

# Quantum Computing and Sustainability

## Some Illustrative Examples and Paths Forward

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### The case for quantum

Climate change poses an ever increasing threat to ecosystems and human civilisation. Although countries and organizations have set incredibly ambitious goals<sup>1</sup>, which would require the investment of an unprecedented amount of capital, they would still fall short of the maximum 1.5°C of global warming that has been deemed as the point of no return by 2050.

Indeed, according to the last figures released by the International Renewable Energy Agency, (IRENA) in its report “World Energy Transitions Outlook 2022: 1.5°C Pathway”<sup>2</sup>, the policies in Place (PES) scenario investments amount to USD 98 trillion between 2021 and 2050, and USD 35 trillion between 2021 and 2030. Thus, this scenario implies a near doubling of annual energy investment, which in 2019 amounted to USD 2.1 trillion.

However, these figures aren’t enough to reach the goals of the 1.5°C scenario. The 1.5°C scenario requires investments of USD 57 trillion in this decade. Therefore, a significant scale up of investments will be required over the next ten years, in all sectors and regions, to reach USD 5.7 trillion a year.

All of this implies that, even if these milestones were fully met, technological advances are imperative to achieve the goal of net-zero emissions. Many of these advances are being limited by the capacity of current and future classical computers, which are unable to deal with the complexity of the problems at hand.

In this context quantum computing emerges as a potential game changer. Even though the technology is still in the so-called noisy intermediate-scale quantum (NISQ) era, the amount of investment and scientific breakthroughs are tangible indicators that quantum advantage and broad impact of quantum will happen during this decade.

As opposed to classical computers, in which  $n$  bits can encode  $n$  values, quantum computers can encode up to  $2^n$  values with only  $n$  qubits, an exponentially higher number. Exploiting the quantum

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<sup>1</sup> *Glasgow Climate Pact*. UN Climate Change Conference, COP26 (2022).

<sup>2</sup> <https://www.irena.org/publications/2022/mar/world-energy-transitions-outlook-2022>

mechanical properties of these processors, it's possible to design algorithms that provide significant speedups on many relevant tasks related to bounded-error quantum polynomial (BQP) problems, which can not be efficiently solved by classical computers, even the most powerful ones.

With this in mind, when will we start seeing the effects of this quantum revolution? With the constant improvement of current quantum devices, NISQ era computers are expected to attain practical use level in the next 5 to 10 years<sup>3</sup>. Although many applications of quantum computing in the sustainability domain require fault tolerant hardware, there are still some relevant use cases where NISQ computers could be more than enough to improve on current classical solutions. These use cases include applications in smart grids, simulations for advancing electric batteries, transportation and logistics, and the development of catalysts for ammonia fixation.

## Smart Grids

Frequently, smart grids involve a huge number of interdependent players, which create a whole myriad of combinatorial optimization problems<sup>4</sup>. Some of them, such as phasor measurement unit (PMU) placement<sup>5</sup> and fault management<sup>6</sup>, can be formulated in a way that makes them suitable for a quantum annealer, a type of non-universal quantum device specially tailored to some combinatorial optimization problems. Power flow<sup>7</sup> and transient analysis<sup>8</sup> problems might even benefit from the exponential speed-up provided by Harrow-Hassidim-Lloyd (HHL) algorithm for solving linear systems of equations, although it requires fault tolerance and high qubit connectivity, and safety in cybersecurity protocols might also be improved with the use of quantum key distribution (QKD)<sup>9</sup> and quantum direct communication (QDC)<sup>10</sup>, as well as post-quantum cryptography (PQC)<sup>11</sup>.

Hybrid variational algorithms, namely the quantum approximate optimisation algorithm (QAOA) and the variational quantum eigensolver (VQE), could be used to avoid the exponential scaling in unit

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<sup>3</sup> J. Bobier, P. Gerbert, J. Burchard, A. Gourévitch. *A Quantum Advantage in Fighting Climate Change*. Boston Consulting Group (2020).

<sup>4</sup> Ajagekar, A., You, F. *Quantum computing for energy systems optimization: Challenges and opportunities*. Energy 179, 76–89 (2019).

