii) a computational resource (e.g. time, space, information), iv) bounds on that resource, and v) the specific evidence context (i.e. theoretical, experimental, operational). By encouraging the identification of these constituent components, this framework facilitates reasoning around how quantum advantages may be applied to real-world use cases in biomedical research. For the biomedical research community, empirical (i.e. experimental and operational) advantages in time and information resources are of principal interest.

Broad application areas where empirical advantages may be realized over the near- to medium-term include quantum simulation and machine learning. For quantum simulation, specific advantages are expected to be experimental and relative to time resources (up to a superpolynomial advantage) and reductions in approximation error for physical and chemical quantities (e.g. molecular ground state energy, binding constants). Use cases where these advantages have the potential to translate into realized operational advantages include drug discovery (e.g. compound screening and lead optimization) [83, 84, 85] and precision medicine. For quantum machine learning, specific advantages are expected to be relative information resources (i.e. lower model generalization error and faster learning by fewer examples, which is relevant to small data contexts [2]) and may readily translate from experimental to operational advantages for certain use cases. While advantages in quantum simulation are supported by robust theoretical evidence the set of use cases is relatively narrow. In contrast, theoretical evidence supporting quantum machine learning advantages remains relatively limited, especially for classical data. Nonetheless, the methodological flexibility of quantum machine learning methods may offer a substantially broader potential scope of application.

Expanding the scope of quantum computing in biomedical research is expected to be contingent on interdisciplinary efforts to identify precise use cases (using the above framework) that are ripe for the development of experimental and operational advantages. While quantum simulation and quantum machine learning methods are expected to be productive areas of exploration, applications using quantum optimization methods merit exploration. Finally, given the early stage of quantum hardware development, it should be expected that identified use cases will continue to be highly sensitive to hardware capabilities for the foreseeable future. New devices may quickly realize new capabilities and, from a process perspective, this dynamism strongly implies that continuous evaluation identified use cases and the feasibility of hardware-specific proof of principles may foster the growth of interdisciplinary efforts.

3.4 Existing Collaborations and Projects in the Field

Various institutions and companies have been exploring the potential of quantum algorithms in analyzing biomedical data. These efforts generally aim to leverage the computational capabilities of quantum computers to address biomedical challenges, from drug discovery to genomics.

For example, some pharmaceutical companies, in collaboration with quantum computing companies, have begun investigating quantum algorithms for molecular modeling and drug discovery. This is due to the exponential complexity of simulating molecular interactions on classical computers. More specifically, AstraZeneca has reported exploring quantum computing to speed up structural chemistry to find "molecules that matter", given that a key element of drug discovery and development relies on establishing the chemical 3D-structure of potential new medicines [86]. More recently, the Alphabet spinoff SandboxAQ has signed up AstraZeneca as users of its drug discovery and development tools [87].

As another concrete example, IBM and the Cleveland Clinic have established a landmark partnership to advance healthcare research using AI, quantum computing, and cloud computing technology. As part of the 10-year partnership, IBM installed its first private sector, on-premises IBM Quantum System One in the United States, in Cleveland. This quantum system was designed to leverage quantum computing's potential in aiding with calculations related to drug discovery and other complex matters that classical computers struggle with [88]. The partnership also involves the establishment of the Discovery Accelerator, a joint Cleveland Clinic and IBM center designed to advance research into critical areas such as genomics, single-cell transcriptomics, population health, clinical applications, and chemical and drug discovery [89].

Not surprisingly, the few examples of existing projects and collaborations such as the ones described above are taking advantage of the most successful and feasible quantum approaches already being used in other scientific areas, such as quantum simulations and hybrid quantum-classical algorithms. Consequently, there is a great opportunity to leverage the combined expertise and research coming from both DOE and NIH to explore other ways to tackle biomedical data (classical and quantum input) problems.

4. Biomedical Use-Cases for Short-Term Quantum Applicability and Impact

4.1 Medical Imaging and Diagnostics

The field of medical imaging could greatly benefit from quantum algorithms as traditional methods for image analysis (e.g., segmentation), reconstruction (e.g., iterative methods), and registration (e.g, feature/intensity/distance- based methods) are computationally demanding, and the need for improved diagnostic accuracy is paramount. Quantum algorithms, including quantum Fourier transform [3], quantum phase estimation, quantum optimization methods [4], quantum machine learning (QML) [5], and quantum image processing techniques [6], can be adapted to enhance medical imaging applications. The demand for quicker, more accurate, and efficient diagnostics is high, and specific applications, such as image denoising and filtering applied to smaller scale classical and quantum input, may be feasible with near-term quantum hardware due to their modest qubit requirements, especially the initial study and development of proof-of-principle demonstrations that can also reduce noise to manageable levels.

Based on the discussions of the roundtable, we discuss the two main promising areas where the development of quantum algorithms may play an important role to overcome the high computational demand of some specific processing steps.

