La España Cuántica: Informe Casos de Uso de Computación Cuántica

Ametic

LA VOZ DE LA INDUSTRIA DIGITAL

Contenido

Prólogo

Es un placer presentar este documento sobre "Casos de uso" y de "éxito" de las tecnologías cuánticas en España.

El "Grupo de tecnologías cuánticas" de AMETIC se ha consolidado como el hub empresarial de referencia en España y Europa. En la actualidad contamos con más de cincuenta empresas asociadas tanto de oferta como demanda.

Uno de nuestros objetivos más importantes para nuestro grupo es ayudar a crear un "mercado" (oferta y demanda) de las tecnologías cuánticas.

Este documento sirve a ese objetivo ya que se muestra cómo las empresas de oferta pueden aportar valor hoy a las empresas que demandan estas tecnologías.

Hemos confeccionado - gracias a las inestimables aportaciones de nuestros asociados - trece casos de uso "reales" que son una muestra realmente representativa de temas y verticales (finanzas, energía, logística, ciberseguridad, defensa y arte.

Los Casos de Uso recogidos son los siguientes:

Caso de Uso 1: Credit valuation adjustments.

Caso de Uso 2: Fraud detection.

Caso de Uso 3: Portfolio optimization.

Caso de Uso 4: Energy production forecasting.

Caso de Uso 5: Smart grids Optimization.

Caso de Uso 6: Hydrogen generation optimization.

Caso de Uso 7: Faster energy market price operation

Caso de Uso 8: Efficient packing in bins.

Caso de Uso 9: Management of empty containers at maritime ports.

Caso de Uso 10: Bus routes optimization.

Caso de Uso 11: ZKP – PQC Layer in Self Sovereign Identity (SSI).

Caso de Uso 12: New Defense Materials through AI and Quantum Simulations.

Caso de Uso 13: Nitrogen fixation.

Caso de Uso 14: Quantum Computer Music.

También es nuestro objetivo que este documento sea útil a las empresas que tienen intención de empezar a usar estas tecnologías; Que tengan referencias reales y actuales sobre lo que están haciendo las empresas de su entorno y que puedan incorporarse a este proceso de adopción de estas tecnologías e incorporarlas a sus procesos de negocio.

En la actualidad, la ventana de oportunidad está focalizada en la intersección entre IA y Cuántica (QuantumAI), la tecnología Quantum Inspired (Tensor Networks) o las tecnologías Post Cuánticas y QKD.

Creo que estos conceptos pueden ser objeto de un nuevo documento del Grupo Cuántico de AMETIC.

Quiero agradecer especialmente la implicación y excelencia de los coordinadores de este documento: Xavier Jordán, FUNDACIÓ I2CAT y Guillermo Gil, TECNALIA.

Y, por supuesto a las empresas y sus profesionales que han cedido desinteresadamente su INFORMACIÓN de sus proyectos reales para confeccionar estas catorce fichas de casos de uso:

- Rafael Martín-Cuevas, EY, por la aportación de Casos de Uso en el sector financiero.
- Iraia Ibarzabal, MULTIVERSE COMPUTING, y Jesús Huertas, QUILIMANJARO, por la aportación de Casos de Uso en el sector energético.
- Enrique Crespo, GMV, por la aportación de Casos de Uso en el sector Ciberseguridad.
- Guillermo Gil, TECNALIA, por la aportación de Casos de Uso en el sector Logística y Movilidad.
- Eneko Axpe, SANDBOX AQ, por la aportación de Casos de Uso en el sector Defensa.
- Adán Garriga, EURECAT, por la aportación de Casos de Uso en el sector de Industrias Culturales y Creativas.

Desde el Grupo “cuántico” de AMETIC tenemos muy claro que la pregunta no es “cuándo”, (que es ahora) sino “quién” y si España será uno de ellos…porque si no somos uno de ellos, que importa cuando ni quien.

Porque, no lo olvidemos, “el mundo es cuántico”.

Alfonso Rubio-Manzanares

VP de la Comisión de Innovación de AMETIC y Coordinador de su Grupo de Trabajo de Tecnologías Cuánticas.

Presentación

Estamos inmersos en el pleno desarrollo de la Computación Cuántica, una nueva disciplina emergente de computación que está llamada a tener un papel esencial en el futuro desarrollo económico y la prosperidad de las sociedades. Aúna aspectos de la física y las matemáticas, y aprovecha las propiedades de la mecánica cuántica para abordar la resolución de problemas computacionales complejos de una manera completamente diferente a los sistemas de computación tradicionales.

Hace más de 75 años, durante la primera revolución cuántica, se sentaron las bases de lo que hoy llamamos Transformación Digital. En ese tiempo, comprendimos la física de semiconductores y aprendimos a construir transistores y otros componentes esenciales que aprovechan las propiedades de la mecánica cuántica, creando gradualmente un sustrato digital indispensable para el funcionamiento de nuestra sociedad actual. Ahora estamos presenciando la llamada segunda revolución cuántica, una nueva fase que supera el mero uso de las propiedades cuánticas. Estamos aprendiendo a manipular directamente la materia para aprovechar procesos basados en características de la mecánica cuántica, como la superposición y el entrelazamiento. Estos avances están dando lugar a nuevas tecnologías para la computación, la comunicación y la detección, que probablemente constituirán una nueva generación de infraestructuras para el funcionamiento de la sociedad en un futuro próximo.

La Computación Cuántica servirá para impulsar la disciplina de Inteligencia Artificial en ámbitos en donde, a medida que el mundo se va haciendo más interrelacionado e instantáneo, las tecnologías convencionales están encontrando cada vez más limitaciones. El nivel de sofisticación necesario para el procesamiento intersistemas en este contexto tan complejo continuará creciendo exponencialmente, así como la necesidad de gestionar y manipular inteligentemente los datos. Como consecuencia, la complejidad computacional resultante será progresivamente intratable para los medios convencionales, y es en este punto donde la computación cuántica ofrece nuevos mecanismos complementarios.

Por estos motivos, esta tecnología es una herramienta formidable en la industria para lograr una transformación digital que combine competitividad, responsabilidad social y respeto al medio ambiente. Posiblemente, de todas las tecnologías en las que estamos trabajando actualmente, la cuántica es la que tiene el potencial de impacto más radical y profundo en ámbitos de nuestra sociedad relacionados con la industria, el transporte, la energía, la seguridad, la salud o el medioambiente. Esta importancia vital nos exige redoblar los esfuerzos desde el plano público y privado para mejorar nuestra posición competitiva. España debe aprovechar sus fortalezas y talento ante esta oportunidad única, capaz de generar un nítido impacto social, económico y medioambiental.

Aunque estamos en una etapa todavía emergente, con desarrollos limitados, inciertos y vertiginosos, las empresas que desarrollen anticipadamente las capacidades necesarias estarán mejor posicionadas para aprovechar este potencial transformador de los negocios, obteniendo una ventaja competitiva significativa en áreas claves de la inteligencia artificial y la optimización de procesos. En este campo se requiere de una sofisticada combinación de talento para crear aplicaciones con impacto, que combina el conocimiento singular de la disciplina, un entendimiento profundo de los grandes problemas organizacionales y la gestión interdisciplinar de diferentes mentalidades y competencias de dentro y fuera de la organización.

Por ello, ya hay muchísimas empresas que están explorando las posibilidades de la computación cuántica como elemento de competitividad en sus negocios. Se trata casi siempre de experimentos sobre problemas reales, pero, debido a las limitaciones del hardware actual, a una escala aún muy pequeña, lejos de la complejidad de los grandes retos que la tecnología promete resolver en el futuro.

En el informe "La España Cuántica"[1] de AMETIC, 2022, se recomendaba establecer una hoja de ruta para la adopción de estas tecnologías por parte de las organizaciones, reconociendo su carácter todavía emergente, Figura 1.

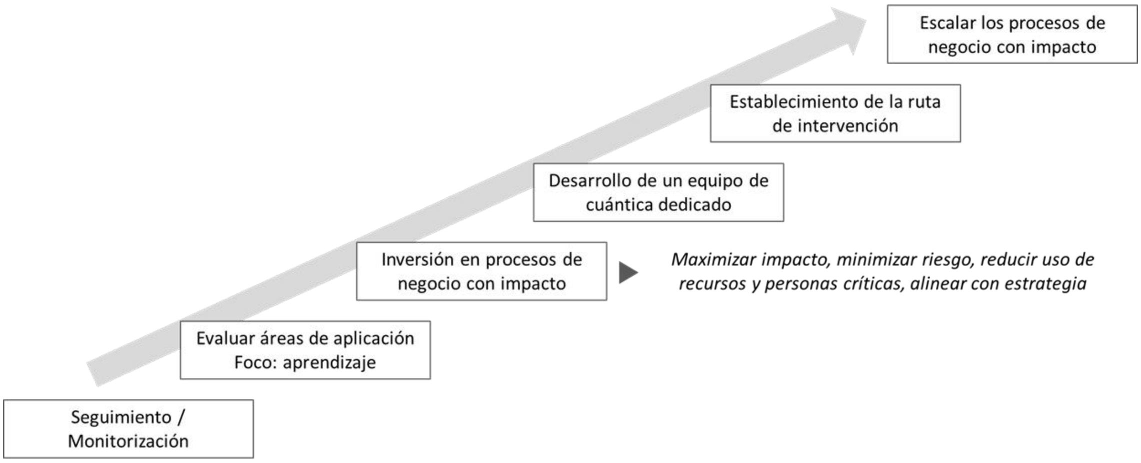


Figura 1. Roadmap de adopción, "La España Cuántica", AMETIC, 2022.

Este catálogo de casos quiere contribuir al primer peldaño de esta ruta, aportando algunas referencias de diferentes sectores.

Los Casos de Uso recogidos son los siguientes:

- Caso de Uso 1: *Credit Valuation Adjustments.*
- Caso de Uso 2: *Fraud detection*.
- Caso de Uso 3: *Portfolio Optimization*.
- Caso de Uso 4: *Energy production forecasting*.
- Caso de Uso 5: *Smart Grids Optimization*.
- Caso de Uso 6: *Hydrogen generation optimization*.
- Caso de Uso 7: *Faster Energy Market Price Operation*
- Caso de Uso 8: *Efficient packing in bins*.
- Caso de Uso 9: *Management of empty containers at maritime ports*.
- Caso de Uso 10: *Bus routes optimization*.
- Caso de Uso 11: *ZKP – PQC Layer in Self Sovereign Identity (SSI)*.
- Caso de Uso 12: *New Defense Materials through AI and Quantum Simulations.*
- Caso de Uso 13: *Nitrogen fixation*.
- Caso de Uso 14: *Quantum Computer Music*.

Para cada uno de estos Casos de Uso se adjunta una ficha en inglés con su descripción y principales identificadores (como sector, nivel de madurez y potencial de impacto), el problema organizacional al que se dirige, la ventaja que se busca lograr y la solución de Computación Cuántica aportada.

Es importante resaltar que la Computación Cuántica está en la misma cadena de valor que la IA, por lo que, dependiendo del nivel de madurez en la adopción de la IA clásica, será más fácil o menos abordar la adopción de la Computación Cuántica. Para aquellas organizaciones que ya tengan un recorrido consolidado en IA clásica, en cualquiera de sus variantes, será más accesible acometer iniciativas con aproximaciones cuánticas.

Los diferentes casos que se ilustran a continuación han servido y están sirviendo para explorar el potencial de estas nuevas tecnologías en el contexto de la organización, entender dónde aportan valor, identificar los ámbitos de intervención, las claves de implantación, comprender los riesgos e incertidumbres, etc. Es decir, es importante comprender, que se han generado en estos últimos tres años en paralelo al desarrollo del hardware existente, todavía muy inmaduro, y que, salvo excepciones, no están "en producción" en procesos de negocio reales. No obstante, con la información disponible de las hojas de ruta de los fabricantes de hardware y de sus servicios vía la nube, es muy probable que se extienda progresivamente la implantación en procesos de negocio en estos próximos 3 años.