<sup>5</sup> Jones, E.B., Kapit, E., Chang, C.Y., Biagioni, D., Vaidhyanathan, D., Graf, P., et al. *On the computational viability of quantum optimization for PMU placement*. IEEE Power & Energy Society General Meeting (PESGM), pp. 1–5. IEEE, Piscataway (2020).

<sup>6</sup> Ajagekar, A., You, F. *Quantum computing based hybrid deep learning for fault diagnosis in electrical power systems*. Appl. Energy 303, 117628 (2021).

<sup>7</sup> Feng, F., Zhou, Y., Zhang, P. *Quantum power flow*. IEEE Trans. Power Syst. 36(4), 3810–3812 (2021).

<sup>8</sup> Zhou, Y., Feng, F., Zhang, P. *Quantum electromagnetic transients program*. IEEE Trans. Power Syst. (2021).

<sup>9</sup> Alshowkan, Muneer, Philip G. Evans, Michael Starke, Duncan Earl, and Nicholas A. Peters. "Authentication of Smart Grid Communications Using Quantum Key Distribution." Scientific Reports 12, no. 1 (July 26, 2022): 12731.

<sup>10</sup> Jiang, Z., Tang, Z., Qin, Y., Kang, C., Zhang, P.: Quantum internet for resilient electric grids. Int. Trans. Electr. Energy Syst. 31(6), e12911 (2021)

<sup>11</sup> Costa VLRd, López J, Ribeiro MV. *A System-on-a-Chip Implementation of a Post-Quantum Cryptography Scheme for Smart Meter Data Communications*. Sensors. 2022; 22(19):7214. <https://doi.org/10.3390/s22197214>

commitment<sup>12</sup> and facility location-allocation<sup>14</sup> problems. Furthermore, different quantum machine learning (QML) algorithms could increase the precision in tasks like energy production forecasting.

## Materials

Quantum simulations could help with the fabrication of new high-density electric batteries for vehicles and energy storage. The Canadian quantum computing start-up Xanadu has recently published a detailed study on how to simulate lithium-ion batteries with a quantum computer<sup>13</sup> which, although requiring fault tolerance, represents the first detailed answer to how these devices can be used to simulate the behavior of these systems, and serve as a first step towards more efficient energy storage. This impact could be increased even more with the development of new solar cells based on perovskite crystal structures. When compared with current crystalline silicon based cells, perovskite ones offer twice as much efficiency, but require deeper chemical understanding to solve their current toxicity issues<sup>14</sup>.

Cement production could also be improved with the use of quantum simulations, since two thirds of carbon emissions come from the calcination processes that create cement clinkers<sup>15</sup>. The use of quantum computers could help with the development of new cement-binding materials, due to their improved ability to simulate molecular properties without requiring costly and time consuming trial-and-error processes<sup>16</sup>. The behavior and resistance of cement is determined by destructive tests, which, again, are costly and time consuming to achieve accuracy to the needed levels. This field could also benefit using quantum computing.

## Transportation & Logistics

The transportation industry is also expected to be radically transformed by emerging quantum technologies. One possible application is to computational fluid dynamics, where quantum computers could help speed-up the design process of vehicles, ships and aircrafts by allowing us to simulate the behavior of fluids on complex surfaces, as well as solving routing and trajectory optimization problems much more efficiently<sup>17</sup>.

In addition to this, supply chain optimization usually involves many interdependent factors that make modeling and solving these systems a very challenging task. The ability of quantum computers to simulate complex interconnected systems is expected to be a game changer in the

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<sup>12</sup> Nikmehr, N., Zhang, P., Bragin, M. *Quantum distributed unit commitment*. IEEE Trans. Power Syst. 37(5), 3592–3603 (2022).

<sup>13</sup> Delgado et al. *How to simulate key properties of lithium-ion batteries with a fault-tolerant quantum computer*. arXiv:2204.11890 (2022).