4.1.1 Basic Image Analysis Operations

Quantum Fourier Transform (QFT). QFT [60, 3] is a linear transformation on quantum bits and it is an essential component of many quantum algorithms. It is a quantum version of the classical discrete Fourier transform (DFT), which is used widely in image processing, especially for tasks like filtering, compression, and noise reduction. QFT could potentially offer exponential speedup in such operations [90, 91]. QFT and its variations [92] and also simular transforms such as the quantum wavelet transform [93, 94] could potentially help in the context of medical imaging and diagnostics in terms of:

- *Speed*: These transformations can theoretically be performed much faster on a quantum computer than their classical counterparts on a classical computer. This speedup could lead to quicker analysis and diagnostics, especially in scenarios where real-time or near-real-time image analysis is crucial, such as during surgery.
- *Efficiency*: The effective implementation of these transforms for image analysis could potentially enable the processing of large and complex images more efficiently. This can be particularly useful in application using high-resolution 3D images, like those produced by an MRI or CT scan.
- *Detail*: By processing images in the frequency domain, it may be possible to isolate and analyze fine details in images that would be challenging to detect in the spatial domain. This could lead to more accurate diagnoses.

Quantum Machine Learning (QML). QML algorithms and quantum classifiers can potentially be used to classify and recognize features in medical images. For example, just like their classical counterparts, QCNNs [24] are a type of quantum machine learning model that can be used for image analysis tasks, like feature extraction and pattern recognition, potentially providing quantum speedups. This could significantly improve the diagnostic process and potentially lead to earlier detection of diseases, for example. QSVMs, which are based on the optimized binary classifier support vector machine (SVM), can be highly efficient when implemented on a quantum computer [22, 95], enabling the possibility of their application to biomedical data classification, with great potential to help with tasks such as the classification and recognition of features in medical images.

Quantum Image Processing (QImP). QImP techniques [96, 97] encode image information into quantum states, allowing operations such as convolution and edge detection to be performed with quantum speedups. For instance, tasks such as image denoising [98], edge detection [99], image segmentation [100] could potentially benefit from these techniques. Moreover, QImP techniques can not only help to improve image quality and extract features, but can also facilitate efficient image storage and retrieval [101]. There is also an interesting interplay between QML and QImP techniques. In the context of biomedical research, QML could be used to analyze and interpret the output of a QImP algorithm. For example, a QML algorithm could be used to classify or detect features in images that have been processed using QImP techniques. Similarly, QML could be used to optimize the parameters of a QImP algorithm. Conversely, QImP could provide pre-processed, high-quality image that could enhance the performance of QML algorithms.

4.1.2 Optimization

Image Registration. Image registration is a process that aligns different sets of data into one coordinate system. In the biomedical field, it is a crucial step in many image analysis tasks, such as comparing patient scans over time or combining data from different imaging modalities. With quantum computing, the image registration process could potentially be accelerated, owing to the inherent parallelism and computational capabilities of quantum systems. This acceleration could be particularly impactful when working with large, high-resolution 3D images, which are commonplace in the biomedical domain.

Quantum optimization algorithms that could potentially be used for image registration include the Quantum Approximate Optimization Algorithm (QAOA) [19], Variational Quantum Eigensolver (VQE) [72], and Quantum Amplitude Estimation (QAE), or more specifically quantum amplitude amplification and estimation [62, 65]. The QAOA can be used for solving combinatorial optimization problems. In image registration, it could be used to find the transformation that best aligns two images, an optimization problem. However, this approach would require formulating the image registration problem in a way that is compatible with QAOA. VQE is a hybrid quantum-classical algorithm used to find the ground state of a quantum mechanical system. It uses a parameterized quantum circuit, the parameters of which are optimized using a classical optimizer to find the lowest eigenvalue (the ground state energy) of a given Hamiltonian. This process of variational optimization could be adapted to tackle image registration problems. QAE is used to estimate the probability of an outcome in a quantum mechanical system, which can be related to the objective function in an optimization problem. While not an optimization algorithm itself, it could form part of a quantum-based image registration process, estimating the probability of a correct alignment.

Other quantum algorithms could potentially be adapted of developed for image registration including QFT, quantum phase estimation (QPE) [66], and QML (using QSVM and quantum principal component analysis (QPCA) [102] to extract features and make the registration process more efficient and robust to variations in the images).

Image Reconstruction. Quantum computers hold potential for advancing image reconstruction methods, which are crucial when dealing with different medical imaging modalities such as CT and MRI. The primary challenge in image reconstruction is to recover an original image from degraded or incomplete data. Quantum algorithms could offer speed-ups and enhanced capabilities for such tasks. Quantum algorithms mentioned before, QAOA and VQE, could also be used in this context. In image reconstruction, where the task can be cast as the optimization problem of finding the most likely image given the observed data, QAOA might be applied. VQE, although used for finding the ground state of a quantum system, can also be adapted for image reconstruction tasks, where the goal would be to minimize the difference between the reconstructed image and the observed data.

It is important to note that this use-case is rapidly evolving with the advance of quantum sensors, as described in [103], given that better reconstruction is expected because of the higher sensitivity compared to classical sensors. Moreover, in this case, quantum algorithms would be applied directly to the quantum data coming from these sensors, which would avoid the data encoding step (see Section 5.1).