Por ello, les invitamos a conocer estos Casos de Uso como inspiración para quieres quieran adentrarse hoy en esta disciplina y anticiparse para explotar todo el potencial de estas tecnologías diferencialmente a medida que se desarrollen.

Introduction

We are immersed in the full development of Quantum Computing, a new emerging discipline of computing that is called to play an essential role in the future economic development and prosperity of societies. It combines aspects of physics and mathematics, and takes advantage of the properties of quantum mechanics to address the resolution of complex computational problems in a completely different way than traditional computing systems.

More than 75 years ago, during the first quantum revolution, the foundations of what we now call Digital Transformation were laid. At that time, we understood the physics of semiconductors and learned to build transistors and other essential components that take advantage of the properties of quantum mechanics, gradually creating a digital substrate indispensable for the functioning of our current society. Now we are witnessing the so-called second quantum revolution, a new phase that goes beyond the mere use of quantum properties. We are learning to directly manipulate matter to take advantage of processes based on characteristics of quantum mechanics, such as superposition and entanglement. These advances are giving rise to new technologies for computing, communication, and detection, which will probably constitute a new generation of infrastructures for the functioning of society in the near future.

Quantum Computing will serve to drive the discipline of Artificial Intelligence in areas where, as the world becomes more interconnected and instantaneous, conventional technologies are increasingly finding limitations. The level of sophistication that is necessary for the intersystem processing in this complex context will continue to grow exponentially, as will the need to intelligently manage and manipulate data. As a result, the required computational complexity will be progressively intractable for conventional means, and it is at this point that quantum computing offers new complementary mechanisms.

For these reasons, this technology is a formidable tool for the industry to achieve a digital transformation that combines competitiveness, social responsibility, and respect for the environment. Possibly, of all the technologies we are currently working on, quantum is the one with the most radical and profound potential impact on areas of our society related to industry, transport, energy, security, health, or the environment. This vital importance requires us to redouble our efforts from the public and private sectors to improve our competitive position. Spain must take advantage of its strengths and talent in the face of this unique opportunity, capable of generating a clear social, economic, and environmental impact.

Although we are still in an emerging stage, with limited, uncertain, and dizzying developments, companies that develop the necessary capabilities in advance will be better positioned to take advantage of this transformative potential of business, obtaining a significant competitive advantage in key areas of artificial intelligence and process optimization. This field requires a sophisticated combination of talent to create impactful applications, which combines the unique knowledge of the discipline, a deep understanding of the major organizational problems and the interdisciplinary management of different mindsets and competencies from within and outside the organization.

For this reason, there are already many companies that are exploring the possibilities of quantum computing as an element of competitiveness in their businesses. These are almost always experiments and proof of concepts on real problems, but, due to the limitations of current hardware, on a still very small scale, far from the complexity of the great challenges that technology promises to solve in the future.

The AMETIC´s report “Spain Quantum Industry”[1], 2023, recommended to establish a roadmap for the adoption of these technologies by organizations, recognizing their still-emerging nature, Figure 2.

---

[1] “Spain Quantum Industry”, AMETIC, 2023, https://ametic.es/publicacion/spain-quantum-industry-report-english-version-2023-edition/

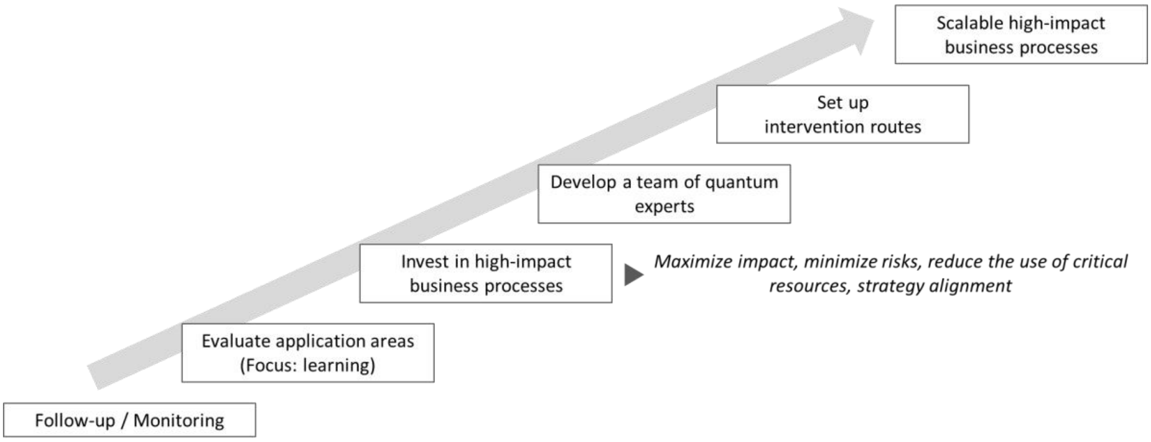


Figure 2. Adoption roadmap, "Spain Quantum Industry Report", AMETIC, 2023.

This catalogue of cases wants to contribute to the first step of this route, providing some references from different sectors.

The Use Cases collected are the following:

- Use Case 1: Credit Valuation Adjustments
- Use Case 2: Fraud detection.
- Use Case 3: Portfolio Optimization
- Use Case 4: Energy production forecasting.
- Use Case 5: Smart Grids Optimization.
- Use Case 6: Hydrogen generation optimization.
- Use Case 7: Faster Energy Market Price Operation
- Use Case 8: Efficient packing in bins.
- Use Case 9: Management of empty containers at maritime ports.
- Use Case 10: Bus routes optimization.
- Use Case 11: ZKP – PQC Layer in Self Sovereign Identity (SSI).
- Use Case 12: New Defense Materials through AI and Quantum Simulations
- Use Case 13: Nitrogen fixation.
- Use Case 14: Quantum Computer Music.

For each of these Use Cases, a form is attached in English with its description and main identifiers (such as sector, level of maturity and potential impact), the organizational problem it addresses, the advantage it seeks to achieve, and the Quantum Computing solution provided.

It is important to highlight that Quantum Computing is in the same value chain as AI, so, depending on the level of maturity in the adoption of classical AI, it will be easier or harder to approach the adoption of Quantum Computing. For those organizations that already have a consolidated journey in classical AI, in any of its variants, it will be more accessible to undertake initiatives with quantum approaches.

The different cases that are illustrated below have served and are serving to explore the potential of these new technologies in the context of the organization, to understand where they add value, to identify the areas of intervention, the keys to implementation, the risks and uncertainties, etc. That is, it is important to consider that they have been generated in these last three years, just in parallel to the development of the existing hardware, still very immature, and that, but exceptions, they are not "in production" in real business processes. However, with the information available from the roadmaps of hardware manufacturers and their cloud services, it is very likely that the implementation in business processes will be progressively extended in the next 3 years.

For this reason, we invite you to know these Use Cases as inspiration for those who want to delve into this discipline today and anticipate exploiting all the potential of these technologies differentially as they develop.

Use Case 1: Credit Valuation Adjustments.

Brief description

Computational Problem Type:	Simulation
Problem Domain:	Financial Services
Subdomain:	Portfolio Management
Industry:	Financial Services, Banking
Time to Maturity (TRL):	Medium: 5-10 years
Potential Impact:	$20-35B
EU Goal alignment:	Industry, innovation and infrastructure
Techniques:	QAE (Quantum Amplitude Estimation), QCBM (Quantum Circuit Born Machine), Monte Carlo simulation.
Source of use case:	BBVA

Summary

Quantum Algorithm for Credit Valuation Adjustments (CVA) is an innovative technique that holds potential for tackling the challenges posed in finance, particularly in risk analysis and derivative pricing. Quantum mechanics, with its potential to accelerate statistical samplings far beyond classical techniques, finds significant application in financial simulations. An important simulation case under discussion here focuses on CVAs, shedding insight on the potential of quantum computing for effective and efficient calculations. CVAs, which require accounting for all possible credit default scenarios, are immensely complex and often computationally expensive on classical computers. However, with quantum computing, a great deal of computational shortcuts and possibilities open up to tackle these massive calculation requirements.

Description

Business Challenge:

Transforming the field of quantitative finance, Credit Valuation Adjustment (CVA) calculations form an integral part of financial risk management. Given its significance in the estimation of counterparty risk and derivative prices, it's important to ensure accuracy and efficiency in these calculations. However, these calculations are immensely demanding, often involving millions of numerical computations with high computational expenses. Classical Monte Carlo simulations, accommodating all possible credit default scenarios, are incredibly resource and time-intensive and often exhibit limitations with high-volume computations. This complex, extensive calculation mandates an advanced computational model, with quantum computing offering a promising solution.

Value Proposition:

The advent of quantum computing offers an innovative solution for these computation-intense processes in financial evaluations. Quantum computing is based on the principles of quantum mechanics, which allow quantum computers to process large amounts of data simultaneously, making them potential candidates for applications that require intense numerical calculations. With the potential to break the classical cost scaling barrier in terms of statistical error, quantum computing can facilitate quicker, more efficient CVA calculations. Even the most complex Monte Carlo simulations could be efficiently handled with quantum algorithmic advancements. However, deploying quantum computations for CVA calculations still represents a complex challenge, requiring sophisticated quantum algorithms and robust quantum hardware.

Solution Approach:

The ideal solution approach involves two fundamental steps. Firstly, the preparation of quantum states that encode the classical data using quantum feature maps, and secondly, the estimation of the statistical average or expectation value. For the former, Quantum Circuit Born Machines (QCBM) and Quantum Circuit Constructions based on Matrix Product States offer potential circuit designs to encode classical data efficiently into quantum states. For the latter, quantum algorithms can estimate operator expectations effectively, significantly reducing the statistical error.

Hybrid quantum-classical algorithms, such as the Variational Quantum Eigensolver (VQE) algorithm or the adiabatic paradigm, can also be leveraged for their combined strengths of both quantum and classical computations. Furthermore, Quantum Amplitude Estimation (QAE) algorithms help to reduce circuit depths, thereby overcoming certain hardware limitations of quantum computers. Another promising technique is the Quantum Circuit Born Machines (QCBM) that generates quantum states encoding a target probability distribution.

The development of such scalable quantum algorithms for CVA calculations fosters the advancement of the financial sector. However, the practical realization of these models would require addressing unique challenges such as reliability, robustness, and accuracy to ensure efficient real-world application.

References

[1] Alcázar, J., Cadarso, A., Katabarwa, A., Mauri, M., Peropadre, B., Wang, G., Cao, Y. (2021). Quantum algorithm for credit valuation adjustments. *New Journal of Physics 24*. https://doi.org/10.1088/1367-2630%2Fac5003

[2] *Un estudio de BBVA y Zapata Computing muestra el potencial de la computación cuántica para el cálculo de derivados*, BBVA, 27 May 2021, https://www.bbva.com/es/innovacion/un-estudio-de-bbva-y-zapata-computing-muestra-el-potencial-de-la-computacion-cuantica-para-el-calculo-de-derivados/. Accessed 5 February 2024.

[3] *Speeding up Monte Carlo simulations, powered by Orquestra*, Zapata Computing Inc., https://zapata.ai/bbva-monte-carlo-simulation-finance-case-study/. Accessed 5 February 2024.

[4] The Quantum Computing Potential to Speed Up Monte Carlo Calculations for Credit Valuation Adjustments, Zapata Computing Inc., https://zapata.ai/cva/. Accessed 5 February 2024.

Use Case 2: Fraud detection.

