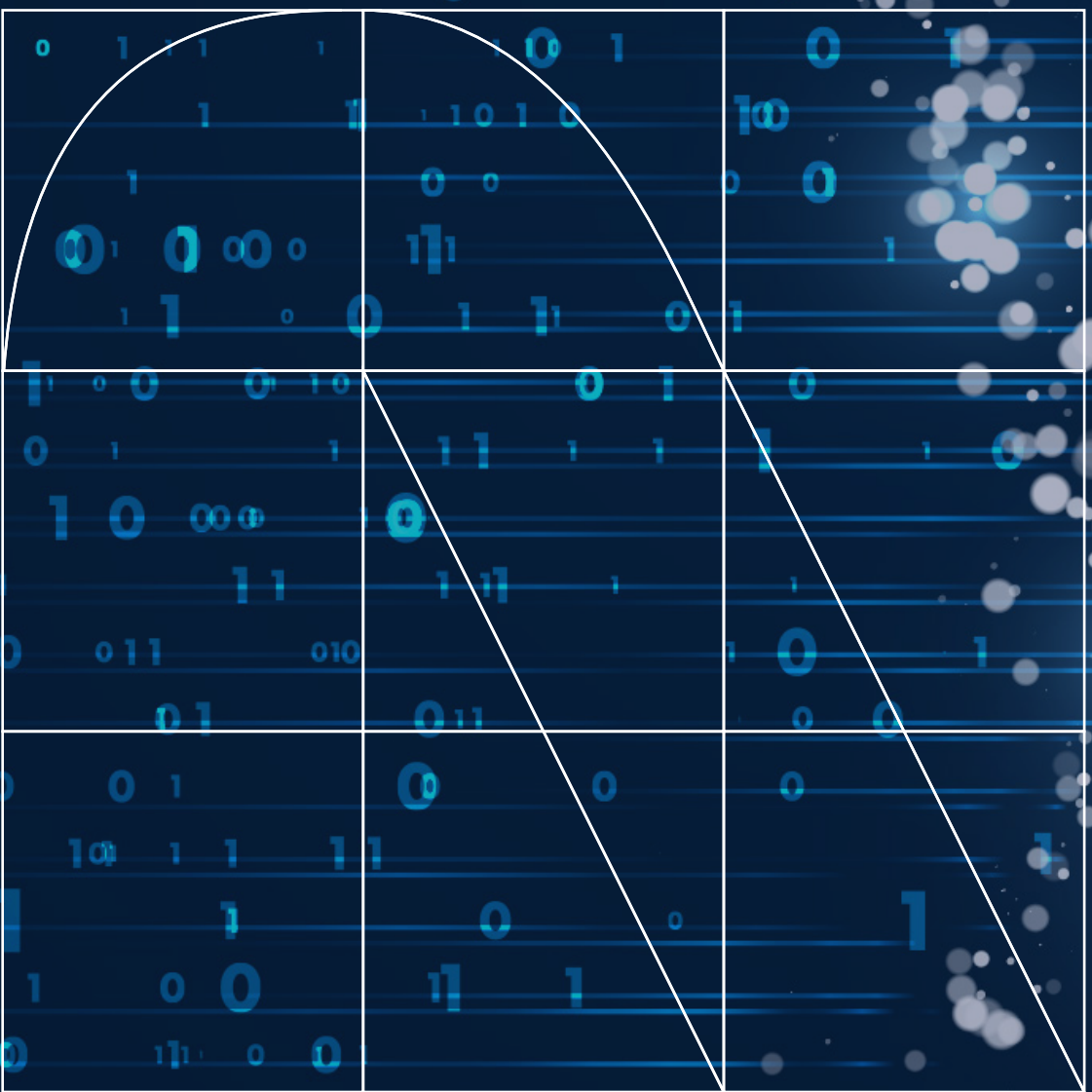
NTT DATA

OPTIMIZATION OF GENOME ASSEMBLY USING QUANTUM COMPUTING



JULY 2023

“Unleashing the power of Quantum Computing: innovative Genome Assembly project breaks down barriers in medical research and explores the potential of quantum technologies in the genetics field.”

Index

0 Executive summary.

Quantum computing, a burgeoning technology, holds immense promise in revolutionizing problem-solving across fields and industries. By leveraging the power of qubits, quantum computers can encode multiple values simultaneously, far surpassing the limitations of classical computing.

In the field of bioinformatics, quantum computing holds great promise. At NTT DATA, quantum technology has been applied to solve the problem of genome assembly. Genome assembly is a complex task in genomics, and quantum computing can provide more accurate and efficient methods for genome assembly. We have developed and implemented an algorithm to solve the genome assembly problem using graph theory and combinatorial optimization techniques. We have run this algorithm on a quantum computing simulator and an actual quantum computer device, and validated its performance compared with classical approaches in terms of speed, accuracy, and scalability on simulated synthetic data sets.

This white paper summarizes our results and discusses the potential, challenges, and limitations of quantum computing to solve problems like this, which rapidly scale beyond the capabilities of classical computing.

1 Introduction.

Quantum computing is a developing technology that promises to revolutionise the way we solve complex problems that are currently impossible to solve with classical computers. It has the potential to transform fields such as finance, cryptography, logistics and pharmaceuticals, among others. In this article we provide an overview of quantum technology, its development and its application specifically in the field of bioinformatics.

Quantum computing aims to solve computational problems using physical systems governed by the laws of quantum physics. Bits are replaced by quantum bits or qubits. Different types of qubits are currently being tested: superconducting, neutral atoms, trapped ions, photonics-based, and others. In all cases, the quantum properties of superposition, interference and entanglement emerge in them, which enables them to encode exponentially many more values, simultaneously, than their classical counterparts. Currently there are two main approaches to making quantum computers: gate-based and adiabatic.

Gate-based quantum computing [1], often called universal quantum computing, uses so-called quantum gates, arranged in sequence to form a quantum circuit, that is, an implementation of a quantum algorithm. These gates act on one or more qubits to perform operations, and are chosen to drive these qubits towards states that, when measured, provide the desired solution to a problem.

Adiabatic quantum computing [2] relies on a very specific type of quantum system, described by the so-called Ising model. Quantum annealers and other types of Ising machines are specially well suited for combinatorial optimization problems, where one is interested in finding the best solution (one that minimizes a problem-dependent cost function), but where the exponentially large number of possible solutions makes it simply impossible to evaluate exhaustively all of them. A set of interconnected qubits is initialized in a state, and then biases and couplings are gradually applied to encode the cost function of the problem. This hopefuly drives the qubits to a state that represents the desired solution. Often a solution that is not optimal, but otherwise good-enough, is found.