4.2 Biological Sequence Data

Biological sequence analysis involves the characterization and interpretation of sequences of biological molecules, particularly DNA, RNA, and protein sequences to understand their structure, function, and evolution. This encompasses sequence alignment, variant/mutation detection, sequence queries, phylogenetic analysis, functional inference and annotation, structural prediction, motif finding, comparative genomics and metagnomics among others. Given the wide scope of potential applications [104, 2, 105], biological sequencing data offers a large sandbox for the development of novel quantum algorithms and quantum computing methods over the near term that may provide greater computational efficiency.

Multiple examples of novel quantum algorithms inspired by biological sequencing data already exist. For example, with regard to biological sequence alignment and pattern matching, modifications of Grover's algorithm have been able to address the problem of repeated sequences [106]. Further extensions of Grover's search algorithm allowed approximate matches needed for read errors in genomics, and a distributed search for multiple solutions over the quantum encoding of DNA sequences gave a quadratic speedup over the classical algorithm [107]. With respect to phylogenetics, quantum simulation of phylogenetic inference and evolution [108] has been developed leveraging quantum walks [109]. In metagenomics, de novo genome assembly is complicated by the variable abundance of species within the sample and modularity optimization in community detection is an NP-hard problem. The application of quantum annealing to de novo genome assembly [110] as well as assessment of empirical run-time of quantum algorithms for community detection [111] provide potential avenues to address these challenges in metagenomics.

4.3 Drug Discovery and Design

Drug discovery and design was seen as a compelling use case for quantum computing due to its potential to significantly accelerate the drug discovery process and address current complex computational challenges. Drug discovery involves modeling and simulating complex molecular interactions between potential drug candidates and target proteins. These simulations require extensive computational resources, making them an ideal candidate for quantum acceleration. Quantum computers could also provide exponential speedup for key drug discovery tasks, such as molecular dynamics simulations, conformational searching, and quantum chemistry calculations, leading to faster identification of drug candidates

Hybrid quantum-classical workflows hold tremendous near-term promise. One example discussed paired classical docking and molecular dynamics with quantum machine learning for finding ligands binding to proteins (accounting for the presence of mutations [13]. A critical step was the identification of the components of the workflow amenable for quantum approaches (in this example, the mutation-impact predictor). The classical machine-learning was mapped to quantum using a neural network constructed from qubit-rotation gates and in both simulation and physical application showed promise compared with classical approaches.

A key challenge in the drug discovery process is that only a small fraction of drug-like molecules are therapeutically relevant [112, 113]. A critical step is hit identification, which involves the identification of small molecules with adequate activity for a specific target that could then be used as a starting point for optimization. Identifying new molecules with a specific desired biological activity, while already challenging is even more difficult when no information about the target is known (e.g, novel target families, orphan targets etc). Molecular de novo design and compound optimization have been aided by artificial intelligence and generative models. Quantum GANs (QuGANs) can improve performance compared with classical GANs through more efficient search in exponentially large chemical space. Scalable quantum generative autoencoder (SQ-VAE) can support simultaneously reconstructing and sampling drug molecules. Comparison with classical counterparts have shown high-dimension molecules generated from quantum generative autoencoders have better drug properties within the same learning period [11].

5. Discussed Cross-Cutting Supporting Research Topics

5.1 Data Preprocessing, Encoding/Decoding, and Input/Output Data

Using quantum computers to process and learn from classical data naturally requires as a first step mapping the classical data (e.g., a medical image) to a quantum state. This encoding step is crucial to guaranteeing the success of the quantum algorithm aimed at processing the classical information. Several methods exist to embed classical data into quantum states such as basis encoding, angle encoding, amplitude encoding, block encoding, and IQP encoding among others [23, 114]. Recently, an efficient method (QPIXL) for encoding classical data has been developed tailored to NISQ devices and capable of encoding different types of data [18]. More interestingly, extensions of QPIXL were developed later and used to develop proof-of-concept analysis algorithms to process images, time-series, and DNA sequences on real NISQ hardware [8]. Due to the limitation of NISQ quantum computers there is usually an intrinsic mismatch between the size of the classical data (i.e., the number of pixels in a image) and the available quantum resources (i.e., encode every pixel value in qubit-qubit interactions). This leads to the requirement of data downsampling methods, where the dimensionality of the classical data is reduced via classical post-processing and only later embedded into a quantum state. Data reduction methods include principal component analysis (PCA), autoencoding, feature learning or feature extractions. While using these techniques can enable quantum computers to process large classical datum, there are several limitations that must be accounted for. On the one side there are data compression limitations one must consider. Similarly, the efficiency of the data reduction scheme must be accounted for in the computational paradigm. More importantly, if one is to understand what are the capabilities and limitations of using quantum computers to process classical data, the use of data reduction protocols raises an important question: What is the true role of the quantum device given that a classical computer has already done a significant and crucial portion of the analysis? From a theoretical perspective, it will be crucial to understand and answer these sorts of questions.