<sup>14</sup><https://www.smart-energy.com/industry-sectors/new-technology/quantum-computing-to-advance-solar-pv-materials/>

<sup>15</sup><https://www.mckinsey.com/industries/chemicals/our-insights/laying-the-foundation-for-zero-carbon-cement>

<sup>16</sup><https://www.mckinsey.com/capabilities/mckinsey-digital/our-insights/quantum-computing-just-might-save-the-planet>

<sup>17</sup> U. Azad, B. K. Behera, E. A. Ahmed, P. K. Panigrahi and A. Farouk, "Solving Vehicle Routing Problem Using Quantum Approximate Optimization Algorithm," in IEEE Transactions on Intelligent Transportation Systems, doi: 10.1109/TITS.2022.3172241 (2022).

logistics industry, with the potential to solve many of the ever-growing large scale supply chain issues<sup>18</sup>.

And, while these advanced and sophisticated use cases will very likely transform entire industries, economies and even societies, there are also more basic problems that, despite being formulated for centuries, we still struggle to solve. A good example of one of these problems is the traveling salesman problem, first mathematically formulated by William Rowan Hamilton and Thomas Kirkman in the 19th century. The traveling salesman problem is central to the transportation and logistics industries, with applications in route scheduling<sup>19</sup>, distribution<sup>20</sup>, traffic management<sup>21</sup>, order picking in warehouses<sup>22</sup> and last-mile distribution<sup>23</sup>.

## Catalysts

The fertilizer industry is expected to be one the first to feel the quantum effect<sup>24</sup>. Since most processes in this domain require simulating complex molecular structures and interactions, having a clear quantum picture of them is a key requirement to obtain optimal solutions. One of the clearest examples of this is the production of ammonia fertilizer, which is currently produced using the carbon-intensive Haber-Bosch process, consuming 3% to 5% of all the natural gas produced globally<sup>3</sup>. This process accounts for 1.4% of global carbon dioxide emissions and consumes 1% of the world's total energy production<sup>25</sup>. In nature, the conversion of atmospheric nitrogen molecules into ammonia, nitrogen fixation, is catalyzed by an enzyme called Nitrogenase, and its primary cofactor is known as FeMoco. A better understanding of the bacterial process that leads to efficient ammonia production could enable us to replicate the FeMoco molecule, allowing green ammonia fabrication<sup>26</sup>. This reduction in cost could also turn ammonia into a carbon-neutral alternative to fossil fuels for the shipping industry<sup>27</sup>.

The development of new catalysts could also transform the carbon capture industry<sup>28</sup>. Designing more efficient carbon binding procedures would lead to a significant reduction in costs, increasing the profitability of these processes within the circular carbon economy, and even the introduction of new direct-air-capture techniques in the long term.

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<sup>18</sup> H. Jiang et al. *Quantum Computing Methods for Supply Chain Management*. ACM/IEEE Workshop on Quantum Computing (2022).

<sup>19</sup>Hulianytskyi, L. et al. *Solving the Problem of Vehicle Routing on Modern QuantumClassical Cloud Services* (2022)

<sup>20</sup><https://www.quantumcomputinginc.com/blog/quantum-computing-distribution/>

<sup>21</sup><https://www.volkswagen-newsroom.com/en/press-releases/volkswagen-optimizes-traffic-flow-with-quantum-computers-5507>

<sup>22</sup>Atchade-Adelomou, P. et al. *qRobot: A Quantum computing approach in mobile robot order picking and batching problem solver optimization* (2021)

<sup>23</sup><https://www.quantumcomputinginc.com/blog/last-mile/>

<sup>24</sup><https://www.mckinsey.com/industries/chemicals/our-insights/the-next-big-thing-quantum-computings-potential-impact-on-chemicals>

<sup>25</sup><https://www.nature.com/articles/s41929-019-0414-4>

<sup>26</sup> Reiher et al. *Elucidating reaction mechanisms on quantum computers*. PNAS 114 (29) 7555-7560 (2017).

