

The Open Quantum Institute

SDG Use Cases White Paper 2023

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Introduction

Quantum computing is still in its early stage of development and computational resources remain limited. For the few applications that can be implemented on current quantum computers, the focus is on applications presenting an immediately graspable commercial or geostrategic advantage, sponsored by organizations with the means to bet on a return-on-investment in the distant future. As a result, too few resources - in terms of computing and expertise - have been allocated to investigating how quantum computing could be harnessed to achieve the UN Sustainable Development Goals (SDGs).

One of the core missions of the Open Quantum Institute (OQI) is to mobilize stakeholders to participate in re-balancing the focus and resources towards applications beneficial to the SDGs and global challenges.

In this 2023 edition of OQI Use Case White Paper, the OQI worked collaboratively with teams from academia, industry, NGOs and International Organizations to further explore use cases related to Food (SDG2), Health (SDG3) and Climate Change (SDG13).



Carbon Reduction

SDG 13

Short Summary:

Quantum Computing simulation to reduce carbon dioxide (CO_2) in the atmosphere by improving catalysis process responsible for the fixation of carbon on the surface of materials.

Context

Approximately 3.3 to 3.6 billion people live in conditions that are highly vulnerable to climate change. The interdependence of human and ecosystem vulnerability to climatic hazards is manifest, and it is exacerbated for regions and people facing considerable development constraints¹.

The window is rapidly narrowing to achieve the goal set by the Paris Agreement of limiting global temperature increase to well below 2 degrees Celsius, while pursuing efforts to limit the increase to 1.5 degrees². To achieve this goal, the immediate and deep reduction of global greenhouse gas emissions (GHGs) is the central target; this requires systems transformations across all sectors and contexts, including scaling up renewable energy while phasing out all unabated fossil fuels, ending deforestation, reducing non-CO₂ emissions and implementing both supply- and demand-side measures³.

Carbon Dioxide Removal (CDR) is no substitute for immediate and deep emissions reductions measures. The Intergovernmental Panel on Climate Change nevertheless acknowledges that it is a required complement to achieve net zero CO₂ and GHG emissions both globally and nationally, specifically to counterbalance 'hard-to-abate' residual emissions⁴.

One of the CDR options, Direct Air Capture and Storage (DACS) could play a key role in achieving and sustaining net negative greenhouse gas emission in the long-term⁵. Widening the implementation of DACS at scale requires resolving geophysical, environmental-ecological, economic, technological, sociocultural, and institutional challenges⁶.

One of such key challenges is to find effective solutions to store and valorize the CO_2 once captured. Technologies exist to capture carbon dioxide and store it underground, but this can only be a temporary solution. It is also possible to reduce CO_2 to single-carbon compounds, notably methane.

¹ IPCC, 2023: Summary for Policymakers. In: *Climate Change 2023: Synthesis Report. Contribution of Working Groups I, II and III to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change* [Core Writing Team, H. Lee and J. Romero (eds.)].

https://www.ipcc.ch/report/ar6/syr/downloads/report/IPCC_AR6_SYR_SPM.pdf (accessed 11 September 2023) ² UNFCCC, *The Paris Agreement*, <u>https://unfccc.int/process-and-meetings/the-paris-agreement</u> (accessed 15 September 2023)

³ UNFCCC, 2023, Technical dialogue of the first global stocktake: Synthesis report by the co-facilitators on the technical dialogue (Advance version)., <u>https://unfccc.int/sites/default/files/resource/sb2023_09_adv.pdf</u> (accessed 15 September 2023)

⁴ UNFCCC, Technical Examination Process: Thematic Area – Carbon capture.,

https://unfccc.int/resource/climateaction2020/tep/thematic-areas/carbon-capture/index.html (accessed 15 September 2023)

⁵ Ibid.

⁶ UNFCCC, 2023: Technical dialogue of the first global stocktake: Synthesis report by the co-facilitators on the technical dialogue (Advance version), <u>https://unfccc.int/documents/631600</u> (accessed 11 September 2023)



The present OQI use case considers how quantum computing could accelerate prospects of recycling carbon dioxide into chemical compounds of value, thus incentivizing stakeholders to invest further in the deployment of Carbon Dioxide Removal technologies.