A different approach to using near-term quantum computers is to analyze the so-called quantum data. Quantum data refers to quantum states encoding some valuable information which are obtained by some quantum mechanical process. In the context of biomedical research one can think about using quantum mechanical systems, allowing them to interact with their environment, and learn something from the environment through this interaction. This sort of approach has been recently identified as one of the potential use-cases of near-term quantum technologies [115].

5.2 Quantum Optimization

Quantum optimization refers to the use of quantum algorithms and quantum computers to solve optimization problems. Optimization problems are pervasive in many fields and typically involve finding the best solution (maximum or minimum) from a set of feasible solutions based on a certain criteria. As mentioned in other sections of this report, quantum optimization methods can have an important impact when developing quantum algorithms for biomedical research. In this section, we briefly summarize some of the existing quantum optimization algorithms that can be used/adapted for the purposes of quantum biomedical applications.

Quantum Annealing (QA): QA is a quantum optimization technique inspired by the classical optimization method called simulated annealing. It is primarily used for solving complex combinatorial optimization problems. The classical simulated annealing is inspired by the annealing process in metallurgy, which involves heating a material and then allowing it to cool slowly to remove defects and finds a low-energy state. The algorithm similarly tries to find a minimum (or maximum) solution to a problem by exploring the solution space, starting with a high "temperature" (meaning solutions can widely vary) and gradually "cooling" to converge on an optimal or near-optimal solution. Instead of temperature, QA uses quantum effects, such as tunneling for example, to explore the solution space. Quantum tunneling allows the system to jump directly through energy barriers rather than climbing over them, potentially speeding up the search for an optimal solution. The goal of QA is to find the ground state (the lowest energy state) of a quantum system, which corresponds to the optimal solution of the optimization problem. QA requires specialized hardware, a well-defined problem (for efficient convergence), and is not typically executed on gate-based quantum computers. There is ongoing debate and research about how much speedup D-Wave's annealers provide over classical algorithms for various optimization problems. Nevertheless, QA has the potential to significantly impact biomedical research by addressing some well-known optimization problems including protein folding, drug discovery (identify drug candidates), genomic data analysis (feature selection, clustering, etc), medical imaging (image reconstruction, segmentation, and registration), optimizing treatment plans, and epidemiological models.

Quantum Approximate Optimization Algorithm (QAOA): QAOA is a heuristic quantum algorithm developed for tackling combinatorial optimization problems, and it is one of the promising techniques in the noisy intermediate-scale quantum (NISQ) era. This hybrid quantum-classical algorithm is a type of variational quantum algorithm, i.e., it iteratively refines a quantum state by adjusting a set of parameters to minimize the expectation value of a Hamiltonian (representation of the problem in question). Compared with QA, both QAOA and QA aim to find low-energy states of problem Hamiltonians, but they approach this task differently. QA relies on the physical process of annealing while QAOA uses a more algorithmic, gate-based approach. Relevant to the NISQ era, QAOA that work with shorter, shallower circuits are of particular interest. QAOA can be applied to the same optimization problems mentioned before for QA, however the way they would be implemented and their suitability for specific problems within the domains mentioned might differ. QAOA can be specifically interesting for problems including combinatorial design of therapies, parameter tuning in bioinformatics tools, dynamic systems optimization, optimal experimental design, network analysis, and pathway analysis in genomics. It is worth mentioning also the Quantum Alternating Operator Ansatz, which is an extension of QAOA that generalizes the QAOA algorithms to address broader optimization problems.

Grover's Algorithm: While not strictly an optimization algorithm, Grover's provides a quadratic speedup for unstructured search problems and it can be adapted for certain optimization tasks. Specifically for biomedical research, Grover's can be relevant for searching problems in a binary solution space, cost function evaluation, amplifying promising solutions, combinatorial optimization, quantum-enhanced metaheuristics, and hybrid approaches.

Variational Quantum Eigensolver (VQE): VQE is an heuristic quantum-classical algorithm that was primarily designed to determine the ground state energy of a given molecular Hamiltonian. It aims to approximate the ground state energy of a quantum system, particularly molecules in the realm of quantum chemistry. VQE can certainly be adapted and applied to various problems in biomedical data analysis including drug discovery and design, molecular dynamics simulations, optimization problems in genomics, structural biology, and pattern recognition in biomedical imaging.

Quantum Random Walks (QRW): QRWs are the quantum analog of classical quantum random walks. Instead of a definite path determined by random events (like coin tosses in classical random walks), QRWs use quantum superposition and interference, allowing for simultaneous exploration of multiple paths. This leads to distinctively different behaviors compared to classical walks, with potential applications in quantum algorithms and information processing. In biomedical data analysis, QRWs have the potential to be applied to problems such as drug discovery, genomic data analysis, protein folding, medical imaging, and epidemiological models.

5.3 Machine Learning and Neural Networks in Biomedical Research

In the near-term, one of the most promising methods for analyzing data embedded in quantum states is through Quantum Machine Learning (QML). QML attempts to leverage quantum computers by adapting a hybrid computational approach where quantum computers are used to estimate (classically hard) quantities, while the power of classical optimizers is leveraged to train the QML model parameters. By pushing some of the computational complexity onto classical devices, QML aims to reduce the requirements on the quantum hardware, making it more amenable for present-day technologies.