<sup>27</sup> <https://www.emsa.europa.eu/publications/item/4833-potential-of-ammonia-as-fuel-in-shipping.html>

<sup>28</sup> G. Greene-Diniz et al. *Modeling Carbon Capture on Metal-Organic Frameworks with Quantum Computing*. arXiv:2203.15546 (2022).

## Multiverse Computing's contribution towards a more sustainable future

While NISQ era quantum technology is expected to deliver the first benefits in the fight against climate change within the short to medium term, Multiverse computing is committed to making an impact now. A pragmatic approach to this is to leverage the currently exploitable capabilities of so-called quantum-inspired technology. Quantum-inspired is a rather broad term which refers to methods that do not rely on nascent quantum hardware but whose design derives from, or takes inspiration from, quantum algorithms. Quantum-inspired algorithms can already improve on classical approaches, and, crucially, are run on High Performance Computing (HPC) premises, like, for example, GPUs (Graphic Processing Units). Additionally, developing them makes strategic sense in the NISQ era since their translation to truly quantum variants is typically straightforward compared to classical algorithms, allowing constantly emerging hardware improvements to be immediately exploited.

In what follows, we explain how Multiverse Computing has been using quantum-inspired technology to further sustainability goals.

### Tensor Networks: a key tool for sustainability

What are tensor networks? In a nutshell, tensor networks are mathematical decompositions of highly correlated data structures. They seek to reduce the dimensionality of a data set by representing it through a set of "instructions" for generating the data rather than describing it exhaustively. At Multiverse Computing, we have been using quantum-inspired technology to move sustainability goals further. Our work shows that tensor networks are a key tool for sustainability.

By applying this idea to machine learning models, such as neural networks, it is possible to dramatically decrease the number of parameters required to build a model. Not only this compression can lead to improved model accuracy, with implications for many of the use-cases mentioned above, but it also leads to a dramatic reduction of model training time and memory consumption. Given that some traditional machine learning algorithms can use up to 3 times the average household's yearly energy consumption<sup>29</sup> to complete one training cycle, improving training efficiency is a sustainability goal in itself. Recently, some efforts have been done to tensorize deep learning models, such as Large Language Models (LLMs)<sup>30,31</sup> and Recommendation Systems (DLRMs)<sup>32</sup>.

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<sup>29</sup><https://www.techtarget.com/searchenterpriseai/feature/Energy-consumption-of-AI-poses-environmental-problems>

<sup>30</sup>Xindian Ma et al. *A Tensorized Transformer for Language Modeling* (2019)

<sup>31</sup> Wang, B., Ren, Y. et al *Exploring extreme parameter compression for pre-trained language models* (2022)

<sup>32</sup><https://analyticsindiamag.com/explained-facebooks-novel-method-to-downsize-recommendation-models-by-112-times/>

In a recent collaboration with a major European bank, we showed that tensorized neural networks used for hedging could be trained in one fifth of the time required for conventional neural networks<sup>33</sup>.

## Timeline and Limitations

It is estimated that the goals set at the 2021 United Nations Climate Change Conference (COP26) would only reduce global warming, in the best case scenario, to 1.7°C<sup>12</sup>. Advances in quantum technologies could bring that value below 1.5°C, but current devices can't tackle most of the problems mentioned in this article at a valuable scale. However, we don't need the full potential of a quantum computer to start obtaining value from this technology. Noisy quantum processors, while unable to deliver some of the theoretical speed-ups that the technology promises, are nonetheless incredibly powerful, with two new claims of quantum advantage being published during 2022<sup>34 35</sup>. Also, several companies, such as IBM<sup>36</sup>, Google<sup>37</sup> and IonQ<sup>38</sup>, expect to unveil the first large-scale fault-tolerant quantum processors before 2030. As quantum hardware providers release their roadmaps towards large-scale fault-tolerant quantum computers, organizations in industry and academia have ramped up their efforts to find useful applications of quantum computers in the short term.

When factoring in accessibility and market awareness, and according to our own estimations, we expect that widespread adoption of the first quantum applications in the sustainability domain will occur between 2030 and 2035. This, together with increasing funding, research and access to educational resources, would put us in pace towards net-zero emissions by the year 2050.