Brief description

Computational Problem Type:	Machine Learning
Problem Domain:	Financial Services
Subdomain:	Fraud Detection
Industry:	Financial Services, Banking
Time to Maturity (TRL):	Short: <5 years
Potential Impact:	$20-30B
EU Goal alignment:	Industry, innovation and infrastructure
Techniques:	Quantum Support Vector Classifier (QSVC), Variational Quantum Classifier (VQC), Estimator Quantum Neural Network, and Sampler Quantum Neural Network.
Source of use case:	BBVA

Summary

Quantum Fraud Detection is a progressive technique that can be employed in financial sectors to detect fraudulent activities which may involve credit card misuse, loan mismanagement, deceptive transfer of funds, and more. This process exploits the computational capability of quantum machine learning models to analyze complex datasets and identify anomalies indicative of potential fraud. Traditional fraud detection methods, while competent, often struggle to handle high-volume, high-velocity data and fail to adapt quickly to evolving fraudulent strategies. Quantum algorithms, on the other hand, pose great potential in efficiently analyzing massive datasets in minimal time. In the long run, this quantum approach could significantly enhance the efficiency of financial fraud detection, but its execution currently involves numerous scientific and business challenges.

Description

Business Challenge:

All methods of fraud detection, especially those related to financial transactions, pose enormous challenges. Traditional Machine Learning models, though effective, require computational resources with growing data volume and complexity. Even the advanced Deep Learning models, dealing with high-dimensional data, require extensive computational power and time. These demanding requirements call for revolutionary technology that can handle such computation-intensive tasks efficiently. Here quantum computing comes into play. It holds the potential to offer exponential speed-up, scalability, and reduced computations, leading to a notably high-performance fraud detection model. Quantum computing means dealing with qubits and leveraging quantum mechanical properties of superposition and entanglement, opening the path to potential opportunities. However, developing a full-scale, practical quantum algorithm for fraud detection requires overcoming several scientific challenges, like high dimensional data handling, real-time data analysis, and dealing with inessential data.

Value Proposition:

Deploying Quantum Machine Learning models for fraud detection could one day immensely increase the speed and efficiency of the detection process. The potential advantage comprises real-time data analysis from vast data volumes, reduction in inessential data, and an enhanced ability to detect complex patterns. Furthermore, it can cut down computational complexity by utilizing quantum mechanical properties like superposition, interference and entanglement. These prospects promise major improvements over traditional fraud detection, potentially saving substantial financial resources and time. However, the practical realization of such a model would involve unique challenges such as reliability, robustness, and accuracy that are yet to be explored and addressed.

Solution Approach:

To build a quantum fraud detection model, an essential step is to encode classical data into quantum states using a suitable feature map. Post encoding, measurement is performed on some or all qubits to obtain classical features. Classical optimization techniques are then employed to find the optimal model parameters, essentially minimizing a cost function. This approach involves a hybrid procedure combining elements from classical computing and Quantum Computing. Quantum algorithms like the Quantum Support Vector Classifier (QSVC), Variational Quantum Classifier (VQC), Estimator Quantum Neural Network, and Sampler Quantum Neural Network offer valuable directions towards developing a high-performance quantum fraud detection model. A noteworthy objective is the comparative study of these Quantum Machine Learning models and the continuous endeavor to optimize them while overcoming limitations. This procedure repeats until the optimal model parameters are found, thereby improving the probability of fraud detection in the given dataset.

References

[1] BBVA Uncovers The Promise Of Quantum Computing For Banking And Financial Services, Forbes, 25 August 2020, https://www.forbes.com/sites/gilpress/2020/08/25/bbva-uncovers-the-promise-of-quantum-computing-for-banking-and-financial-services/. Accessed 5 February 2024.

[2] How may quantum computing affect Artificial Intelligence?, BBVA, 20 January 2020, https://www.bbva.com/en/innovation/how-may-quantum-computing-affect-artificial-intelligence/. Accessed 5 February 2024.

[3] Innan, N., Al-Zafar Khan, M., Bennai, M. (2023). Financial Fraud Detection: A Comparative Study of Quantum Machine Learning Models. International Journal of Quantum Information. https://doi.org/10.1142/S0219749923500442

Use Case 3: Portfolio Optimization.

Brief description

Computational Problem Type:	Optimization
Problem Domain:	Financial Services
Subdomain:	Portfolio Management
Industry:	Financial Services, Banking
Time to Maturity (TRL):	Medium: 5 - 10 years
Potential Impact:	$20-50B
EU Goal alignment:	Industry, innovation and infrastructure
Techniques:	Adiabatic Paradigm, VQE (Variational Quantum Eigensolver), QAOA (Quantum Approximate Optimization Algorithm), QPE (Quantum Phase Estimation)..
Source of use case:	BBVA

Summary

Quantum computing and quantum-inspired methods show promising potential for optimizing investment portfolios. Aimed at maximizing returns and reducing risk, these initiatives could greatly transform the financial landscape, possibly offering scalability metrics superior to classical alternatives. By utilizing principles of quantum computing, the classic financial challenge of portfolio optimization using real market data can be efficiently tackled, thanks to its direct correspondence with the optimization capabilities of quantum computing. Recent research in this field has introduced new methodologies that can vastly speed up relevant calculations.

Description

Business Challenge:

The special challenge in this scenario is optimizing the weights allocated to varied assets in an investment portfolio to maximize returns. The proposed solutions leverage quantum computing and other quantum-inspired technologies, which have vast potential to improve existing financial tools. These techniques are currently being assessed from a computational viewpoint. Financial institutions are beginning to utilize a mix of quantum-based technologies and conventional methods to dynamically optimize investment portfolios based on market data. This innovative line of work has already led to the creation of pioneering methods designed to enhance these calculations.

Value Proposition:

Applying quantum computing to this specific task has the potential to yield results that surpass those achieved with traditional methods. Research in this field suggests that substantial investment portfolios could be optimized using quantum and quantum-inspired tools. This could be a game-changing development as it would enable institutions to optimize portfolios of a size that holds commercial value, offering an advantage over traditional methods which often depend on heuristics and simplifications. Computational tests conducted thus far by various players have relied on implementing several quantum and quantum-inspired algorithms on multiple hardware platforms. This helps determine the optimal trading direction for an investment portfolio and discern the leading quantum technologies.

Solution Approach:

For the gate-model paradigm, the Variational Quantum Eigensolver (VQE) is one of the favored algorithms. This hybrid algorithm combines the strengths of both quantum and classical computation and can be executed on currently available quantum systems, yielding potentially better results than traditional methods. Other approaches rely on the Quantum Approximate Optimization Algorithm (another instance of a variational quantum algorithm that blends quantum and classical computing methods), and Quantum Phase Estimation (which relies solely on universal quantum computers). As for the adiabatic paradigm, the preferred solution is based on the use of quantum annealers, which naturally seek the global minimum of the supplied optimization problem.

These innovative methods open the possibility to boost potential investment returns by leveraging real market data, marking a significant advancement in applying quantum technologies in finance. This quantum-inspired computation adoption could cause a significant shift in the financial industry by redefining the rules of the game. The ability of quantum computing to manage large systems places it in a unique category, potentially enabling previously impossible real-time data handling. Consequently, users can significantly reduce computational times, bringing immediate benefits to portfolio management.

The future holds ample possibilities for this rapidly expanding field, especially considering the swift advancements within quantum computing. Firms acknowledge this and have begun using quantum and quantum-inspired optimizers in the field of finance. Therefore, continued investment and research in this area could potentially transform the realm of financial computing as we know it.

References

[1] Mugel, S., Kuchkovsky, C., Sánchez, E., Fernández-Lorenzo, S., Luis-Hita, J., Lizaso, E., Orús, R. (2022). Dynamic portfolio optimization with real datasets using quantum processors and quantum-inspired tensor networks. *Phys. Rev. Research* 4, 013006. https://doi.org/10.1103/PhysRevResearch.4.013006

[2] *BBVA y Multiverse demuestran cómo la computación cuántica puede optimizar la gestión de las carteras de inversión*, BBVA, 19 July 2022, https://www.bbva.com/es/bbva-y-multiverse-demuestran-como-la-computacion-cuantica-puede-optimizar-la-gestion-de-las-carteras-de-inversion/. Accessed 29 January 2024.

[3] *Multiverse Computing: Optimizing Financial Portfolios with Quantum Computing*, D-Wave Systems Inc., 2021, https://www.dwavesys.com/media/5qahck2o/multiverse_case_study_v8.pdf. Accessed 29 January 2024.

Use Case 4: Energy production forecasting.

Brief description

Computational Problem Type:	Quantum Machine Learning
Problem Domain:	Prediction
Subdomain:	Energy Production
Industry:	Energy
Time to Maturity (TRL):	Medium: >5 years
Potential Impact:	High – disruptive
EU Goal alignment:	Affordable and clean energy
Techniques:	Quantum Annealing, Adiabatic Paradigm
Source of use case:	MULTIVERSE COMPUTING

Summary

Quantum Computing in Energy Production Forecasting leverages quantum algorithms for precise energy output predictions, particularly from renewable sources like solar and wind. The inherent volatility of these sources complicates energy management, necessitating advanced forecasting methods. Quantum computing, capable of handling extensive data sets and complex calculations at unparalleled speeds, offers a robust solution. It not only predicts energy production fluctuations with higher accuracy but also facilitates the integration of renewable sources into the energy mix, promoting a more sustainable energy landscape.

Description

Business Challenge:

Integrating Quantum Computing into Energy Production Forecasting presents significant challenges, primarily the merger of this cutting-edge technology with established forecasting systems. This integration demands considerable investment in R&D, training in quantum computing and meteorology, and the development of a skilled workforce. The collection, processing, and interpretation of large-scale meteorological and energy data pose additional challenges in computational capacity, data accuracy, and security. Ensuring the reliability and accessibility of quantum computing resources for continuous, real-time forecasting also remains a critical concern.

Value Proposition:

The adoption of Quantum Computing in Energy Production Forecasting offers substantial benefits. It enhances the precision of predicting renewable energy outputs, leading to more efficient grid management, reduced operational costs, and a decrease in dependence on fossil fuels. For energy providers, this advanced forecasting capability allows for better resource allocation and risk management, adapting swiftly to energy production changes. Consumers benefit from a more reliable energy supply, potentially lower costs, and a shift towards a more environmentally responsible energy infrastructure.

Solution Approach:

The implementation strategy for Quantum Computing in Energy Production Forecasting involves the creation of bespoke quantum algorithms to analyze and interpret complex weather patterns and energy production data accurately. These quantum algorithms, operating on state-of-the-art quantum computing platforms, offer rapid and comprehensive data analysis capabilities far beyond classical computing methods. The collaborative effort between energy sector specialists, meteorologists, and quantum scientists is key to developing effective and accurate forecasting models. This approach not only aims at enhancing the accuracy of predictions but also at establishing a scalable and adaptable framework for future advancements in quantum computing and energy forecasting.

References

[1] Stavros Efthymiou, Jack Hidary, and Stefan Leichenauer. 2019. “Tensor Network for Machine Learning”
[2] Caio B. D. Goe, Thiago O. Maciel, Eduardo I. Duzzion, Giovani G. Pollachini, Rafael Cuenca and Juan P. L. C. Salazar. 2021. “QBoost for regression problems: solving partial differential equations.”
[3] Maria Schuld, Ilya Sinayskiy and Francesco Petruccione. 2016. “Prediction by linear regression on a quantum computer”.
[4] Mansoor Khan, Tianqi Liu and Farhan Ullah. 2019. “A New Hybrid Approach to Forecast Wind Power for Large Scale Wind Turbine Data Using Deep Learning with TensorFlow Framework and Principal Component Analysis”
[5] Paweł Piotrowski, Dariusz Baczy ´nski, Marcin Kopyt and Tomasz Gulczy´nski. 2022. Advanced Ensemble Methods Using Machine Learning and Deep Learning for One-Day-Ahead Forecasts of Electric Energy Production in Wind Farms”.

Use Case 5: Smart Grids Optimization.