By utilizing the Hilbert space of quantum states as a quantum-enhanced feature space [23, 82] QML is able to generalize many classical machine learning methods to the quantum realm. For instance, quantum computers can be used to estimate similarity measures between quantum states, and thus construct a kernel which can be used in kernel-based techniques such as support vector machines (SVM) [23]. Similarly, quantum versions of several quantum neural networks (QNNS) have been proposed and developed [77, 78, 79, 80, 81]. At their core, a quantum and a classical neural network perform a similar role. They take input data, which is processed through a series of layers, and finally mapped to some output space. Despite this similarity, their modus operandi are drastically different. Classical neural networks rely greatly on non-linearities and the ability to copy classical data. On the other hand, quantum learning models are constrained by the no-cloning theorem [116] and quantum neural networks are usually instantiated via parametrized quantum circuits meaning that they can only act linearly, and unitarily, on the input data. As such, non-linearities in QML are usually implemented at the data-embedding level, through data re-uploading schemes [114], or by accessing multiple copies of the input data states [117, 118].

A crucial aspect to note is that while deep learning has gained significant attention in classical machine learning, its quantum counterpart has several limitations that must be accounted for. For instance, the absence of backpropagation methods for QNNs makes gradient-based training of quantum models computationally expensive, as every single gradient entry must be individually computed. Moreover, deep quantum circuits are prone to exhibit barren plateaus (i.e., vanishing gradients) [119, 120] or large amounts of local minima in their parameter training landscape [121]. Despite such limitations QNNs have shown promise to outperform their classical counterparts [79], and more work is needed to understand their capabilities in domain specific applications such as biomedical research. Specifically, it has been recently shown that by creating QNNs with sharp inductive biases one can mitigate issues and lead to efficiently trainable models [80].

5.4 Foundational Mathematical Concepts

Several foundational mathematical concepts underpin the development of new quantum algorithms for biomedical data analysis. Here are some of them:

- Linear Algebra: Quantum states are described using vectors, and quantum operations are represented by matrices. So understanding vector spaces, matrix operations, eigenvalues, and eigenvectors is crucial. Linear algebra is the mathematical language of quantum mechanics and quantum computing.

- Probability Theory: Quantum mechanics is inherently probabilistic. When we measure a quantum state, we get one of several possible outcomes, each with a different probability. Understanding the theory of probability is necessary to make sense of this.

- Fourier Analysis: Quantum computing uses Fourier analysis in many algorithms, like Shor's algorithm or the Quantum Fourier Transform. Understanding the basics of Fourier series and the Fourier transform is critical.

- Differential Equations: Quantum systems evolve according to the Schrödinger equation, which is a differential equation. Having a solid grasp of how to solve and analyze such equations is beneficial.

- Graph Theory: Some quantum algorithms, like the quantum walk, are based on graph theory. Moreover, many problems in biomedical data analysis, such as understanding genetic networks or the structure of chemical compounds, can be framed as problems in graph theory.

- Group Theory: Quantum computing uses group theory, especially in algorithms for solving the hidden subgroup problem. This is an important mathematical concept in the field.

- Sampling: Sampling, the process of extracting classical information from quantum states, is crucial in quantum computing. Used in algorithms like Shor's and QFT, it leverages quantum superposition to generate probabilistic results. In biomedical applications, it can aid in generating complex models, simulating random processes, and solving optimization problems.

These mathematical tools, among others, form the building blocks for developing and understanding quantum algorithms for biomedical data analysis. They provide the language and framework needed to describe and manipulate quantum states, design quantum circuits, and analyze their behavior. Table 5.1 shows the intersection between these foundational mathematical concepts and the quantum algorithms and applications discussed in this report.

5.5 Addressing Noise

When it comes to the development of machine learning algorithms, considering noise associated with the data is an important part of the process in a number of ways. *Sample noise* can help to improve the robustness of models by making them less sensitive to small changes in the data. *Intentionally added noise* can be used to regularize models and prevent overfitting. *Unwanted noise* can be mitigated through techniques such as data cleaning and feature selection.

Sample noise refers to random or inherent variability in the data, which can significantly impact the performance of algorithms. It often leads to reduced model accuracy due to overfitting, where the model learns noise as if it were a significant part of the data, resulting in poor generalization to new data. Sample noise, although often challenging, can be beneficial by promoting model robustness and preventing overfitting. It encourages models to focus on significant