We are currently in the so-called noisy intermediate-scale quantum (NISQ) era, which means that although there are already a number of quantum computers

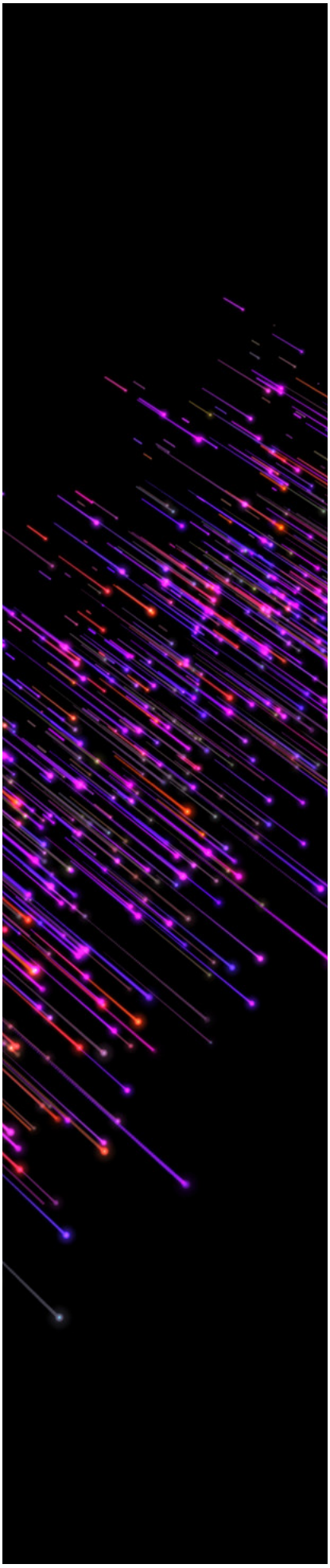
available, they are still very limited in the number of qubits (30–500 in gate-based, 500–5000 for quantum annealers) and in their connectivity (one qubit is connected to only a few other qubits), while also being noisy and prone to errors when measured.

Quantum computing is still in its early stages of development, and there are currently several limitations, in particular hardware limitations, as the technology for building quantum computers is still in the early stages of development, and the current qubit systems make many errors, requiring complex error-correction techniques to remain stable. Another issue is scalability: it is uncertain whether quantum computing can be scaled up to solve large-scale problems, as the number of qubits required for solving complex problems increases exponentially.

Despite the limitations of the technology, significant progress is being made in the development of quantum computers and quantum algorithms. It has unique features that make it a promising technology for solving complex problems. For example, quantum computers can perform many calculations simultaneously through the use of superposition and quantum entanglement, allowing them to explore multiple solutions at the same time. This allows quantum computers to perform certain types of computations with great computational power and much faster than classical computers. In addition, quantum computers can perform calculations that are impossible for classical computers, such as factoring large numbers.

At NTT DATA Health and Life Science industries, we have carried out a first approach to quantum technologies, by taking advantage of the unique and exclusive properties of quantum computers to solve the problem of genome assembly. The problem of genome assembly is a complex challenge in bioinformatics, involving the reconstruction of an organism's DNA sequence from fragments of genetic material. With the increasing availability of advanced sequencing technologies, there is a great demand for efficient and accurate methods for genome assembly.

In this whitepaper, we provide an overview of NTT DATA's quantum strategy. We then identify specific use cases where the adoption of quantum computing could involve and add value to the healthcare and life sciences industries. It follows a discussion on the proof of concept on the application of quantum computer to the genome assembly problem and the results, challenges, and limitations of quantum computing to solve problems like this, which rapidly scale beyond the capabilities of classical computing.



2 NTT DATA's quantum strategy.

The market for services in quantum optimization, quantum simulation and quantum machine learning in EMEAL is expected to reach $360m by 2029 [3]. The main drivers of growth are the expected ability to solve completely new types of problems, anticipation of reduced resource usage for solving currently challenging problem, limits in digital processor performance, and rising investment by governments. This growth is currently opposed by intense competition from established optimization software and algorithms, a gap in quantum hardware performance, and a lack of understanding of quantum solvers.

At NTT DATA we believe that Quantum Computing is a long-term endeavor. Our vision is to become a trusted Quantum System Integrator and support our customers by providing in-depth analysis of their business problems and identifying, implementing, and operating Quantum Computing and Quantum Inspired end-to-end solutions following an optimal solution strategy. To this end, our consulting strategy stands on the followings four pillars:

01 FIRST, FIND YOUR FIT

Quantum computing will not be for everyone. But if your business is in a data-intensive industry or a sector where simulations of complex and dynamic real world scenarios are relevant, we recommend that you start to engage with this advanced technology. A good first step is to launch an initiative to build an understanding of quantum algorithms and gain experience using the existing quantum (and quantum inspired) platforms and tools. Then again, if the transformative value of quantum computing is at least five to ten years away, why should we consider investing now?

02 STEEP LEARNING CURVE

First, this is a radical technology that presents daunting acceleration challenges. Both quantum programming and the quantum technology stack bear little resemblance to their classic counterparts (although the two work together closely). Early adopters achieving expertise, visibility into knowledge and technological gaps, and even intellectual property, will gain a structural advantage as quantum computing gains commercial traction.

03 EXPECT SUDDEN BREAKTHROUGHS

More importantly, progress towards maturity in quantum computing is not expected to follow a smooth, continuous curve. Rather, quantum computing is a candidate for a sharp turnaround that can come at any time. Companies that have invested to integrate quantum computing into their workflow are far more likely to be able to capitalize quickly, and the gaps they open will be difficult for others to close. This will offer a substantial advantage in industries where classically intractable computational problems lead to bottlenecks and lack of revenue opportunities.