Brief description

Computational Problem Type:	Optimization
Problem Domain:	Energy Optimization
Subdomain:	Smart Grids
Industry:	Energy
Time to Maturity (TRL):	Medium: >5 years
Potential Impact:	High – disruptive
EU Goal alignment:	Affordable and clean energy
Techniques:	Quantum Annealing, Adiabatic Gate Paradigm
Source of use case:	MULTIVERSE COMPUTING

Summary

Quantum Computing for Smart Grid Optimization presents a cutting-edge approach to enhancing the efficiency and reliability of electrical grid systems. By harnessing the unparalleled computational power of quantum computers, this application tackles complex optimization problems in grid management that are beyond the reach of classical computing methods. Quantum algorithms can rapidly analyze vast amounts of data, predict energy demand patterns, and optimize energy distribution in real-time. This not only leads to a more efficient use of renewable energy sources but also significantly reduces energy wastage and improves the overall stability of the power supply. Additionally, quantum computing aids in the integration of decentralized energy resources, enabling a more dynamic and responsive grid system. This technology marks a significant leap towards a sustainable, efficient, and resilient energy future.

Description

Business Challenge:

Implementing Quantum Computing in Smart Grid Optimization presents multifaceted challenges, primarily in integrating cutting-edge quantum technology with traditional electrical grids. This integration demands substantial investment in research and specialized workforce development, as expertise in both quantum computing and energy systems is currently scarce. The task involves not only technological adaptation but also a fundamental shift in grid management practices to fully exploit quantum computing's potential. Additionally, managing the vast data generated by smart grids and ensuring its security is crucial. Another significant hurdle is the high cost of implementation and maintenance, posing a particularly daunting challenge for smaller energy providers. Balancing these upfront expenses against the anticipated long-term benefits in efficiency and environmental impact remains a critical business decision.

Value Proposition:

Integrating Quantum Computing into Smart Grid Optimization offers transformative benefits, significantly enhancing grid efficiency and reliability through advanced data processing and optimization capabilities. For utility companies, this translates into cost savings, improved demand management, and greater resilience, leading to higher customer satisfaction. Consumers benefit from more stable and potentially lower energy costs. Critically, this technology aligns with global sustainability goals, facilitating efficient energy use, reducing emissions, and supporting a greener energy mix. Despite being in early development stages, quantum computing in smart grids represents a substantial economic and environmental opportunity, underscoring its potential as a key driver in the evolution towards sustainable energy systems.

Solution Approach:

The implementation of Quantum Computing in Smart Grid Optimization is centered around the utilization of Quantum Annealing, a technique particularly suited for solving complex optimization problems that are typical in modern electrical grid management. Quantum Annealing excels in finding the optimal configuration among a vast set of possibilities, making it ideal for balancing and optimizing energy distribution across a dynamic and ever-changing grid landscape.

This approach involves integrating Quantum Annealing with current grid management systems to enhance real-time decision-making. The technology will enable the grid to adapt efficiently to varying energy demands and the intermittent nature of renewable energy sources. Continuous development and refinement of grid management software are essential, combining Quantum Annealing's powerful optimization capabilities with classical computing resources for seamless operation.

The integration of Quantum Annealing promises not only a more efficient and reliable electricity grid but also a forward-looking solution that is scalable and adaptable to future energy challenges and advancements in quantum technology.

References

[1] Aiswariya L., T. P Imthias Ahamed, Sheik Mohammed S. 2020. “Optimal Microgrid Battery Scheduling Using Simulated Annealing”.
[2] Fernando Postigo Marcos, Carlos Mateo Domingo, Tomás Gómez San Román and Rafael Cossent Arín. 2020. “Location and Sizing of Micro-Grids to Improve Continuity of Supply in Radial Distribution Networks”.
[3] Marina Fernandez-Campoamor, Corey O’Meara, Giorgio Cortiana, Vedran Peric and Juan Bernabe-Moreno. 2021. “Community Detection in Electrical Grids Using Quantum Annealing”.
[4] Yifan Zhou, Zefan Tang, Nima Nikmehr, Pouya Babahajiani, Fei Feng, Tzu-Chieh Wei, Honghao Zheng and Peng Zhang. 2022. “Quantum computing in power systems”.
[5] Fernando Postigo Marcos, Carlos Mateo Domingo, Tomaś Gomeź San Roman. 2022. “Improving distribution network resilience through automation, distributed energy resources, and undergrounding”.

Use Case 6: Hydrogen generation optimization.

Brief description

Computational Problem Type:	Optimization
Problem Domain:	Quantum Optimization
Subdomain:	Green hydrogen and hydrogen generation plants
Industry:	Energy
Time to Maturity (TRL):	Medium: >3 years
Potential Impact:	High – disruptive
EU Goal alignment:	Affordable and clean energy
Techniques:	Quantum Annealing, Adiabatic Gate Paradigm
Source of use case:	MULTIVERSE COMPUTING, IDEA INGENIERÍA

Summary

Improve efficiency and reduce costs in green hydrogen production through electrolysis optimization. This is achieved by combining the digital twin, which allows the creation of an accurate virtual replica of the electrolysis system, and quantum computing, which helps solve complex optimization problems. This development has the potential to have a positive impact on industry and society.

Description

Business Challenge:

The current landscape in energy demands a significant shift towards sustainability, necessitating the adoption of cleaner energy sources and reducing reliance on fossil fuels. In this context, hydrogen holds immense promise as a clean energy carrier. However, the conventional methods of producing hydrogen through electrolysis are encumbered by inefficiencies and high energy consumption. The critical challenge facing the industry is the inherent inefficiency of the electrolysis process for hydrogen generation. This traditional method requires substantial energy input, primarily from non-renewable sources, leading to elevated operational costs and impeding its widespread adoption. The energy-intensive nature of electrolysis poses economic barriers, hindering the scalability and economic viability of green hydrogen, crucial for large-scale integration into sustainable energy ecosystems. Moreover, the escalating global demand for sustainable energy solutions intensifies the urgency to optimize hydrogen production processes. The industry faces mounting pressure to streamline operations, reduce carbon footprints, and enhance energy efficiency while ensuring cost-effectiveness. These challenges create a formidable barrier to achieving the full potential of green hydrogen technology. Addressing these hurdles is paramount to realizing a sustainable energy future. Thus, optimizing electrolysis processes to make green hydrogen economically competitive and environmentally viable stands as a pressing business challenge for the industry.

Value Proposition:

Our pioneering initiative offers a transformative solution poised to revolutionize the landscape of green hydrogen production by addressing critical challenges and unlocking unparalleled opportunities. At the heart of our value proposition lies the fusion of cutting-edge technologies: the digital twin and quantum computing. This innovative fusion propels us to deliver significant value to the industry and broader sustainability objectives. By leveraging the digital twin technology, we create an exact virtual replica of the electrolysis system. This precise emulation enables real-time monitoring, analysis, and optimization of the hydrogen generation process. Concurrently, the integration of quantum computing capabilities enables us to apply advanced algorithms for optimizing these complex chemical processes. This synergy between the digital twin and quantum algorithms results in a paradigm shift, empowering us to fine-tune electrolysis operations with unprecedented precision and efficiency.

Our solution doesn't solely aim at optimizing processes; it fundamentally reshapes the perception of green hydrogen's feasibility. We offer a sustainable, scalable, and economically viable approach to hydrogen production. By significantly enhancing operational efficiency, we reduce energy consumption while maximizing hydrogen output, effectively mitigating the cost barriers that hinder widespread adoption. Moreover, our value proposition extends beyond immediate operational enhancements. We catalyze the transition towards a more sustainable energy future by making green hydrogen economically competitive and widely accessible. This innovation aligns with global sustainability agendas, positioning stakeholders at the forefront of a burgeoning industry while contributing substantially to environmental preservation. In essence, our value proposition transcends mere technological advancements. It represents a catalyst for transformative change—an opportunity to not only optimize hydrogen production but also revolutionize the energy sector by paving the way for a more sustainable and economically feasible future.

Solution Approach:

Our solution embodies a groundbreaking approach, merging state-of-the-art technologies to tackle the challenges hampering efficient hydrogen production through electrolysis. The strategic integration of the digital twin and quantum computing represents a pioneering path towards optimizing the entire hydrogen generation process.

The foundation of our solution lies in the implementation of a digital twin—a highly accurate virtual replica of the electrolysis system. This digital replica provides a comprehensive and real-time representation of the physical setup, facilitating in-depth analysis, monitoring, and simulation of the electrolysis process. Concurrently, our solution leverages the capabilities of quantum computing, employing advanced algorithms designed to optimize processes with unparalleled precision. Through the digital twin, we replicate and monitor the intricacies of the electrolysis process, capturing minute details and variables that influence hydrogen generation. Quantum-inspired algorithms are then employed to fine-tune these processes, seeking optimal configurations and conditions that maximize hydrogen output while minimizing energy consumption.

Our approach is holistic, focusing not only on process optimization but also on scalability and economic viability. By harnessing the potential of quantum computing within the digital twin framework, we aim to revolutionize the efficiency and cost-effectiveness of hydrogen production. This synergy enables us to identify, test, and implement highly efficient operational parameters, resulting in substantial improvements in both output and energy efficiency. Moreover, the strategic integration of these cutting-edge technologies positions our solution as a catalyst for broader industry transformation. By optimizing electrolysis processes and making green hydrogen production economically viable, we pave the way for its widespread adoption. This solution not only addresses immediate operational challenges but also aligns with global sustainability goals, contributing significantly to a cleaner, more sustainable energy ecosystem.

In summary, our solution represents a paradigm shift in hydrogen production methodologies, offering a comprehensive, technologically advanced, and economically feasible approach that not only optimizes processes but also champions the transition towards a more sustainable energy future.

References

[1] Institute for Energy Technology, P.O. Box 40, N-2027 Kjeller, Norway “Modeling of advanced alkaline electrolyzers: a system simulation approach”.

[2] Jesús Rodríguez and Ernesto Amores, December 2020, “CFD Modeling and Experimental Validation of an Alkaline Water Electrolysis Cell for Hydrogen Production”.

[3] Monica Sanchez, Ernesto Amores, David Abad, Lourdes Rodríguez, Carmen Clemente-Jul, 2029, “Aspen Plus model of an alkaline electrolysis system for hydrogen production”.

[4] Georgios Sakas, Alejandro Ibanez-Rioja, Vesa Ruuskanen, Antti Kosonen, Jero Ahola, Olli Bergmann, 2021, “Dynamic energy and mass balance model for an industrial alkaline water electrolyzer plant process”.

[5] Alejandro Ibáñez-Rioja, Pietari Puranen, Lauri Järvinen, Antti Kosonen, Vesa Ruuskanen, Jero Ahola, Joonas Koponen, "Simulation methodology for an off-grid solar–battery–water electrolyzer plant: Simultaneous optimization of component capacities and system control".

[6] Manuel Tobias Baumhof, Enrica Raheli, Andrea Gloppen Johnsen, and Jalal Kazempour, 2023, "Optimization of Hybrid Power Plants: When Is a Detailed Electrolyzer Model Necessary?".

Use Case 7: Faster Energy Market Price Operation.

Brief description

Computational Problem Type:	Combinational Optimization
Problem Domain:	Energy
Subdomain:	Market Price Operation
Industry:	Energy
Time to Maturity (TRL):	Medium: 5 years
Potential Impact:	High – disruptive
EU Goal alignment:	Energy and the Green Deal
Techniques:	Quantum Annealing, Quantum inspired.
Source of use case:	QILIMANJARO QUANTUM TECH

Summary

The day-ahead market (DAM) problem represents a key challenge in the management of contemporary electricity markets. It consists of efficiently scheduling and dispatching electrical energy for the upcoming 24-hour period. The DAM serves as a platform where electricity producers and electricity consumers participate by submitting offers to sell or bids to buy electricity for specific time intervals in the following day.

The objective is to determine the set of offer orders required to meet hourly demand while optimizing social welfare by maximizing both consumer and producer surpluses, subject to network topology and hourly transmission capacity constraints.

In the constantly evolving and competitive energy industry, the need for faster and more efficient models has become increasingly apparent. This use case introduces a quantum-inspired algorithm developed for an electrical company that achieved a significant time reduction whilst maintaining the optimality of the solutions found.