Mathematical Concept	**Quantum Algorithms**	**Potential Applications**
Linear algebra	Quantum Phase Estimation (QPE), Quantum Fourier Transform (QFT), HHL Algorithm, Quantum Singular Value Decomposition (QSVD), Shor's Algorithm, Variational Quantum Eigensolver (QVE), Swap Test, Amplitude Amplification	Medical Imaging, Molecular Dynamics, Pattern Recognition, Protein Folding, Drug Design, Phylogenetic Trees
Probability Theory	Grover's Algorithm, Quantum Phase Estimation (QPE), Quantum Counting, Amplitude Estimation, HHL Algorithm, Quantum Random Walks, Quantum Machine Learning, Swap Test	Drug Interactions, Drug Discovery, Molecular Dynamics, Protein Folding, Pattern Recognition, Disease Classification, Drug Target Identification
Fourier Analysis	Quantum Fourier Transform (QFT), Shor's Algorithm, Quantum Phase Estimation, HHL Algorithm, Simon's Algorithm, Quantum Walks in the Fourier Basis	Medical Imaging, Genomic Data Analysis, Protein Structure Estimation, Drug Interactions, Linear Systems in Biomedical Modeling, Biomarker Discovery, Biological Systems Modeling
Differential Equations	Quantum Simulation Algorithms, HHL Algorithm, Quantum Machine Learning, Adiabatic Quantum Computing and Quantum Annealing	Epidemiological/Neurological/Cardiovascular Modeling, Protein Folding, Genomic Data Analysis, Image Analysis, Predictive Modeling, Systems Biology
Graph Theory	Quantum Walks on Graphs, Quantum Search on Structured Data, Quantum Algorithms for Graph Problems, Quantum Approximation Algorithms, Adiabatic Quantum Computing and Quantum Annealing, Quantum Error-Correction, Graph States, Quantum Algorithms for Shortest Path and Related Problems	Genetic Linkage Maps, Protein-Protein Interaction Networks, Disease Modeling, Brain Connectivity Networks, Medical Imaging, Metagenomic Data Analysis, Protein Structure Prediction
Group Theory	Shor's Algorithms, Simon's Algorithm, Quantum Phase Estimation (QPE), Hidden Subgroup Problem (HSP), Quantum Algorithms for Non-Abelian Hidden Subgroup Problems, Jones Polynomial and Topological Quantum Computation, Quantum Walks on Cayley Graphs, Solovay-Kitaev Algorithm	Protein Folding, Molecular Symmetry Analysis, Genomic Data Analysis, Medical Imaging, Drug Interaction and Design, Phylogenetic Trees
Sampling	Quantum Fourier Transform (QFT), Quantum Amplitude Estimation (QAE), Quantum Approximate Counting, Boson Sampling, Random Circuit Sampling, HHL Algorithm, Variational Quantum Eigensolver (VQE), Quantum Random Walks	Drug Discovery, Genomic Data Analysis, Adaptive Trial Design, Disease Spread Sampling, Proteome Sampling, Statistical Model Sampling, Evolutionary Pathway Sampling, Behavioral Pattern Sampling, Medical Imaging

Table 5.1

patterns rather than minor fluctuations, enhancing their generalization to real-world data. Training on noisy data also helps in simulating practical scenarios and can lead to more sophisticated feature selection and realistic model validation.

To prevent overfitting, which occurs when a model learns the training data too well and does not generalize well to new data, intentionally added noise forces the model to learn the underlying signal instead of the noise. This can be done by adding Gaussian noise, salt and pepper noise, or other types of noise to the data.

Unwanted noise refers to any random, irrelevant, or extraneous information or disturbances that corrupt the signal or data. It is something that is not part of the intended signal or data and is usually considered detrimental. This type of noise can be caused by a number of things, such as sensor noise, measurement error, and random fluctuations. There are a number of techniques that can be used to mitigate unwanted noise, such as data cleaning and feature selection. Data cleaning is the process of removing or correcting errors in the data. Feature selection is the process of selecting the most relevant features for the model.

In summary, noise can be both a positive and negative factor in machine learning. It is important to understand the different types of noise and how they can affect machine learning models, which can highly impact the development of new quantum machine learning algorithms for biological problems. Specifically, considering these types of noises when encoding classical data becomes crucial.

In addition to noise associated to the data, the noise found in quantum systems is equally important. Fully understanding realistic noise in quantum computers can help with tailoring specific problems in machine learning for biological problems to the underlying noise inherent to quantum systems. More specifically, it would enable the development of more accurate and noise-resistant quantum algorithms, significantly enhancing the efficiency and reliability of machine learning models for complex biological data analysis. Such advancements could help advancing fields like genomics and personalized medicine by enabling more sophisticated data processing and handling of larger, more complex datasets with greater fidelity.

It is crucial to remember that realistic noise limits the simulable regime of quantum algorithms by reducing the coherence time and introducing errors, which constrain the duration, complexity, and accuracy of simulations. This limitation restricts the scalability of quantum algorithms, defining the current boundaries of feasible quantum computations (under 50 qubits) and the range of problems that can be effectively addressed. To support the development of quantum algorithms taking into account noise, several noise models can be simulated such as, for example, decoherence, dephasing, crosstalk, low frequency, among others.

Some quantum algorithms explicitly take advantage of the noisy nature of the underlying quantum hardware for the design of noise-robust algorithms or error mitigation methods [122]. But a similar attempt has yet to be made in the domain of machine learning and biological applications.