How could quantum help

One approach to recycling of carbon dioxide is to sequester it in energy production (e.g., coal power plants) or industrial processes (e.g., burning of cement), and then to transform it into other compounds, such as formic acid, methane, methanol, ethanol, or ethene. This chemical transformation can be accelerated by the interaction of carbon dioxide molecules with copper surfaces, through the process so-called heterogenous catalysis⁷.

Although the catalysis process is relatively well adopted, it is still unclear how these chemical reactions are accomplished locally on a copper surface. This lack of clear understanding limits the ability to scale in production what would be an efficient tool for carbon dioxide recycling.

Computer simulations are used to systematically screen for the structure of local active sites⁸. The computational challenge relies on two key ingredients: 1) automated tools to explore for a wide range of structures (local surface structures as well as adsorbed molecular species and reactive intermediates including transition state structures) and 2) accurate assignment of electronic energies to the optimized molecular structures obtained.

Quantum computing is a natural tool to simulate chemical systems⁹. After systematically screening adsorption sites and energies at differently prepared copper surfaces using density functional theory calculations, quantum computations would lead to collect sufficiently accurate energy estimates.

A roadmap to impact

Classically, one would rely on density functional theory (DFT) calculations for the elucidation of the relevant molecular structures. A key bottleneck of the classical approach is the lacking accuracy of the energy assignment to the structures and the huge number of structures that need to be inspected.

In fact, tens of thousands of structures need to be optimized in order to assemble a comprehensive reaction network that would deliver sufficient details for understanding the carbon dioxide fixation chemistry at copper centers on the surface. The energy assignment to these structures is affected by potentially large errors, which are, most importantly, not known for every individual structure. The lack of accuracy compromises the modelling of the chemical process, and no valid conclusion can be drawn from data affected by errors that are too large.

Quantum algorithms, such as adaptive variational quantum eigensolver algorithms in the short-term, and quantum phase estimation algorithms in the longer run, may be used for this problem. The exploration of adsorbed structures and reactions of those adsorbed species with accurate energies will lead to efficient search of reaction paths and provide all details to control chemical selectivity and guide experiment.

⁷ Nitopi, S., Bertheussen, E., Scott., S., et al., 2019, Progress and Perspectives of Electrochemical CO2 Reduction on Copper in Aqueous Electrolyte., Chemical Reviews. <u>https://doi.org/10.1021/acs.chemrev.8b00705</u> (accessed 15 September 2023)

⁸ Steiner, M., Reiher, M., 2022, Autonomous Reaction Network Exploration in Homogeneous and Heterogeneous Catalysis. Top Catal 65, 6–39. <u>https://doi.org/10.1007/s11244-021-01543-9</u> (accessed 15 September 2023) ⁹ Von Burg, V., Low, G., Haner, T., et al., 2021, Quantum computing enhanced computational catalysis. <u>https://doi.org/10.1103/PhysRevResearch.3.033055</u> (accessed 15 September 2023)



Accuracy will be gained with quantum computing approaches, which is key to deriving a correct mechanism of the chemical processes that will support efficient carbon dioxide reduction solutions. This will likely require fault-tolerant quantum computers with a very large number of qubits that will only be available in many years.

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Mitigating Antimicrobial Resistance

SDG 3

Short Summary:

Addressing global public health challenges, by developing a quantum computing solution to improve current AI models, predict more quickly and accurately patterns of resistance and identifying new chemical compounds with low resistance on more targeted bacteria.

Context

WHO declared antimicrobial resistance (AMR) as one of the top ten threats to global public health¹⁰.

Antimicrobials include antibiotics, antivirals, antifungals, and antiparasitics. These compounds are used to combat infections not only in humans, but also in livestock, agriculture, and aquaculture. Antibiotics in particular have been largely misused and overused, which has led to emergence of multi-drug resistant bacteria. This also leads to rising levels of antibiotic pollution in wastewater, with serious threats to human health and significant disruption in downstream ecosystems.