Description

Business Challenge:

The algorithm considers a set of orders, consisting of both bidding offers and demands, for different plants distributed across various bidding zones. These zones are interconnected via a power transmission network that accommodates different capacities of energy flow for different interconnections, time windows, and direction, without considering losses or tariffs for these lines. Each offer has a different type and merit order based on the source of energy and priority. The selection of orders from the offerings optimization problem determines the final flow of each traffic line, fulfilling that the total amount of accepted offers must be equal to the demand and respecting the topology and hourly transmission network capacities.

Value Proposition:

The quantum algorithm's formulation starts by defining which values and variables are needed in the problem's Hamiltonian, i.e., a mathematical construction that relates to the energy of the problem), encoding such variables in the Quadratic Unconstrained Binary Optimization (QUBO) model, which is widely used in solving optimization problems with quantum annealing.

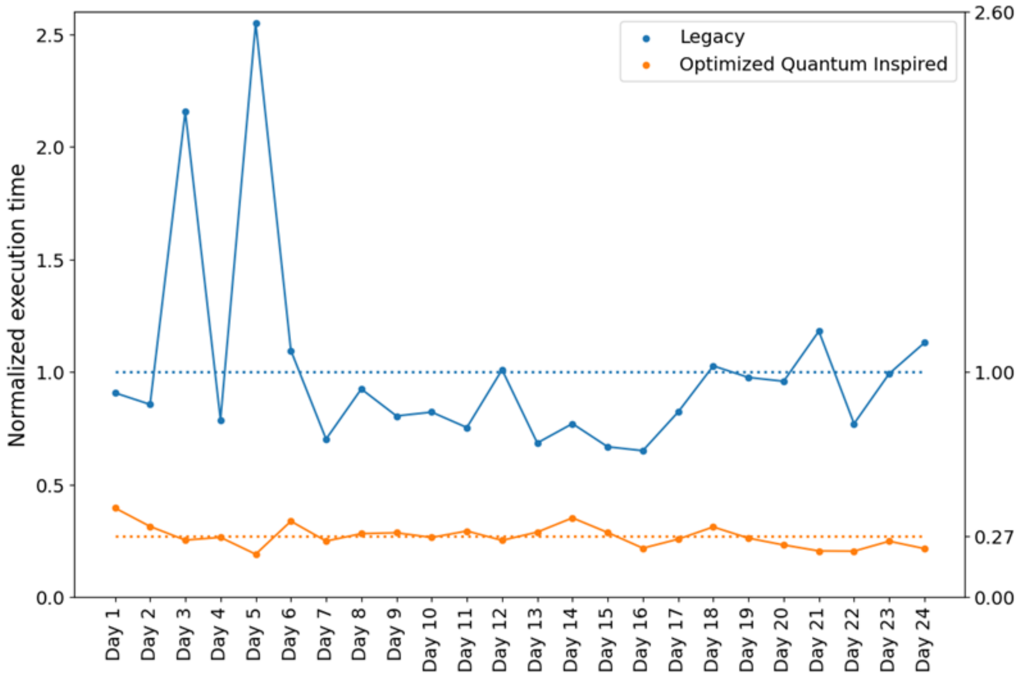
The Hamiltonian contains all the constraints and variables to guarantee that the solution of the optimization problem is in the system's state of lower energy (ground state) according to the basics of quantum annealing. Each constraint in the Hamiltonian has an associated coefficient that defines its strength and that must be assigned before optimization begins. Determining these optimal coefficients can be challenging but, as a rule of thumb, the stricter a constraint is—such as physical constraints linked to the network flow capacity—the larger its coefficient should be.

Since finding the optimal solution that satisfies all the constraints may be computational expensive for certain sizes of the problem, e.g., during hours with large offer and demand volumes, we extended the algorithm to find approximated solutions, i.e., those that slightly break the constraints of the problem. Relaxing the constraints enlarges the space of solutions, resulting in a trade-off between optimality and speed. These error margins are introduced as parameters that are controlled by the user and that can be easily tuned at each execution.

After the formulation was properly refined, an in-depth assessment of several candidate optimization solvers and algorithms was performed. This implied extensive testing of multiple algorithmic combinations and configurations to identify the most effective setup to achieve optimal results.

Solution Approach:

The solution developed relays on a Quantum-Inspired algorithm that resulted 4x faster (75% time reduction, see image below) than the company's current algorithm, whilst maintaining the optimality of the solutions found. The problem formulation was designed to suit current commercial quantum and quantum-inspired platforms, and the solver algorithm included several heuristics that allowed for a significant reduction in the number of variables required to solve the problem.



Use Case 8: Efficient packing in bins.

Brief description

Computational Problem Type:	Combinational Optimization
Problem Domain:	Logistics
Subdomain:	Bin Packing Problem
Industry:	Mobility & Logistics (vertical market) and industry (horizontal market)
Time to Maturity (TRL):	Medium: <5 years
Potential Impact:	High – disruptive
EU Goal alignment:	Industry, innovation and infrastructure
Techniques:	Quantum Annealing, Adiabatic Paradigm
Source of use case:	SERIKAT, TECNALIA

Summary

Efficient packing of items into bins or containers is a common daily task for industry and logistic companies. Known as Bin Packing Problem, it has been intensively studied in the field of optimization and Artificial Intelligence. Since decades, many variants have been proposed, with the three-dimensional Bin Packing Problem as the closest one to real-world use cases. This Use Case introduces a hybrid quantum-classical framework for solving real-world three-dimensional Bin Packing Problems, considering different realistic characteristics, such as: package and bin dimensions, overweight restrictions, affinities among item categories and preferences for item ordering.

Description

Business Challenge:

The widespread interest in combinatorial optimization problems such as the Bin Packing Problem (BPP) can be divided into two distinct facets. Firstly, there is a notable business interest inherent in these problems, stemming from their origins in real-world, everyday challenges. Various practical scenarios can be effectively modelled as Bin Packing combinatorial optimization problems for more efficient treatment and resolution. Secondly, a significant subset of these problems presents formidable complexity in their solutions, presenting an enticing challenge for operational businesses. These problems fall under the classification of NP-Hard problems. Following the principles of computational complexity theory, the Bin Packing Problem earns the NP-Hard designation, meaning that there is no technique capable of determining an optimal solution for all instances within polynomial time. The one-dimensional BPP is considered the simplest packing problem. This problem involves a set of packages, each with an associated size, and an unlimited supply of containers with the same capacity. The goal of the one-dimensional BPP is to pack all the packages into the fewest possible containers, thereby minimizing the number of containers used. Starting from this simple formulation, numerous variations of the BPP have been proposed in recent literature to address real-world situations within the logistics and industrial domains. These variants have a variable number of constraints and conditions, increasing the complexity of problem resolution.

Value Proposition:

The objective of the BPP is to minimize the number of containers (or bins, or cargo vehicles) of a specified capacity (dimension, maximum load) needed to pack a set of items. Although it is a problem traditionally associated with the logistics field, its application can quickly extend to other areas such as content allocation to storage tapes or disks, allocation of virtual machines to servers, optimization of cutting variable-sized pieces in fabrics, wood, or metals (equivalent to a 2-dimensional problem), etc.

In its common formulation, the problem involves packing a given number N of items (i1, i2, ... in) into the smallest possible number of containers, each with a capacity of q. Naturally, the dimension of these items is less than q.

The variety and typology of cases within this type of problem are also extensive, based on factors such as dimensionality, type of elements, homogeneity or characteristics, constraints, handling costs, etc. Even though there are many variations based on these criteria, a representative case of the problem is the optimization of packing N 3-dimensional items (x, y, z) into M containers of, for example, equal dimensions and specified limitations (e.g., weight). The objective is to identify the location and orientation of the items to minimize container usage while meeting applicable constraints. This problem can be simplified for 1-dimensional problems, such as the weight of the items and the container's capacity limit—like a vehicle, for instance; or for 2-dimensional problems, to place elements in a single layer, such as on a pallet, or for more than 3 dimensions, if, for example, optimizing the 3-dimensional case includes the container's centre of gravity (as in the case of air transport of the container).

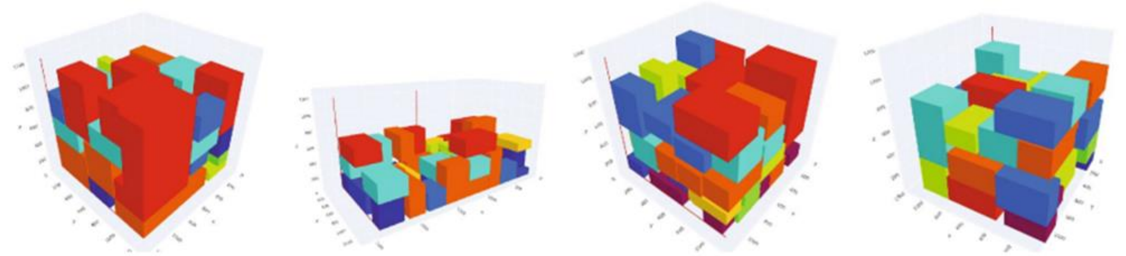
The type of constraints applicable in these cases can be equally extensive: related to handling operations (e.g., if the item needs to be removed from the container early or late), the order or arrival time of items, and whether they eventually need to be processed in small groups at specified times, with intrinsic constraints (they cannot be close to the surface due to temperature-related issues), expiration issues, resistance or fragility for stacking, depending on the size of the base, grouping issues (if an item has to be associated with others and, therefore, in the same or near containers), etc.

Solution Approach:

The proposed solution is a hybrid quantum-classical framework for solving real-world three-dimensional Bin Packing Problems, coined *Q4RealBPP* or Quantum for Real Bin Packing Problems. The Q4RealBPP solution is geared towards real applications in industrial and logistics fields, addressing challenges such as organizing port containers, optimizing the loading of delivery vans and trucks, or arranging food items on distribution pallets, among others. Utilizing a hybrid quantum-classical approach, Q4RealBPP marks a significant advancement in solving 3-dimensional Bin Packing Problems (3 dBPP) with the explicit goal of addressing real-world issues valued by end-users and companies. This framework resorts to the Leap Constrained Quadratic Model (CQM) Hybrid Solver (LeapCQMHybrid) of D-Wave. At the same time, Q4RealBPP is built on an existing code (D-Wave Ocean Developers Team: 3d-bin-packing, GitHub repository, 2022, https://github.com/dwave-examples/3d-bin-packing - last retrieved 2023/02/27). In this code, the problem is framed in a way that requires numerous variables, leading to a high demand for qubits. This poses a challenge in terms of feasibility, particularly within the context of quantum hardware during the Noisy Intermediate-Scale Quantum (NISQ) era. Consequently, optimizing the code becomes imperative when tackling intricate problems. The refinement in the mathematical formulation done in Q4RealBPP allows problems for being formulated using fewer variables, directly enhancing the framework's capability to handle larger instances.

Furthermore, the previous code was also oriented toward solving the most basic variant of the 3dBPP by only considering the dimension of both packages and bins. Taking this situation into consideration, the mathematical formulation in Q4RealBPP has been extended in order to address real-world oriented settings. Key features encompassed by Q4RealBPP include (1) dimensions of packages and bins, (2) maximum allowable weight per bin, (3) positive and negative affinities among item categories, and (4) preferences for package ordering in terms of load-bearing and load balancing. To showcase its applicability, several experiments were conducted using 12 different instances as illustrative examples. Moreover, Q4RealBPP enables users to easily construct flexible and well-defined instances, adapting a multitude of real-world situations for quantum computer-based solutions.

(a) Colour palette scheme used to relate `id` (item categories) with colours in the illustrative examples.