5.6 Privacy Preserving

Current challenges in biomedical data privacy. Modern biomedical databases are mostly massive and include complex data from multiple sources incorporating both phenotype and genotype (e.g., biobank data, EMRs, and general behavior data). These databases are continuously updated, may be retained for indefinite periods of time, and can serve in unlimited research endeavors. This modern context presents multiple challenges to the classical notions of "consent or de-identify": (i) Scholars have cast doubts on the ability of participants to exert control in complex big data scenarios (leading to a rise in non-informed forms of consent such as broad and opt out consents), additionally, (ii) the detailed participants' data available in these modern databases compounded by the rise in publicly available information (online) made it possible to re-identify what was thought to be properly de-identified data. As a result data curators are moving away from data sharing in favor of more restrictive and virtual data access. Current research directions in this area include:

1. An increasingly popular way to overcome the issues of data privacy and availability is to use fully synthetic data. The application of synthetic data to the biomedical domain is recent yet increasing in popularity. Synthetic data is still in the experimental stage and is often used to carry out preliminary research such as exploratory analyses as their utility is not well established. Current research is exploring new synthetic data generation mechanisms based in machine learning as well as quantifying the utility and privacy of such generators in real-life scenarios.

2. Another research direction is the use of federated learning, which allows multiple data curators to collectively

build high-quality machine learning models on their distributed data while keeping their raw data private. FL suffers from multiple shortcomings, they require intense communication between the data holders to achieve the final model, they rely on heavy cryptographic protocols (secure communication) to achieve results with good accuracy while maintaining privacy, and the accuracy of the resulting models is dependent on the original data distributions.

Quantum research directions. Privacy research can greatly benefit from the promise of quantum computing. Examples include: the exploration of more efficient secure communications, designing efficient encryptions that enable analysis on encrypted data and designing superior synthetic data generators:

1. Encryption is used to secure communications in federated learning models. It is preferred over other privacy preserving mechanisms as it does not distort intermediate parameter calculations. The impact of quantum machines on the efficiency of secure communications is something to anticipate, provided a quantum secure encryption is used.

2. Fully homomorphic encryption (FHE) is an ideal tool for the private analysis of sensitive data. It allows any analysis (any function) to be applied on encrypted data while providing the same encrypted results if the analysis were to be applied on plain data (imagine having experts analyze your genomic data without obtaining any information about the data or the results). Fully homomorphic encryption is not in use due to its high inefficiency in real life scenarios. Quantum computing could be explored to:

   (a) Study the impact of quantum machines on the efficiency and security of existing FHE's

   (b) Generate novel efficient FHEs

   (c) On the Synthetic data generation front, an interesting direction is to explore the use of quantum machine learning to design SDGs of higher efficiency and utility

5.7 Quantum Simulation and Real Quantum Hardware

Understanding where, and how, quantum technologies can be used to enhance biomedical computations will likely require large amounts of benchmarking and model testing. At a first stage, one can simulate the quantum algorithm via classical methods to understand what are its capabilities in an ideal setting. Techniques such as tensor networks, or sparse matrix calculations allow for the simulation of generic quantum computation for systems of up to 20 or 30 qubits in standard-sized machines (larger simulations are possible under certain assumptions). These simulations can be used to benchmark the algorithm's performance in a noiseless setting (i.e., no hardware noise, and no sampling noise), and thus study its performance without other sources of uncertainty. Here, it will be crucial to leverage these early simulations to study the scalability of the quantum algorithm. That is, in order to guarantee that the methods will perform well in realistic problems, one should perform analysis of the number of resources (e.g., number of training iterations) needed to achieve a given solution accuracy as a function of the problem size. Such study will guarantee that the quantum algorithm complexity will not scale prohibitively for large scale problems. At a second stage, noise should be included in these classical simulations. Since near-term quantum hardware is intrinsically noisy, algorithms aimed at NISQ computers should be studied with sampling and hardware noise. Including sampling noise in a simulation allows one to study the number of calls to a quantum computer needed to solve a given task. Crucially, by adding hardware noise one can understand the robustness of the algorithm, as well as the need to integrate error mitigation techniques along with the algorithm itself.

Once the aforementioned classical simulations have been performed, one can use quantum hardware to test in a real device the performance of the quantum algorithm. Given that different platforms exist –superconducting qubits, trapped ions, neutral atoms, photonics-based– the practitioner should identify what is the device that best suits its algorithm needs. Here there are several factors that come into play and that must be accounted for, such as the number of qubits, the gate error rates, and the qubit topology and connectivity. In all cases, the classical benchmarking of simulations will be crucial in estimating the performance of the algorithms, as well as its run cost (i.e., how many shots are needed, or how much quantum computer run-time is needed). While real quantum hardware implementations are the ultimate goal, current devices are still in development stages. Even if available devices are not suited for implementing a given algorithm, this does not preclude the possibility that their near-future versions will be. As such, a useful analysis that one can perform is: how good does the hardware need to be for the algorithm to succeed? This kind of study can be further used to co-design hardware amenable for a given task.