We must not forget, however, that the adoption of quantum technologies is in no way enough to achieve our common goal. Without the adoption of sustainable measures and policies by governments and organizations, no technology, present or future, has the power to single-handedly solve all environmental issues by itself. To avoid the catastrophic consequences of global warming, a joint effort is needed on a global scale, of which quantum technologies would be a crucial step towards a sustainable future.

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<sup>33</sup> Patel, Raj G., Chia-Wei Hsing, Serkan Sahin, Samuel Palmer, Saeed S. Jahromi, Shivam Sharma, Tomas Dominguez, et al. "Quantum-Inspired Tensor Neural Networks for Option Pricing." arXiv, December 28, 2022.

<sup>34</sup> Huang et al. *Quantum Advantage in Learning from Experiments*. <https://arxiv.org/abs/2112.00778>

<sup>35</sup> Madsen, L.S., Laudenbach, F., Askarani, M.F. et al. Quantum computational advantage with a programmable photonic processor. *Nature* 606, 75–81 (2022). <https://doi.org/10.1038/s41586-022-04725-x>

<sup>36</sup> <https://www.ibm.com/quantum/roadmap>

<sup>37</sup> <https://www.theverge.com/2021/5/19/22443453/google-quantum-computer-2029-decade-commercial-use-ful-qubits-quantum-transistor>

<sup>38</sup> <https://ionq.com/posts/december-09-2020-scaling-quantum-computer-roadmap>

## About the Authors

Gianni Del Bimbo's current role in Multiverse is Chief Operations Officer. Gianni is a quantum physicist, holding a MSc in Condensed Matter Physics from the Ludwig Maximilian University (LMU) of Munich and a BSc in Physics and Astrophysics from the University of Florence. In Gianni's own words: "At Multiverse, I started as a quantum machine learning specialist and later worked as head of quantum engineering managing teams and leading client projects in finance, energy, manufacturing and chemistry. As COO, I'm now responsible for designing, implementing and overseeing day-to-day operations to drive the company's strategy. I'm also responsible for designing and building the company's ESG plan".

Rodrigo Hernández Cifuentes is Multiverse Computing Chief Growth Officer. Rodrigo is a mechanical engineer from the Polytechnical University of Madrid and MSc in information Sciences from the Complutense University of Madrid. Rodrigo also serves as faculty member at the Artificial Intelligence Finance Institute (AIFI, NYU Tandon School). Rodrigo is also a former researcher in satellite plasma thruster design and precision metrology at the Higher Technical School of Aeronautical and Space Engineering, Polytechnical University of Madrid.

Esperanza Cuenca Gómez is Head of Strategy and Outreach at Multiverse Computing. She is a digital transformation enthusiast with more than 12 years of experience in consumer finance and banking, and more than 5 years in strategy and operations consulting. Quantum mechanics has always fascinated Esperanza, so she decided to study and research in quantum computing and communications. As an engineer, Esperanza sees applied science and engineering as ways to build new technologies, solve problems, and contribute to society. Esperanza is a member of Bankinter Foundation for Innovation FIBK Voices, an ecosystem of experts who are international referents and give the Foundation their vision on how innovation is revolutionizing areas such as science, technology, entrepreneurship or education. Esperanza also serves as Head of Change Navigation at the Quantum Strategy Institute.

Daniel García Guijo is a Technical Project Manager in Multiverse Computing. Daniel holds a BSc in Physics at the University of Oviedo, final project on fluid simulations using Deep Convolutional Neural Networks. Daniel has participated in key projects in the energy, life sciences and manufacturing sectors in Multiverse specializing in quantum and quantum-inspired machine learning, and contributes decisively to Multiverse's efforts in sustainability.

Angus Dunnet is a Quantum Inspired Software Engineer in Multiverse Computing. Angus is a quantum physicist with a special interest in Tensor Networks. Angus holds a MPhys in Theoretical Physics from the University of St Andrews and a PhD in Computational Physics from the Institut des NanoSciences de Paris, working on novel Tensor Network methods and their application to Open Quantum Systems.