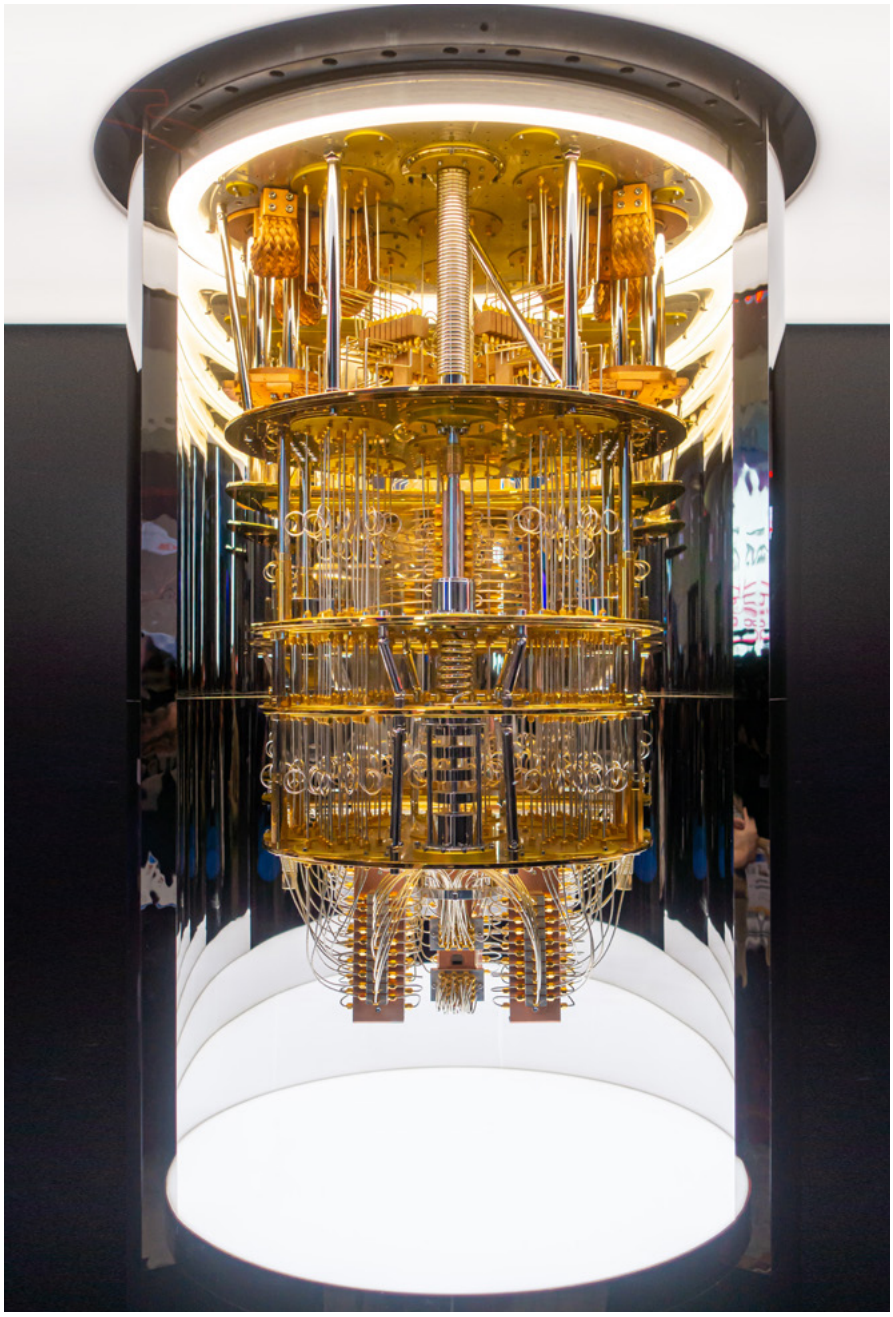
04 MANY ALTERNATIVE APPROACHES

Finally, although today's quantum race focuses on the realization of universal quantum computers as theorized by Feynman and Deutsch in the 1980s, alternative approaches to quantum and non-Von Neumann techniques are already available on the market. They are not general purpose, but they prove effective in solving a wide range of usually intractable combinatorial optimization tasks. Furthermore, the development of "quantum-inspired" algorithms is gaining traction, in turn leading to the realization of new digital (i.e., classical) hardware architectures capable of taking full advantage of them.

3 Quantum computing in the life sciences and healthcare industries. A long term vision.

Quantum computing has experienced a significant boom in the last decade, making it possible to start addressing real-world problems that were previously impossible or impractical to solve using classical algorithms.

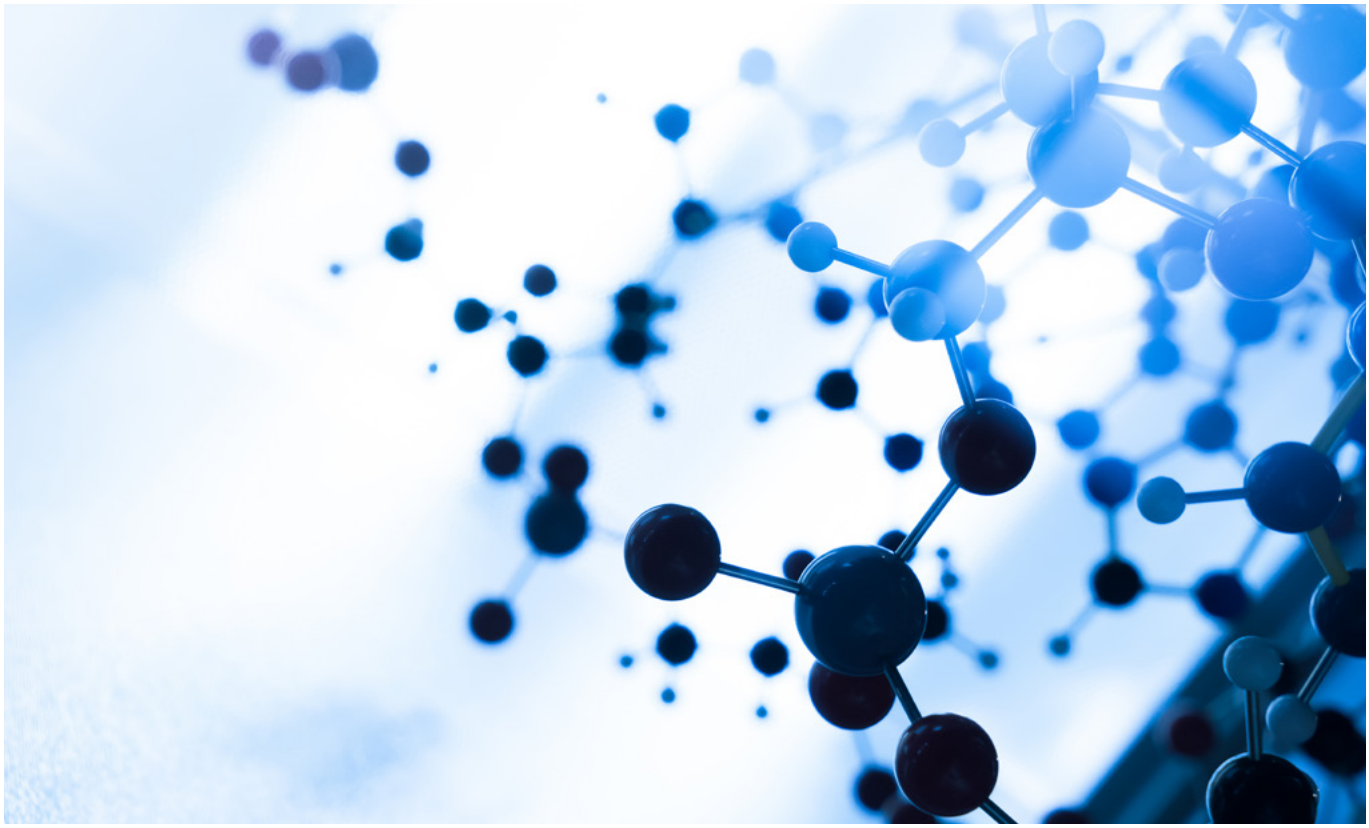
Quantum optimization algorithms are particularly relevant to the healthcare sector and may offer a competitive advantage when dealing with complex computing problems as well as those requiring high computational capacity. This is the case of genomics, where there are currently genome optimization problems [4], [5], [6] (such as genome assembly) whose computational complexity is rapidly increasing, and the classical computing approaches encounter great difficulties when trying to solve them. Quantum computing in this field can lead to more accurate genome assemblies and faster diagnoses of genetic diseases. In healthcare, quantum computing can also be used for medical imaging and personalized medicine. Quantum algorithms could analyze large sets of medical images, allowing doctors to detect anomalies and diagnose diseases more quickly. Personalized medicine involves tailoring treatments to an individual's specific genetic makeup, and quantum computing can help analyze large datasets of genetic information to identify optimal treatments. Also, health analytics could become faster and more accurate in the analysis of large-scale healthcare data sets by using quantum computing-based technologies. For instance, it may speed up the analysis of Electronic Health Records (EHRs) and enable health and care professionals to perform more accurate analyses while identifying patterns and trends in disease outbreaks and contributing to better-informed decisions on, for example,