5.8 Workforce Development and Accessibility

The span of applications for quantum computing in biomedical data science will not be met by a single pedagogical approach nor a single workforce persona. There is a need for a variety of expertise and education levels to create a balanced technical workforce. In addition, the continually evolving innovations in the field pose additional challenges for standardized curriculum, requiring a continual learning mindset for those in this field.

To date, the focus of training and workforce development has been on Quantum Information Science (QIS). In 2021, a DOE Office of Science working group developed a plan to establish the knowledge base and competencies needed for developing a curriculum in QIS [123]. In the report, two communities were identified who should contribute to curriculum development for QIS: the "demand side" (industries supporting development and manufacturing of technologies based on QIS as well as government laboratories and universities conducting research and development in QIS) and the "supply side." (educational, degree granting institutions, as well as the National Science Foundation which directly supports educational research). While this is critical for quantum workforce development, additional skills and competencies need to be considered for applied quantum biological data science.

Key components of such training must include interdisciplinary training (both with respect to mentoring and pairing of trainees), hands-on training, emphasis on team science and critical thinking in order to appropriately evaluate applications of quantum approaches in the context of biology and medicine. Accessibility in terms of QIS is often focused on access to technology through the cloud and quantum simulators. While this is absolutely critical, in order for the uptake of quantum computing and algorithms in biological data science to be meaningful, there must also be a focus on cognitive accessibility. This requires to first understand the potential users of these approaches in biology and medicine and then focus on user experience and user interface design when developing software and toolkits. Software development is not enough - these approaches must be integrated into existing domain specific workflows (as well as developed for those use cases). Leveraging the expertise and existing work in both NIH and DOE could allow this to be accomplished in the near-term through joint training programs and curriculum development.

5.9 Ethics and Governance

It is clear that Quantum computing presents new ethical and governance issues that must be considered [124] . For example, encryption and security breakdowns could lead to unprecedented security breaches and privacy violations. Quantum sensors could enhance surveillance capabilities, raising ethical questions about privacy, and civil liberties. In addition, access to quantum computing hardware could enable certain groups and organizations, as well as nations to gain significant advantages in areas such as cryptography, optimization, and drug discovery leading to ethical concerns about power concentration, inequality and access to the technology [125] .

There are also ethical and governance aspects of quantum computing that are shared with fields such as AI/ML. These include bias and fairness, transparency and accountability, with a need for ethical governance structures to ensure responsible development and deployment. There is also an interplay between quantum computing and AI that must be considered. Quantum computing will enhance AI capabilities, making it essential to consider the ethics of AI within the context of quantum computing as well.

Preparing for the ethical and governance challenges of quantum computing requires a proactive and strategic approach. We are in a critical window to develop the ethical and governance frameworks and before the full potential of quantum is realized. While the ethical landscape is evolving as quantum technologies advance, there is much that can be learned from the ethical issues raised by the advent of AI/ML to ensure past mistakes are not repeated. Proactively development of comprehensive ethical frameworks must be undertaken to establish clear ethical principles and guidelines. Engagement with ethicists and interdisciplinary collaboration must be encouraged to integrate ethical considerations into quantum research and development processes. Robust governance structures must be established to oversee quantum computing research and development and establish mechanisms for sharing knowledge, technology, and insights while addressing security concerns. Transparency and inclusivity must be integral components of governance processes, involving diverse stakeholders, including academia, industry, nonprofits and government. Finally, there needs to be major investment in education and public awareness as well as promoting ethical literacy within organizations and institutions engaged in quantum research and application to encourage the responsible use of quantum computing.

Establishing a solid ethical foundation and robust governance structures early that guides the development and deployment of quantum computing technology is key. By proactively addressing ethical concerns, the benefits of quantum computing can be realized while minimizing risks and ensuring that the technology serves the broader interests of society

6. Conclusion

In conclusion, the intersection of quantum computing, data science, and biomedical research represents an exciting frontier with immense potential. The collaborative efforts between the Department of Energy (DOE) and the National Institutes of Health (NIH) hold the promise of transformative breakthroughs in the near-, medium-, and long-term. From addressing the computational challenges in medical imaging and diagnostics to advancing biological sequence analysis and streamlining drug discovery, quantum computing holds the hope to make a significant impact. Cross-cutting research topics such as data preprocessing, quantum algorithms, noise mitigation, privacy preservation, and quantum hardware development further underscore the potential of this collaboration. As we embark on these research directions, it is essential to focus on workforce development, accessibility, ethics, and governance to ensure responsible and equitable progress.

7. Addendum

During the review of this report, a proof-of-principle 48 qubit fault tolerant quantum computer (FTQC) was demonstrated with the potential to readily scale to as many as 1000 logical qubits over the near term [126]. This result gives significant reason for optimism over the near- to medium-term and implies that the challenges due to NISQ error rates and NISQ-only algorithmic paradigms (e.g. certain variants of QAOA) may be obviated in the coming years. For the timing, this work may prove critical to advancing the viability of quantum computing in the biomedical data sciences and guiding the development of near-term practical quantum advantages.

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