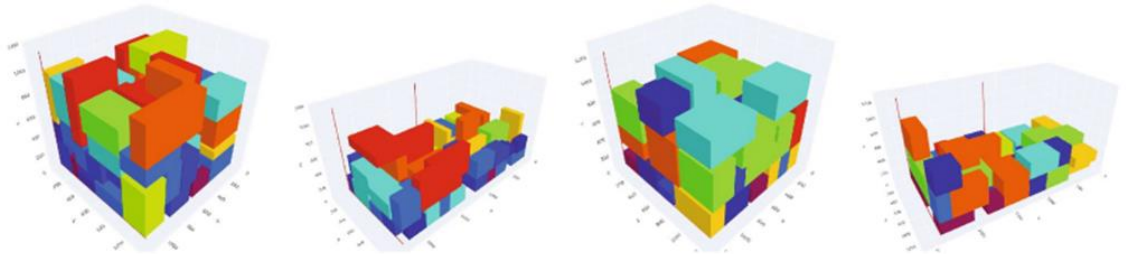


(b) 3dBPP_1: 51 items without restrictions and $\sum_{i\in I}\mu_i = 1776$.

(c) 3dBPP_2: inst. 3dBPP_1 with $M = 1000$.

(d) 3dBPP_3: 52 items without restrictions.

(e) 3dBPP_4: inst. 3dBPP_3 with $\eta = 2$. {0:■, 1:■, 9:■} weight more than twice of {3:■, …, 8:■}.

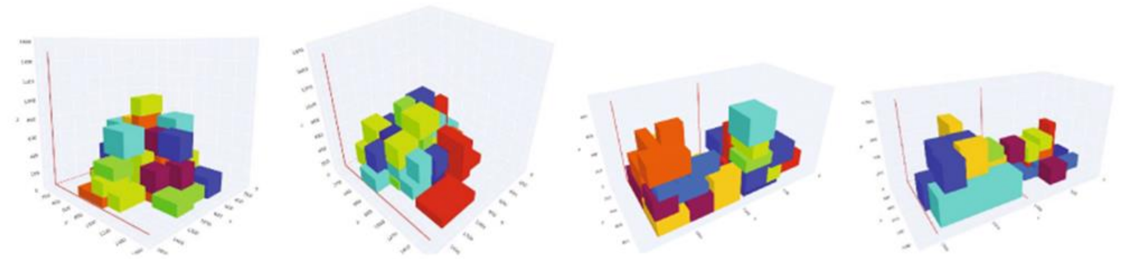


(f) 3dBPP_5: 54 items without restrictions.

(g) 3dBPP_6: inst. 3dBPP_5 with {(4:■, 7:■), (7:■, 9:■)} incompatible.

(h) 3dBPP_7: 46 items without restrictions.

(i) 3dBPP_8: inst. 3dBPP_7 with (4:■, 8:■) incompatible and {(0:■, 3:■), (0:■, 8:■)} together.



(j) 3dBPP_9: center of mass at $(\tilde{L}, \tilde{W}) = (750, 750)$, the middle of the bin.

(k) 3dBPP_10: center of mass at $(\tilde{L}, \tilde{W}) = (900, 500)$.

(l) 3dBPP_11: $M = 800$; $\eta = 2$ and {0:■, 7:■} weight more than twice of the rest; (7:■, 9:■) incompatible; {(0:■, 3:■), (0:■, 8:■)} together; $(\tilde{L}, \tilde{W}) = (750, 750)$.

(m) 3dBPP_12: $M = 900$; $\eta = 2$ and {3:■, 4:■} weight more than twice of the rest; (4:■, 8:■) incompatible; (2:■, 4:■) packed together; $(\tilde{L}, \tilde{W}) = (500, 500)$ (the middle).

Lastly, the most recent version of Q4RealBPP also includes the following new characteristics: i) the existence of heterogeneous bins, ii) the extension of the framework to solve not only three-dimensional, but also one- and two-dimensional instances of the problem, iii) the inclusion of requirements for item-bin associations, and iv) restrictions regarding delivery priorities.

References

[2] Romero, S., Osaba, E., Villar-Rodriguez, E., Oregi, I., Ban, Y., "*Hybrid approach for solving real-world bin packing problem instances using quantum annealers*", Sci Rep 13, 11777 (2023). https://doi.org/10.1038/s41598-023-39013-9

[3] Romero, S. V., Osaba, E., Villar-Rodriguez, E., & Asla, A. (2023). "*Solving Logistic-Oriented Bin Packing Problems Through a Hybrid Quantum-Classical Approach*". In *2023 IEEE Intelligent Transportation Systems Conference (ITSC)*. IEEE. , https://arxiv.org/abs/2308.02787

[4] Osaba, E., Villar-Rodriguez, E., & Romero, S. V., "*Benchmark dataset and instance generator for Real-World Three-Dimensional Bin Packing Problems*", 2023, *Data in Brief*, 109309, https://www.sciencedirect.com/science/article/pii/S2352340923004286?via%3Dihub

Use Case 9: Management of empty containers at maritime ports.

Brief description

Computational Problem Type:	Combinational Optimization
Problem Domain:	Logistics
Subdomain:	Management of empty containers at maritime ports
Industry:	Mobility & Logistics (maritime)
Time to Maturity (TRL):	Medium: <5 years
Potential Impact:	High – disruptive
EU Goal alignment:	Industry, innovation and infrastructure
Techniques:	Quantum Annealing, Adiabatic Paradigm
Source of use case:	QUANTUM MADS

Summary

During the logistics chain, maritime containers go through different stages, whether with or without cargo, commonly known as the container cycle. Global logistics involved in this process is highly complex and is focused on achieving efficient management of the container fleet by minimizing transportation costs and environmental impact and maximizing container usage.

An essential part of global container logistics is empty container logistics. This type of logistics studies the process of transportation, storage, and distribution of these containers, which begins once the container is emptied at the recipient's facilities and ends when the container is deployed for loading at the loading facilities.

Within this logistics framework, the Use-case focuses on the local level, i.e., on the internal movement of empty containers between port terminals, empty container depots (where empty containers are temporarily stored), consignees (who receive imported full containers that are emptied there), and shippers (who receive empty containers loaded for export).

Description

Business Challenge:

The inefficiency of managing empty containers represents one of the most significant costs for companies in the maritime sector. Around 21% of the containers in the total traffic on the main trade routes are empty and more than 50% of their lifespan is spent empty, either in storage or during transportation. Finding innovative ways to optimize this management with a significant economic and environmental impact is, therefore, a priority. Every container movement has an associated economic and environmental cost that depends on the operations required to perform the transport. The problem is to decide how many containers are set in motion, where they originate and where they are headed to meet the demand with the existing supply capacity within a time window.

Value Proposition:

The solution provides a tool for the efficient management of empty containers at local level, based on the daily needs of shippers, terminals, and consignees, and using classical optimization and machine learning. It incorporates quantum nodes to execute computationally expensive subroutines.

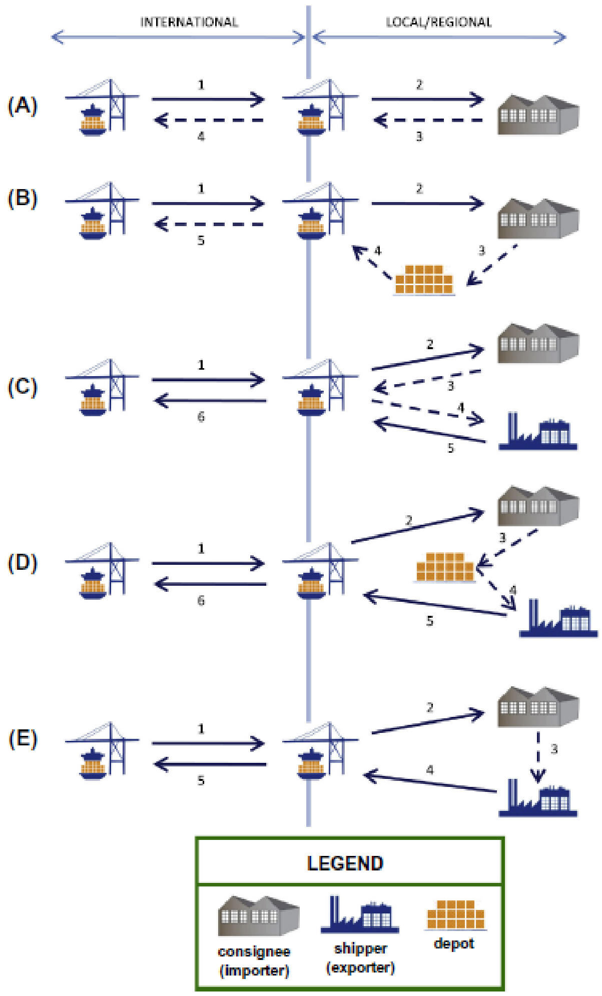
Solution Approach:

The problem of empty container repositioning falls into the NP-hard problems class, requiring exponentially more computational resources as the size of the problem grows. Thus, the solution provides a logistic-port optimization solver based on classical-quantum hybrid algorithms to efficiently tackle real-world sized problem instances. It manages the entire process to consistently meet the demand for empty containers while minimizing the required economic and environmental cost. This translates into deciding how many containers are set in motion, where the empty containers come from (who the suppliers will be) and where they should go (to serve which demanders or supply which warehouses) so that present and future demand is satisfied with the lowest possible cost.

The solution focuses on the internal movement of empty containers between port terminals, empty container depots (where they are temporarily stored), consignees (who receive the imported filled containers with the aim of unloading), and shippers or dispatchers (who receive the empty containers for loading for future export) are included. The movements of empty containers occur in different scenarios:

- A container has been emptied at the consignee's location and needs to be stored. Storage takes place in an intermediate depot or at the port terminal. When the container is exported empty (leaving abroad through the terminal), the cycle is considered within the category of container repositioning -cases A and B in the figure below.
- The empty container, after being emptied at the consignee's location, is assigned to a new loading process at a shipper, with the aim of exporting it through the port terminal. The assignment can occur after temporary storage in a depot or, less often, directly after being emptied in the consignee's warehouses. This latter scenario is what is referred to as a "street-turn", and both cases fall into the "match back" category.

The following figure provides the patterns of container movement with dashed lines indicating movements of empty containers and continuous lines indicating loaded container transport.



The mathematical formulation comprises the origin-destination tuple (between consignees, shippers, depots or port terminals), time windows, number and container types for each time slot, the demand and supply of empty containers at the ends of the cycle to be managed, the storage capacities and the initial inventory of facilities that enable storage at the depots or port terminals, and the costs incurred in the storage of empty containers and in their transportation.

The objective of the solution cost function is to minimize the economic and environmental costs associated with the transport and storage of empty containers, given:

- A specified availability of empty containers leaving consignees after unloading.
- A demand for empty containers from the shipper-exporters that needs to be met.
- A storage capacity in depots and port terminals that cannot be exceeded and, in the case of depots, must also be kept.
- A set of inventories in depots and port terminals that need to be updated with the entries and exits of empty containers over time and that contribute to the availability of containers.

References

[1] Furió, S., Andrés, C., Adenso-Díaz, B., Lozano, S., “Optimization of empty container movements using street-turn: Application to Valencia hinterland”. Computers & Industrial Engineering, Volume 66, Issue 4, 2013, pages 909-917, ISSN 0360-8352, https://doi.org/10.1016/j.cie.2013.09.003.

[2] Wang, B., & Wang, T., “Research on the optimization of intermodal empty container reposition of land-carriage”. Journal of Transportation Systems Engineering and Information Technology, Volume 7, Issue 3, 2007, pages 29-33, ISSN 1570-6672, https://doi.org/10.1016/S1570-6672(07)60020-8

[3] González-Torre, P., Sarkis, J., & Adenso-Díaz, B., “Shipping agents and container management: An exploratory analysis of infrastructural and cost concerns”. International Journal of Shipping and Transport Logistics, (IJSTL), Vol. 5, No. 3, 2013.

[4] Hosseini, A., Sahlin, T., “An optimization model for management of empty containers in distribution network of a logistics company under uncertainty”. J. Ind. Eng. Int. 15, 585–602 (2019). https://doi.org/10.1007/s40092-018-0286-2.