prescription optimization and effectiveness.

In the scope of life sciences, concrete impacts have also been identified where quantum computing could make a difference. This is the case of drug discovery: Quantum computing could be used to simulate the behavior of molecules and predict how they will interact with other molecules, which could accelerate the drug discovery process [7]. This could lead to the development of new treatments for diseases that are currently difficult to treat. Precision medicine [8] is also a discipline that could benefit from quantum computing, as it could be used to analyze large amounts of genomic and clinical data to develop personalized treatment plans for patients. This could improve the effectiveness of treatments and reduce the risk of adverse side effects. Regarding protein folding, quantum computing has the potential to be used to simulate the folding of proteins, which is a critical process in understanding how proteins function and how they can be targeted by drugs [9], [10]. This could lead to the development of new treatments for diseases such as cancer and Alzheimer's.

Overall, quantum computing has the potential to accelerate scientific discovery and improve our understanding of complex biological systems, leading to new treatments for diseases and better health outcomes for patients. It represents a revolutionary paradigm shift in the field of life sciences and offers researchers and practitioners unprecedented opportunities to accelerate scientific discovery, improve our understanding of complex biological systems and unlock the mysteries of biology. As the technology matures and investment in quantum research continues to accelerate, the potential of quantum computing to revolutionize healthcare and drive medical innovation is truly limitless. While challenges remain, quantum computing will play a crucial role in shaping the future of healthcare and transforming the way we think about the fundamental workings of life itself.



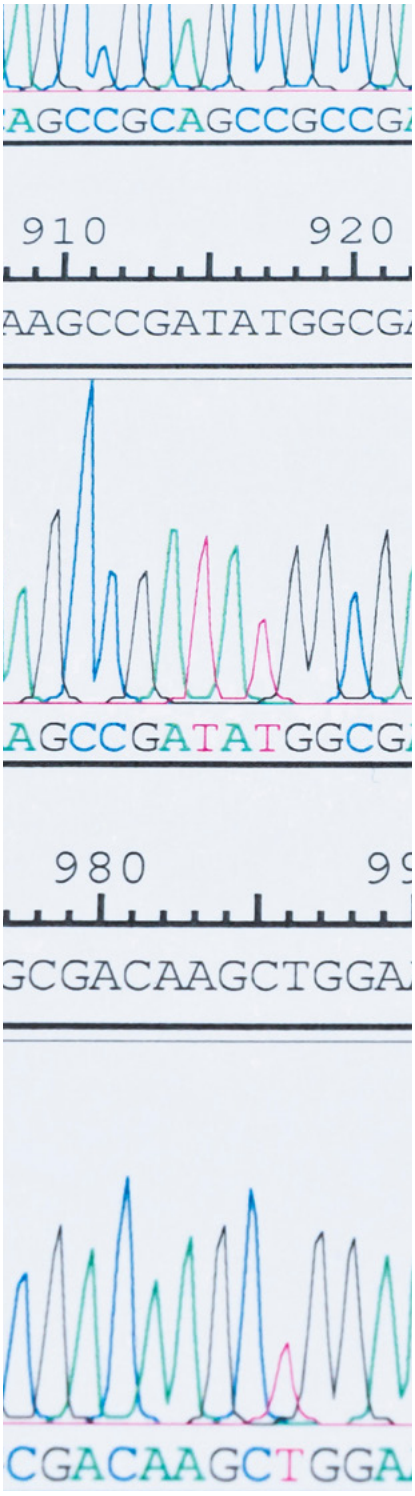
4 Optimization of genome assembly using quantum computing.

4.1 PROBLEM BACKGROUND

Genome assembly is a fundamental task in genomics, allowing researchers to reconstruct a complete genome from short fragments of DNA sequences obtained with sequencing techniques. This process is crucial to advance our understanding of genetics and biology, because by sequencing and assembling the genomes of individuals, scientists can identify genetic variations that may be associated with certain diseases or conditions. This information can be used to understand pathogens populations, investigate diseases, develop new treatments, create therapies that target the underlying genetic causes of diseases, or create new strains with desirable traits, such as increased disease resistance or improved performance of a particular product.

Genome sequencing technologies generate a vast amount of data that is fragmented into short pieces (reads). In addition, genomes often contain repetitive sequences and polymorphisms that, together with the errors introduced by sequencing technologies, makes de novo genome assembly an extremely challenging task (NP-hard) [11]. Solving these problems involves arranging many combinations of DNA fragments, leading to a large search space. Finding the optimal arrangement is computationally intensive [12], [13], [14]. As the size increases, the complexity increases rapidly, and classical computational approaches face limitations, computational difficulties, and slow computational speed to meet ever-increasing sequencing demands. Even with advanced classical algorithms, genome assembly remains a difficult and time-consuming process that can take days, even weeks, or in some cases remains an unsolved problem.

Quantum computing can help solve these problems more accurately and efficiently, as it has made significant advances in the last decade, opening doors to solving real-world problems that were previously impossible or impractical to solve using classical algorithms. Quantum algorithms have demonstrated their potential to accelerate genome assembly by exploiting the unique properties of quantum systems (superposition and quantum entanglement). This could lead to faster and more accurate genome assemblies, allowing researchers to study the genetic information of organisms with greater detail and precision.



4.2 PROBLEM STATEMENT

In this proof of concept on the adoption of quantum computing to the problem of genome assembly, we address one of the biggest challenges in genomics today: the computer-assisted assembly of fragmented genomic sequences, the so-called reads. The 'de novo' genome assembly is a technique for reconstructing the genome of an organism without a reference genome. Starting from the fragmented genome sequences or reads (Figure 1a), one must figure out how to arrange them in the correct order and reconstruct the genome.

The genome assembly problem can be formulated as a combinatorial optimization problem in a graph (Figure 1b), where the nodes represent the reads, and the connections between pairs of nodes depend on the mutual overlaps between the reads.

Figure 1a. *Example genome sequence. Reads of length 16 base-pairs.*

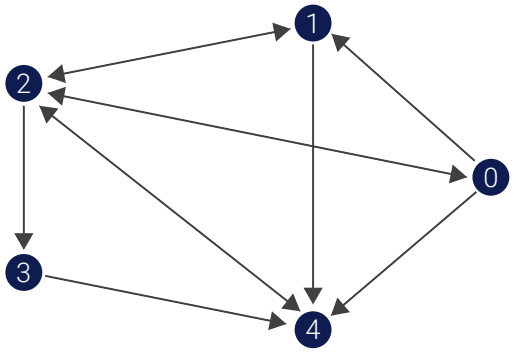
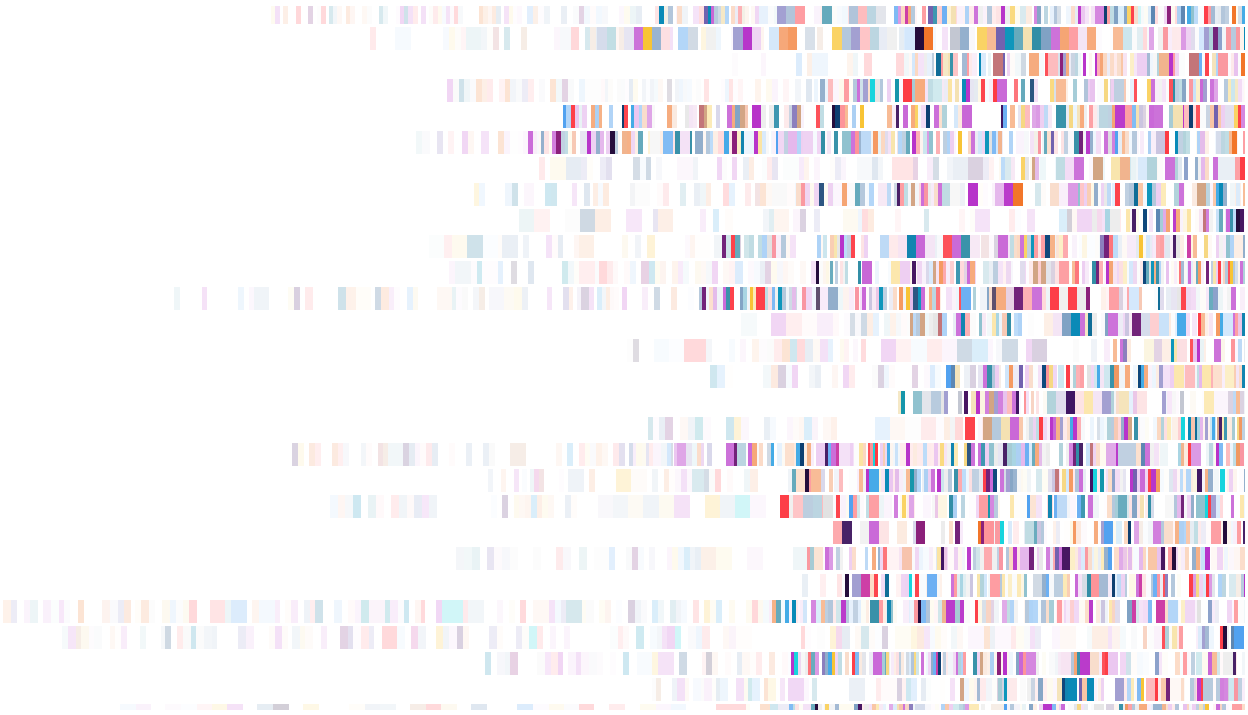


Figure 1b. *Directed Graph encoding the overlaps between the pairs of reads.*



There are multiple ways to solve such optimization problems. In this specific case, we are basing our approach on the Traveling Salesperson Problem (TSP), where the minimum total distance path that connects all the nodes (subject to some constraints) provides the correct ordering of the reads, thus allowing the assembly of the original genome (Figure 2a).

This sort of distance between two reads can be calculated as the total length of a read minus the degree of overlap between them. That is, the greater the overlap, the smaller the distance. It is important to note that the distance from node 1 to node 2 is not equal, in general, to the distance from node 2 to 1.

By mathematically formulating the above problem as a quadratic unconstrained binary optimization problem, or QUBO (a special type of combinatorial optimization problem), it can be submitted to a quantum computer to solve it. In this case, we assume there is an optimal shortest path that connects the reads, indicating their correct order.

Once we know the model and the formulation of our problem, we launch it into the different solvers that we will discuss below to solve the algorithm and obtain solutions to the genome assembly as we can see in Figure 2b, to finally get the genome assembly (Figure 3):

Figure 2a. *The example genome sequence reads, arranged to show their mutual overlaps.*

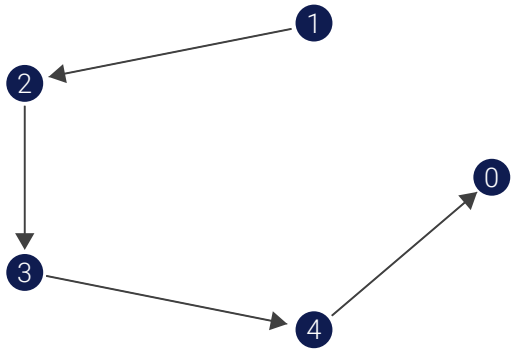


Figure 2b. *An optimal path in the Directed Graph that depicts correct order of the reads.*

GGATGGTGTCCTCATCTAATGATGTCGGTAAAGAGTCTAC

Figure 3. *The genome assembled, with the overlapping reads arranged in the correct order.*

4.2.1 Quantum algorithms and solvers

We explored two types of quantum and quantum-inspired solvers for this problem: quantum annealing and coherent Ising machines. Both are examples of so-called Ising machines.