[5] Gusah, L., Cameron-Rogers, R., Thompson, R. G., “A systems analysis of empty container logistics – a case study of Melbourne, Australia”. Transportation Research Procedia, Volume 39, 2019, pages 92-103, ISSN 2352-1465, https://doi.org/10.1016/j.trpro.2019.06.011.

[6] Meseguer Llopis, J., Furio Prunonosa, S., Llop Chabrera, M., Cubas Rodriguez, F.J. (2021). “Artificial Neural Network Based Empty Container Fleet Forecast”. In: Rutkowski, L., Scherer, R., Korytkowski, M., Pedrycz, W., Tadeusiewicz, R., Zurada, J.M. (eds) Artificial Intelligence and Soft Computing. ICAISC 2021. Lecture Notes in Computer Science, vol 12854. Springer, Cham. https://doi.org/10.1007/978-3-030-87986-0_10.

Use Case 10: Bus routes optimization.

Brief description

Computational Problem Type:	Combinational Optimization
Problem Domain:	Mobility
Subdomain:	Public Urban Transport
Industry:	Mobility & Logistics
Time to Maturity (TRL):	Medium: <5 years
Potential Impact:	High – disruptive
EU Goal alignment:	Industry, innovation and infrastructure
Techniques:	Variational Quantum Eigensolver (VQE)
Source of use case:	ACCENTURE

Summary

Within this public transportation framework, the Use-case focuses on a simplified optimization process for selecting the minimum number and best environmental-friendly routes to cover several bus stops. This Use-case is particularly useful for planning a new bus route service.

Description

Business Challenge:

Efficient optimization of bus routes to the demand plays a crucial role in the planning of public transport systems from a social, economic, and environmental perspective. The general goal of this optimization process is to reduce the number, size or cost (economic or environmental) of bus routes, rearrange bus stops, prioritize low or no-emissions vehicles, optimize the bus passenger capacity, or decrease the idle time of empty buses on the road. Other specific aspects may be included as well, for instance those related to varying schedules due to special events that may influence the normal provision of public transportation, or the accommodation to special requirements such as accessibility needs.

There is also an increased need to adapt bus route planning to dynamic conditions. These conditions can include fluctuations in passenger demand, traffic patterns, weather events, and unforeseen incidents. To address these challenges, transit agencies are demanding more powerful tools that allow for making on-the-fly adjustments to bus routes. This current optimization processes and solutions tend to be slow with classical technologies and requires high processing capabilities.

Value Proposition:

The proposed solution with quantum technologies, together with classical optimization and machine learning, could led in the medium term to solutions that provide effective planning of public transportation adapted to dynamic conditions in near real-time or even in real-time.

Solution Approach:

The solution provides a bus routes optimization function to enhance the economic and environmental sustainability of public transportation. This type of optimization functions is primarily associated with two well-known and studied optimization problems: the TSP (Travelling Salesman Problem) and the VRP (Vehicle Routing Problem):

- The general TSP problem addresses the optimization of the route a person must take to visit all different points once and return to the origin with the shortest distance (or in the least amount of time). It is relevant to goods planning and logistics, as well as other related services such as SAT (Technical Assistance Services) planning. This is a problem that quickly escalates in complexity. Specifically, it is an NP-hard combinatorial optimization problem. For N nodes, the general number of combinations is (N-1)!/2.

Beyond 25-30 nodes (about 10^30 combinations), the problem becomes impractical for classical computing. Moreover, the problem becomes more complicated with the introduction of constraints that may exist in a real-world context: one-way streets, tolls, risk probabilities (traffic congestion, accidents, temperatures, and weather conditions), carrier time windows, etc.

- The VRP problem, similar to the TSP, addresses the total cost optimization for routes of a fleet of vehicles serving a set of customers, bus stops or destinations. In this case, the applicable constraints become significant: vehicle capacities, consumption and emissions, customer time restrictions, location restrictions (restricted roads, for example), number of stops, whether delivery and pickup are combined, etc.

The solution focuses on a hybrid classical – quantum approach, with the VQE – Variational Quantum Eigensolver algorithm in the quantum part. This type of algorithm is suited for finding the ground state energy of a given quantum system. Applied to the Use-case problem It allows to find a solution to a combinatorial problem through the quantum tunnelling effect. This effect enables the calculation of gradients across the problem's surface without getting stuck in a local minimum or plateau. VQE is effective for calculating global minima but not for local minima. This is the advantage over its classical counterparts, which often struggle to reach the global minimum of the problem. VQE uses a parameterized quantum circuit to calculate the cost and combines it with a classical optimizer to iteratively improve the parameters of the quantum part. This hybrid approach makes VQE a promising algorithm for near-term quantum computers to solve real-world problems.

The approach was implemented for the bus routes problem with the following constraints:

- All stops must be covered by at least one bus.
- The same route cannot be repeated for a journey.
- All arrivals must end at the same point.
- All departures must start from the same point.
- The possibility of sub-routes within the graph is eliminated.
- Journeys exceeding a certain carbon footprint are not allowed (approximate data).

References

[7] E. Osaba, E. Villar-Rodriguez and I. Oregi, A Systematic Literature Review of Quantum Computing for Routing Problems. IEEE Access, vol. 10, pp. 55805-55817, 2022, 10.1109/ACCESS.2022.3177790

Use Case 11: ZKP – PQC Layer in Self Sovereign Identity (SSI).

Brief description

Computational Problem Type:	Cryptography
Problem Domain:	PQC
Subdomain:	ZKP Protocols / Information Security
Industry:	Transversal
Time to Maturity (TRL):	Short <3 years
Potential Impact:	High – disruptive
EU Goal alignment:	Industry, innovation and infrastructure
Techniques:	PQC // AEAD Techniques / eIDAS 2 // EU Digital Identity
Source of use case:	GMV

Summary

One of the more challenge topics in current state of art Digital identity is focused on development of SSI (self-Sovereign Identity), mainly because of its very advanced anonymous schemes based on ZKP (Zero knowledge Protocols) and Oblivious knowledge Transfer techniques. However, these techniques are currently based on Pre Quantum cryptography so moving to PQC is essential to resist the Quantum Challenge and soar SSI upon the Quantum disruption.

SSI depicts and provides an updated and disruptive Digital Identity Framework to deal with wider Use Cases than current DI Schemes One of the main SSI foundations is its very strong cryptographic Layer, mainly in order to ensure ZKP (Zero Knowledge Protocols) , Anonymous Digital Signature (DS) Schemes based on current crypto and PQC Crypto.

This Layer also deals with AEAD (Authenticated Encryption with Associated Data) technics and is fully embedded in Hybrid schemes to ensure Crypto Agility and ensure a minimum impact in other SSI Layers, mainly business and government.

In addition, a Key element in SSI frameworks is the so-called Id Wallet, which is deployed in mobile devices as an App, turning to be a critical element from the point of view of overall security and supported cryptography.

One very specific SSI Use Case is the Adult Age Verification preserving Anonymous (Adult Sites, Alcohol and Drugs acquisition in web, Weapon and para-Pharmacies Control, dangerous CHEMICAL AND ELECTRIC components, ….) as, for example, in Spain recently has come recently into public discussions becoming a government objective to ensure, but this is just one flavour of a this very important topic.

Description

Business Challenge:

SSI frameworks are not new but as all disruptive topics dealing with Digital Identity need and important time not only to standardize (which in this case is quite mature) but to gain market acceptance trough meaningful Public (government) and social and industry useful and valuable Use Cases.

We focus on the Use Cases develop on Industry as Public Uses cases are under EU Public funding umbrella. Synergies with this public funding umbrella must be consider also to speed up acceptance on the industry – Private Use cases to widen market for SSI and associated technologies Vendors.

In addition, the full SSI shows its whole capacity when anonymous techniques are deployed allowing us to advance technical mechanisms sufficient to implement Privacy Personal Identity (PPI) Management preventing us from falling into PPI uncontrolled clearance.

The avoid coming QT threatens the whole SSI Crypto Layer and enable SSI dealing with Privacy Information must be written with PQC technics. The very specific use cases of SSI and in some cases, the overlapping with PKI technics and mobile elements (like for the ID - wallets) make for the whole SSI framework a critical framework to handle the PQC challenge.

Value Proposition:

The Value proposition has as main aim to gather SSI vendors and Private Sector to define minimum requirements for useful and disruptive Uses Cases

To clearly define minimum requirements and framework for PQC ZKP in SSI mechanism

To develop Private Sector valuable use cases involving state of art SSI ecosystem technologies and check current compliance with SSI (Vendors) n order to define minimum requirement to enable GAP identifications and proper stakeholder coverage and synergies.

To ease meeting of Industry early adopters and SSI Vendors: PQC SW / HW Providers, Network HSM, Hybrid CA and Post-Quantum Digital certificate Management, eIDAS 2.0 environment, SSI, Mobile Technologies, wallets and PQB based blockchains.

Solution Approach:

To gather Industry (HSM; SW SSI Vendors, Mobile APP developers), OPI, Security Expertise, Digital Identity Providers to build and declare a successive successful steps to move into valuable Use Cases facing current challenges.

To gather relevant stake holders to move into H2202 / next Generation EU tenders.

References

[1] Workgroup: Web Authorization Protocol Internet-Draft: draft-ietf-oauth-sd-jwt-vc-00 Published: 16 August 2023
[2] SD-JWT-based Verifiable Credentials (SD-JWT VC) ISO/IEC JTC 1/SC 27 NXXXXX Date: 2023-07-28
[3] ISO/IEC DIS 20008-3 ISO/IEC JTC 1/SC 27/WG 2 A Signature Scheme with Efficient Protocols Jan Camenisch, IBM Research, Zurich Research Laboratory Workgroup: Web Authorization Protocol
[4] draft-ietf-oauth-selective-disclosure-jwt-05 Published: 30 June 2023 Intended Status: Standards Track K. Yasuda Microsoft B. Campbell
[5] Ping Identity Selective Disclosure for JWTs (SD-JWT) Abstract
[6] Verifiable Credentials Data Model v1.1 W3C Recommendation 03 March 2022
[7] Verifiable Credentials Data Model v2.0 14 ZKP Clare Nelson (1) (Serie SSI MeetUp. ORG)
[8] Information Security – Security techniques – Anonymous digital signatures – Part 3: Mechanisms using multiple public keys IT Technologie de sécurité — XXX — Partie 3: XXX
[9] Lattice Signature with Efficient Protocols, Application to Anonymous Credentials Toward a Post-Quantum Zero-Knowledge Verifiable Credential System for Self-Sovereign Identity
[10] PKCS#11 Cryptographic Token Interface Base Specification Version 3.0, OASIS Committee Specification Draft 01 / Public Review Draft 01 29 May 2019
[11] PKCS#11 Cryptographic Token Interface Base Specification Version 2.20, RSA Laboratories, 28 June 2004
[12] KMIP

Use Case 12: New Defense Materials through AI and Quantum Simulations

Brief description

Computational Problem Type:	Simulation
Problem Domain:	Materials innovation
Subdomain:	Chemistry, molecular and materials properties
Industry:	Manufacturing, Chemical, Materials, Defense
Time to Maturity (TRL):	Long: >10 years
Potential Impact:	High – disruptive
EU Goal alignment:	Industry, innovation and infrastructure
Techniques:	Hamiltonian Simulation, Variational Quantum Eigensolver (VQE), Quantum Annealing
Source of use case:	SANDBOXAQ

Summary

The initiative leverages advanced computational methodologies combining AI and quantum simulations to expedite the discovery and development of innovative materials. This fusion of technologies, spearheaded by SandboxAQ, aims to address critical challenges in the defense sector by enabling the creation of materials with enhanced properties, such as increased durability, lighter weight, and improved performance under extreme conditions.