An Ising model is a physics model used in statistical mechanics to describe several types of phenomena in ferromagnetic materials. The energy in these physical systems acts as the cost function to be minimized, called the Ising Hamiltonian.

There is a trivial transformation between a QUBO expression and its corresponding Ising Hamiltonian so, in essence, a combinatorial optimization problem (or other type of problem) expressed as a QUBO could be solved in an Ising Machine.

QUANTUM ANNEALING WITH D-WAVE

Quantum annealers are a particular type of quantum

computer that internally maps the QUBO problem into an Ising problem. D-Wave Systems is a company that provides APIs, software libraries and tools to interface with its pure quantum computers (such as the 2000Q or the more recent Advantage series) and hybrid quantum-classical computers.

We used the D-Wave Advantage series of quantum computers, with more than 5000 qubits and 15 couplers per qubit, or more than 35000 couplers in total.

In addition, we used the D-Wave hybrid quantum-classical solver, which combines the power of classical and quantum computing to solve optimization problems that would not fit on the current Advantage QPUs, due to their size (number of variables and coefficients).

NTT DATA'S COHERENT ISING MACHINE

Coherent Ising machines (CIM) use networks of so-called degenerate optical parametric oscillators (DOPO's), an alternative physical system for solving the Ising problem. NTT Basic Research Laboratories is conducting research and development of a CIM implemented by NTT using photonics technologies.

Due to the intrinsic complexity of CIM, it is common to use simulation algorithms in CPU or GPU. Specifically, chaotic amplitude control (CAC) is one such algorithms used in this project.

BASELINE: CLASSICAL MODELS

To compare the performance of the quantum algorithms and solvers, we used two types of classical solvers to find solutions to the genome assembly problem. The first one is a linear model implemented in Gurobi, a state-of-the-art software package for solving mathematical optimization problems.

The second is the simulated annealing algorithm, a heuristic algorithm very similar to a hill-climbing algorithm to search for optimal solutions of a cost function. It is one of the most widely used algorithms when comparing the performance of quantum and quantum-inspired approaches. We used D-Wave's simulated annealing solver implementation to run this solver on common hardware using the default settings.

4.2.2 Dataset

Currently, short length reads (100–200 base-pairs) predominate in sequencing technologies. Some recent sequencers can produce longer reads (10k base-pairs), but they tend to contain more sequencing errors. However, for our approach, and given the still very limited capabilities of current quantum computers, this complicates the possible application, as the problem size (number of variables) scales very quickly, as N^2, where N is the number of nodes or reads. We have generated simulated data with varying numbers of reads, read lengths and overlaps, making it easier to control the capacity of our algorithm and obtain accurate results.

We started with the circular genome of the bacteriophage phiX174, which has 5.386 base pairs [15]. With these data we represent different scenarios of varying complexity:

- The number of reads or nodes range from 5 to 30 at 5-nodes intervals. We also adjusted the length of the reads to ensure that they fully cover the genome.
- The overlaps between consecutive reads were randomly generated following a uniform distribution within min-max intervals.
    - 15–25 %: Very small average overlaps, very concentrated around the mean.
    - 45–55 %: Moderate average overlaps, very concentrated around the mean.
    - 40–60 %: Moderate average overlaps, with some spread around the mean.
    - 20–80 %: Moderate average overlaps, with much more spread around the mean, with important fractions of very small and very high overlaps.
    - 75–85 %: Very big average overlaps, very concentrated around the mean.

By controlling these parameters, we generated a dataset with 30 scenarios that is tailored to our specific needs, allowing us to test the scalability and accuracy of our algorithm under different conditions.

4.3 POC RESULTS

We compared the results obtained with the different approaches used to solve the genome assembly problem. Given a set of solutions obtained from the different solvers and approaches, we focus our evaluation on two main aspects:

- Firstly, the energy of the solutions, which is an indicator of how optimal they are.
- Secondly, the computing time required by each solver in each scenario.

The solutions found may fall into one of the following categories:

- Optimal solutions, which have an energy equal to the optimal energy for the specific problem scenario. These are the best possible solutions.
- Feasible solutions, which do not reach the optimal energy, but at least satisfy all the problem constraints. Depending on their energy, they can be close to the optimal solution, or they can be far away from it.
- Unfeasible solutions, which do not meet some of the problem constraints, although their energy could be lower than the optimal energy (we discard them for our analysis).

4.3.1 Ability to find optimal or good-enough solutions

Reaching the optimal energy with at least one solution is important to prove that a certain approach can find the best possible solutions, given the constraints and parameters. We computed the ratio of the solution energies with respect to the expected optimal energies, for each solver. For the feasible solutions, this shows how far they are from the optimal solutions.