Description

Business Challenge:

The defense industry is constantly in pursuit of materials that can offer better protection, efficiency, and functionality while minimizing costs and environmental impact. Traditional material discovery methods are slow, costly, and often hit the limits of computational capabilities when trying to model complex quantum interactions essential for understanding material properties at the molecular level. This process can take over a decade and cost up to $100M with a success rate of less than 1% for new material discovery.

Value Proposition:

The integration of AI and quantum simulations proposes a groundbreaking approach to overcome the computational barriers faced by the defense industry. By harnessing the power of quantum mechanics and AI-driven insights, this approach significantly reduces the time and financial investments required for material discovery and development. It enables the exploration of a vast chemical space with greater precision and speed, leading to the identification of novel materials that meet the demanding requirements of defense applications.

Solution Approach:

This AI x Quantum strategy –a blend of tensor networks, quantum chemistry, generative modeling, and other AI technologies to simulate and predict material properties and behavior– allows for the rapid, accurate modeling of molecular interactions and the exploration of new material combinations that were previously unattainable. Key focus areas include the development of high-temperature superconductors, energy storage materials, nonlinear optical materials, and advanced catalysts for environmental remediation. The approach not only accelerates the discovery phase but also extends to the synthesis and production stages, ensuring that the materials are viable for large-scale manufacturing and deployment in defense applications.

References

[1] IBM Research Blog. (n.d.). New Sustainable Materials. Retrieved from https://research.ibm.com/blog/new-sustainable-materials
[2] Phys.org. (2023, October). Chemical Compounds Discovered. Retrieved from https://phys.org/news/2023-10-chemical-compounds-discoveredhere-world.html

[3] Nature. (2023, November). DeepMind's AI for Materials Discovery. Retrieved from https://www.nature.com/articles/s41586-023-06735-9
[4] SandboxAQ. (2024). Chemicals & Materials SB_EY Deck vJL Jan 2024. Retrieved from the provided document.

Use Case 13: Nitrogen fixation.

Brief description

Computational Problem Type:	Simulation
Problem Domain:	Chemistry Simulation
Subdomain:	Electronic structure problem
Industry:	Manufacturing, Chemical, Materials, Agriculture
Time to Maturity (TRL):	Long: >10 years
Potential Impact:	High – disruptive
EU Goal alignment:	Industry, innovation and infrastructure
Techniques:	Variational Quantum Eigensolver (VQE), Adiabatic Paradigm
Source of use case:	University Leiden

Summary

Nitrogen Fixation is a very important technique to produce fertilizers which are used in agriculture to increase the crop yield. This process consists of converting molecular nitrogen (N2) as contained in the air into ammonia (NH3). It is an essential reaction for life as biosynthesis of all nitrogen-containing organic compounds such as amino acids or proteins. In that sense, some industrial processes, like the Haber-Bosch process, are used to reproduce this reaction outside a biological environment. But all of those processes are very expensive in terms of energy, using over 1% of worlds total produced energy [2], as well as they produce a huge number of residues that are not good for the sustainability of nature. Because of this, it is very important to tackle this problem to find a way to replicate these processes in a more efficient way.

Description

Business Challenge:

All nitrogen fixation processes are very costly. They require a huge amount of energy to reproduce the nitrogen fixation reaction. Because of this, it is very important to find new enzymes where the same process could be reproduced in a more efficient way (performing it with less energy). Two approaches using quantum computers are understanding and developing improvements to the Haber-Bosch process [2] and understanding nature's method of nitrogen fixation. (Understanding the enzyme nitrogenase [3]). The effort for calculating the energy density grows exponentially with the number of molecules involved. A recent paper [5] attempted to calculate the number of qubits necessary to simulate the FeMoCo element of the nitrogenase MoFe protein [5] would take 10 days using a the AutoCCZ approach on a 7.5×10^6 qubits with a 1 μs code cycle time. This puts the calculation on par with the number of qubits needed for Shor's algorithm [6]. It is likely to take more than 10 years of development effort to attain the computational capacity to tackle this level of problem. In the meantime, developing the basic algorithms to model smaller molecules will be an important research topic (see Drug Discovery – Binding Energy Calculation).

Value Proposition:

It is difficult to estimate the value and timeline of this use-case, it is a representative of similar use-cases that promise enormous value to society. The main reason is that all of these kinds of problems are tackled by heuristic algorithms, where no theoretical advantage can be demonstrated. Even though, it is very important to demonstrate that these algorithms can solve these use cases better than their classical counterparts. (Also see UC50 CO2 recapture). It is also not clear if quantum computers can ever be realized that would have sufficient computing ability to model these complex module chemical processes. But, given how much impact the Haber-Bosch process has made to our lives on Earth [6], there is a necessity to understand nature in order to preserve it. This last reason might be the most important argument why we need to invest in the development of high-performance quantum computers.

Solution Approach:

The high number of qubits needed to simulate these complex molecules will not be available for several decades. Even that, it is important to start approaching this kind of problems with this emerging technology, as it is the only one that promises to solve it in the future. Because of this, the development of the underlying modelling software needs to continue using a combination of classical and quantum computing hardware.

For that purpose and to the aim of solving this use case, the Variational Quantum Eigensolver (VQE) algorithm is recommended for the gate model paradigm, and the adiabatic paradigm itself is also suggested.

From the gate-model paradigm perspective, the VQE is a hybrid algorithm that uses the best of both worlds to get better results than their classical counterparts. It could estimate the energy of different enzymes and comes out with a more efficient process than the Harber-Bosch process. On the other side, the adiabatic paradigm is mainly based to solve this kind of optimization problems, and that's why it is a perfect fit for that.

References

[1] Dukatz, Carrel-Billiard, Garrison, Accenture 2017, "Think beyond ones and zeros".
[2] Capdevila-Cortada, M. Electrifying the Haber–Bosch. Nat Catal 2, 1055 (2019). https://doi.org/10.1038/s41929-019-0414-4 .
[3] Reaction mechanisms on quantum computers, Markus Reiher, Nathan Wiebe, Krysta M. Svore, Dave Wecker, Matthias Troyer, Proceedings of the National Academy of Sciences Jul 2017, 114 (29) 7555-7560; DOI: 10.1073/pnas.1619152114.
[4] American Institute of Physics. "How big does your quantum computer need to be? What size will a quantum computer need to be to break Bitcoin encryption or simulate molecules?." ScienceDaily. ScienceDaily, 25 January 2022. http://www.sciencedaily.com/releases/2022/01/220125112556.htm.
[5] Mark Webber, Vincent Elfving, Sebastian Weidt, Winfried K. Hensinger. The impact of hardware specifications on reaching quantum advantage in the fault tolerant regime. AVS Quantum Science, 2022; 4 (1): 013801 DOI: 10.1116/5.0073075.
[6] How fertiliser helped feed the world By Tim Harford, 2 January 2017 https://www.bbc.com/news/business-38305504.

Use Case 14: Quantum Computer Music.

Brief description

Computational Problem Type:	Simulation, Quantum Machine Learning (QML)
Problem Domain:	Music Simulation
Subdomain:	Generative QML
Industry:	Culture and Creative Industries (CCI)
Time to Maturity (TRL):	Long: >10 years
Potential Impact:	Medium – at a scale
EU Goal alignment:	Good health and well-being
Techniques:	Quantum Gates Algorithms
Source of use case:	EURECAT

Summary

The origin of computer-generated music is associated with the beginning of computing itself. Its rise began in the 1950s with the creation of the first computers capable of producing sound, followed by the development of synthesizers (both analog and digital) [1]. Since then, computers have been present in almost every aspect of the music industry.

In recent years, a new field of research has emerged, *Quantum Computer Music*, which seeks to harness the unique features of quantum computing for applications in music [2]. This new technology will enable the development of new instruments and new ways of creating music and synthesizing sounds [3].

Description

Business Challenge:

Nowadays, Artificial Intelligence techniques, mainly Deep Learning, are employed for music generation and composition. These techniques focus on the development of systems that mimic the style of existing music [4]. An overview of Deep Learning models for musical composition can be found in [5].

Value Proposition:

In the field of music creation, quantum computers can accelerate the processing of the large amounts of data required by Deep Learning architectures, which can have a significant impact on music recommendation systems [6]. Furthermore, and more significantly, quantum computing will enable new ways of creating music, some of which have already being tested [7,8].

Solution Approach:

Cellular Automata are abstract computational models that simulate changing patterns in space and time [9]. These patterns can be translated into music [10,11].

In the same way that quantum versions of Cellular Automata have been developed to simulate quantum phenomena, quantum versions are also being developed for applications in music creation [12].

References

[1] Roads, C. (1996). The computer music tutorial. MIT press.
[2] Miranda, E. R. (Ed.). (2022). Quantum Computer Music: Foundations, Methods and Advanced Concepts. Springer Nature.
[3] Miranda, E. R., Thomas, P., & Itaboraí, P. V. (2023). Q1Synth: A Quantum Computer Musical Instrument. Applied Sciences, 13(4), 2386.
[4] Miranda, E. R. (Ed.). (2021). Handbook of artificial intelligence for music. Cham: Springer International Publishing.
[5] Hernandez-Olivan, C., & Beltran, J. R. (2022). Music composition with deep learning: A review. Advances in speech and music technology: computational aspects and applications, 25-50.
[6] Kerenidis, I., & Prakash, A. (2017). Quantum Recommendation Systems. In 8th Innovations in Theoretical Computer Science Conference (ITCS 2017). Schloss Dagstuhl-Leibniz-Zentrum fuer Informatik.

[7] Oshiro, S. (2022). QuiKo: A Quantum Beat Generation Application. In Quantum Computer Music: Foundations, Methods and Advanced Concepts (pp. 131-158). Cham: Springer International Publishing.
[8] Clemente, G., Crippa, A., Jansen, K., & Tüysüz, C. (2022). New Directions in Quantum Music: concepts for a quantum keyboard and the sound of the Ising model. In Quantum Computer Music: Foundations, Methods and Advanced Concepts (pp. 433-445). Cham: Springer International Publishing.
[9] Wolfram, S. (1984). Cellular automata as models of complexity. Nature, 311(5985), 419-424.
[10] Beyls, P. (1989). The musical universe of cellular automata. In Proceedings of the 1989 International Computer Music Conference, San Francisco, September 1989.
[11] Miranda, E. R. (1993). Cellular automata music: An interdisciplinary project. Journal of New Music Research, 22(1), 3-21.
[12] Miranda, E. R., & Shaji, H. (2023). Generative Music with Partitioned Quantum Cellular Automata. Applied Sciences, 13(4), 2401.

Agradecimientos

- Rafael Martín-Cuevas, EY, por la aportación de Casos de Uso en el sector financiero.
- Iraia Ibarzabal, MULTIVERSE COMPUTING, por la aportación de Casos de Uso en el sector energético.
- Enrique Crespo, GMV, por la aportación de Casos de Uso en el sector Ciberseguridad.
- Guillermo Gil, TECNALIA, por la aportación de Casos de Uso en el sector Logística & Movilidad.
- Eneko Axpe, SANDBOX AQ, por la aportación del Caso de Uso en el sector Defensa.
- Adán Garriga, EURECAT, por la aportación del Caso de Uso en el sector de Industrias Culturales y Creativas.
- Jesús Huertas, QILIMANJARO, por la aportación del Caso de Uso en el sector del mercado energético.

Editores

Colaboradores

EY

MULTIVERSE COMPUTING

gmv INNOVATING SOLUTIONS

tecnalia MEMBER OF BASQUE RESEARCH & TECHNOLOGY ALLIANCE

SANDBOXAQ

eurecat Centre Tecnològic de Catalunya

QILIMANJARO QUANTUM-TECH

Entanglement Partners_ >

accenture

Únete al grupo de trabajo de Tecnologías Cuánticas de AMETIC

Remite tu interés a innovacion@ametic.es

Ametic
LA VOZ DE LA INDUSTRIA DIGITAL

Ametic

LA VOZ DE LA **INDUSTRIA DIGITAL**