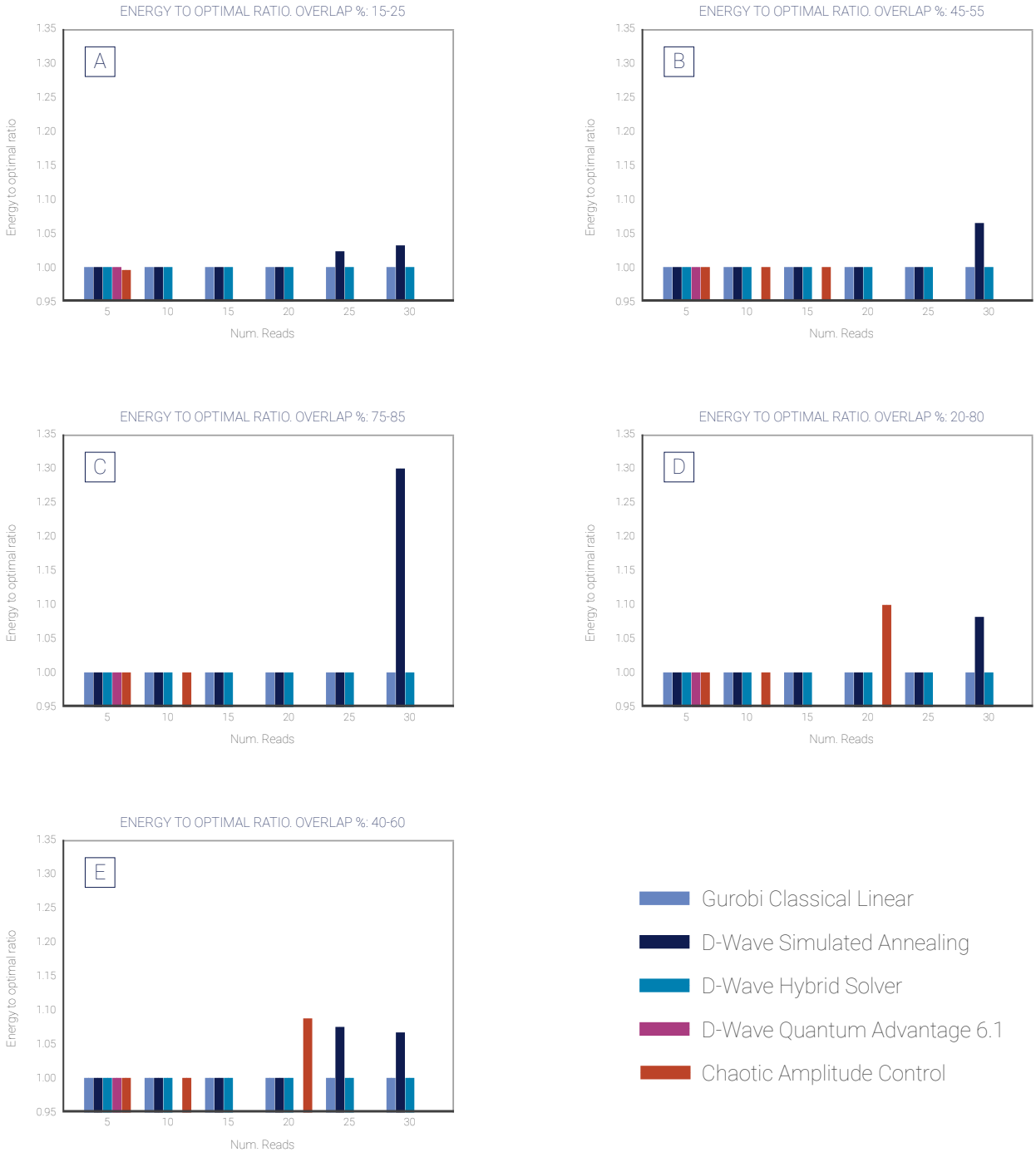


Figure 4. *Energy to optimal ratio as a function of number of nodes for overlap between A) 15–25%. B) 45–55%. C)75–85%. D) 20–80%. E) 40–60%.*

4.3.1 Computing time and cost of finding solutions

Next, the execution times (Wall clock time) of each solver in all the scenarios have been compared. The following figures show various interesting trends.

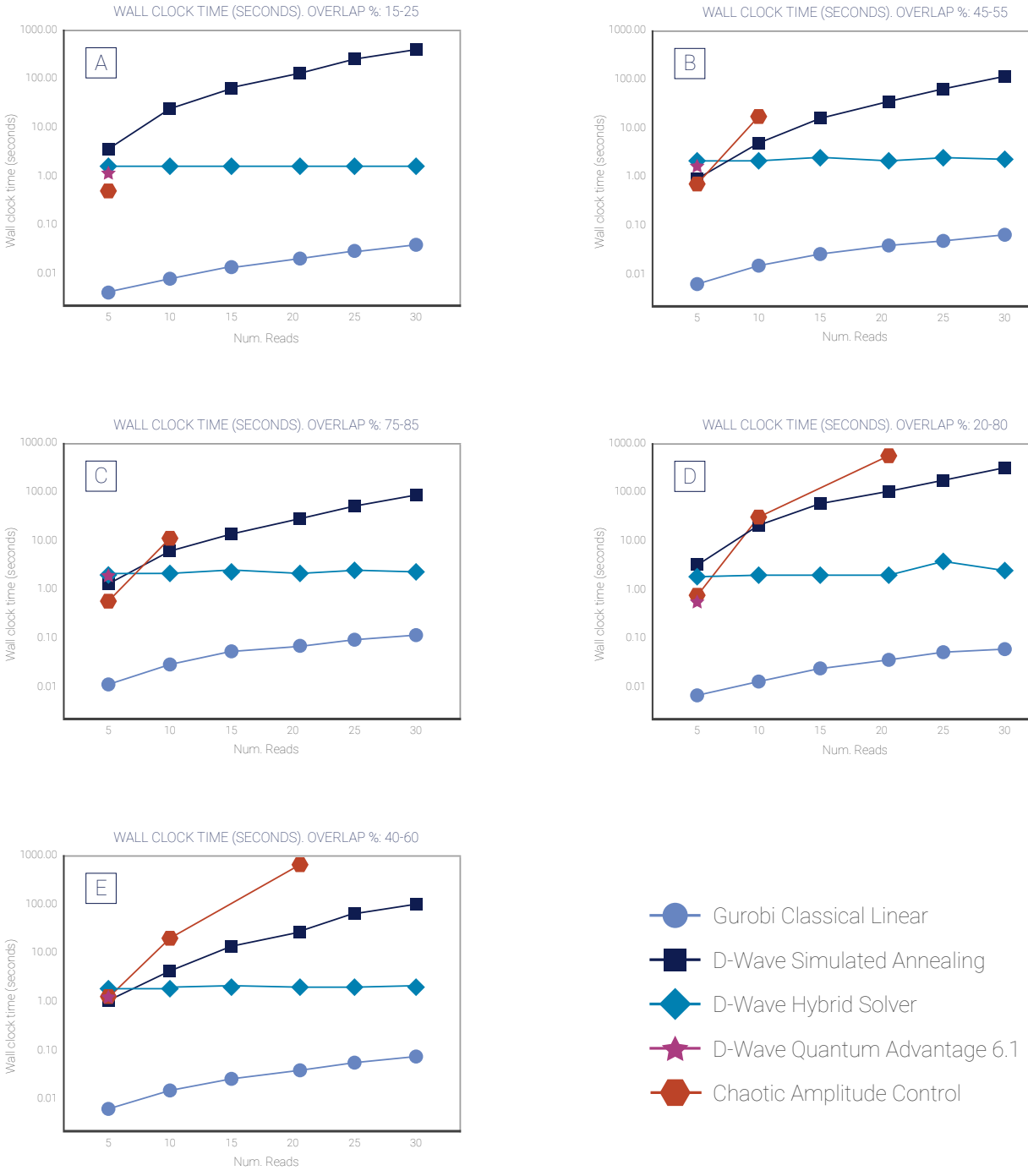


Figure 5. *Wall clock time as a function of number of nodes for overlap between A) 15–25%. B) 45–55%. C)75–85%. D) 20–80%. E) 40–60%.*

The results for each of the approaches were the following:

GUROBI LINEAR SOLVER

This classical solver obtained optimal solutions for all the proposed scenarios with all the overlapping ranges. Looking at the computing times, it can be observed that it is the fastest, with a linear dependency of time with respect to number of reads, for our scenarios.

D-WAVE SIMULATED ANNEALING

This solver found the optimal solutions for the scenarios of up to 20 nodes, and some in the 25-node scenarios (Figure 4). As the number of nodes increases (25, 30), we obtain mostly feasible (not optimal) solutions. The computing times increase with the number of reads and with the overlap ranges that are a priori more difficult to solve (Figure 5). The results indicate that it is easier for this solver to perform genome assembly when the overlaps between reads are higher.

D-WAVE ADVANTAGE6.1 QPU

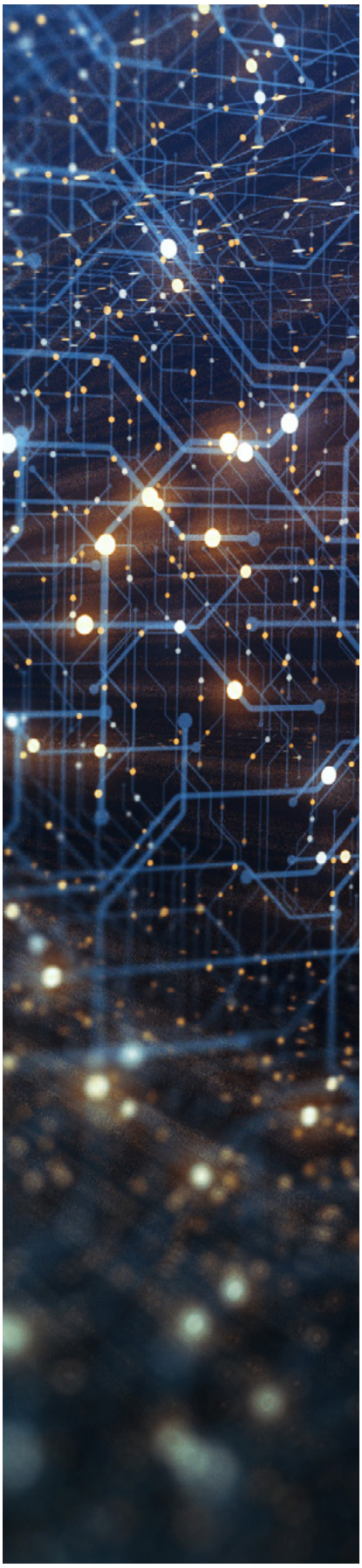
We obtained solutions with this QPU only for the 5-node cases, for 10 nodes we only obtained unfeasible solutions (therefore not shown in the Figure 4). The scenarios with more than 10 nodes exceeded the limit for this type of QPU. To some extent, this was to be expected, due to the limited capacity to encode this kind of problem in D-Wave QPUs, because of the number of variables and high connectivity required.

D-WAVE HYBRID SOLVER

Figure 4 shows how the D-Wave hybrid solver also obtained optimal solutions for all the proposed scenarios with all the overlapping ranges, and maintains a constant trend in the duration times, as the number of nodes increases.

CHAOTIC AMPLITUDE CONTROL QUANTUM-SIMULATOR SOLVER

This solver found optimal solutions for all overlapping scenarios up to 10 nodes (Figure 4), and feasible solutions in other cases. Larger problems could not be solved due to the solver timing out.



5 Conclusions and next steps.

We have shown the results obtained from the solvers we have used, in the quantum and classical approaches. To conclude, we enumerate the main advantages and limitations of the quantum approach and some potential future directions for research in this field.

- The D-Wave hybrid solver and the classical Gurobi linear solver have shown the best performances in obtaining optimal solutions for all the proposed scenarios.
- The purely quantum D-Wave Advantage6.1 QPU solver was only able to obtain optimal solutions for the five-node case due to its scale limitations for this type of problem.
- The D-Wave simulated annealing solver obtains optimal solutions for scenarios with small number of nodes, but has difficulty maintaining optimality as the number of nodes increases.
- Overall, the results obtained with the different solvers look promising in many respects, but at the same time highlight the importance of choosing an appropriate solver for the problem and the need for further research to improve the scalability of the quantum and quantum-inspired solvers.

The scope of this report and the limitations we have encountered lead us to think about new ideas and potential next steps to optimize the mathematical formulation of the model and its implementation for the solvers, to be able to tackle problems with higher computational power and to apply our model to real genomic sequencing data. They include:

1 INCREASE THE NUMBER OF NODES AND EXPLORE SCENARIOSWITH MORE READS (NODES)

In this report, we have generated scenarios with up to 30 nodes, but what happens when we increase the number of nodes and run the scenarios on the hybrid quantum-classical device? How does it behave in comparison to the classical solvers? Is there any indication that they could reach the same performance at some point?

2 GRAPH PARTITIONING

To solve larger graphs, we can use graph partitioning techniques that divide the graph into smaller, more manageable subgraphs, solve these individually, and combine the solutions into a master solution for the full-graph problem.

3 ALTERNATIVE FORMULATIONS THAT REDUCE SCALABILITY ISSUES

To ensure the scalability of the model, we can optimize the algorithm reducing the number of qubits required. This can be achieved by developing a more efficient model and exploring other approaches to genome assembly.

4 IMPROVED SIMULATED SEQUENCES GENERATION

By simulating more reads and filtering them, similarly to how real sequencing techniques work, we can better understand the potential of quantum computing for genome assembly.

5 HANDLING READS WITH RANDOM ERRORS

Finally, we can explore the potential of quantum computing to handle reads with errors. To do this, we can develop algorithms capable of detecting or correcting errors in reads, which could lead to more accurate genome assemblies.

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NTT DATA – a part of NTT Group – a trusted global innovator of IT and business services headquartered in Tokyo. We help clients transform through consulting, industry solutions, business process services, IT modernization and managed services. NTT DATA enables clients, as well as society, to move confidently into the digital future. We are committed to our clients' long-term success and combine global reach with local client attention to serve them in over 50 countries.

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