Low- and middle- income countries, and certain population groups such as children and the elderly, are hit the hardest by AMR. One in five deaths attributed directly to AMR occurred in children under five years¹¹. South Asia and Sub-Saharan Africa showed the highest rates of deaths associated and attributable to AMR on a population basis. AMR causes suffering for millions, and nearly 1.3 million annual deaths are attributed to bacterial resistance alone¹². AMR also has an economic cost, as it affects productivity and economic growth. The World Bank estimates that if AMR is unchecked, by 2030, an additional 24.1 million people could be forced into extreme poverty¹³.

Given the alarming situation, the WHO global research agenda has given priority to the research topics with the greatest impact on mitigating antimicrobial resistance in the human health sector. In response to this ambitious goal, the Global Antibiotic Research & Development Partnership (GARDP), a not-for-profit global partnership, was launched to tackle the complex problem of AMR and develop treatments for drug-resistant infections¹⁴.

Despite the significant economic, environmental, and societal costs, the development of new antimicrobials has not kept pace with the emergence of resistance, leaving healthcare providers with fewer options for treating infections.

No new classes of antibiotics have been discovered in the past decades. The last new class of antibiotics approved by the US Food and Drug Administration (FDA) was in the mid-

¹⁰ WHO, 2021, Global Antimicrobial Resistance and Use Surveillance System (GLASS) Report., <u>https://www.who.int/publications/i/item/9789240027336</u> (accessed 15 September 2023); The Lancet, 2021, Antimicrobial resistance: a top ten global public health threat.,

https://www.thelancet.com/journals/eclinm/article/PIIS2589-5370(21)00502-2/fulltext (accessed 15 September 2023)

¹¹ The Lancet, 2022, The burden of bacterial antimicrobial resistance in the WHO European region In 2019: a cross-country systematic analysis., <u>https://www.thelancet.com/journals/lanpub/article/PIIS2468-2667(22)00225-0/fulltext</u> (accessed 15 September 2023)

¹² Ibid.; Gajdács M., 2021, Antimicrobial resistance in the context of the Sustainable Development Goals: a brief review. Eur J Investig Health Psychol Educ. 2021; 11: 71-82 <u>https://doi.org/10.3390/ejihpe11010006</u> (accessed 15 September 2023)

¹³ World Bank, 2017, *Drug-Resistant Infections: A Threat to Our Economic Future.*, Washington, DC: World Bank. License: Creative Commons Attribution CC BY 3.0 IGO,

https://documents1.worldbank.org/curated/en/323311493396993758/pdf/final-report.pdf (accessed 15 September 2023)

¹⁴ GARDP, *GARDP website.*, <u>https://gardp.org/</u> (accessed 15 September 2023)



1980s¹⁵. The antibiotics that have been brought to market in the past 30 years are variations on existing drugs discovered before that time. Advanced AI – which is already used to scan large libraries of molecules - and quantum computing could be leveraged to foster the exploration of novel areas for future discoveries. One of such promising areas is novel approaches to natural product discovery¹⁶, leveraging advances in next-generation genome sequencing, bioinformatics, and analytical chemistry combined with new strategies in antibiotic discovery, including inhibition of resistance, novel drug combinations, and new targets.

Beyond the required acceleration of research and development of new compounds, AMR mitigation requires a holistic approach, with integrated measures to reduce misuse for both human health and agriculture, to improve infection prevention and control measures, to remediate the presence of residual AMR substances in the environment for instance. Quantum computing could also be leveraged in this last area.

How could quantum help

Response to AMR is multifold. One way is to mitigate the disruption created in the ecosystem, by designing new materials and chemicals to remove antibiotics from wastewater. Computer simulations help accelerate the discovery and design phases. However, it requires substantial computational resources to accurately simulate the complex chemical reaction involved in the interaction of materials and chemicals that 'filter' antibiotics from wastewater. Quantum computing is a rare natural candidate for providing powerful tools to bring better accuracy in these critical chemistry simulations. This quantum chemistry approach could be further developed by OQI in the future¹⁷.

Another approach to AMR research identifies new drugs that have more targeted action to specific diseases and that are efficient against any known resistance mechanism. Machine learning methods are used to find new and efficient combination of compounds¹⁸. Such predictive models learn relationships between large chemical diversity found in libraries of chemical compounds and experimental in vitro observations, and then predict novel mixes with improved efficacies (in terms of targeted disease treatment and resistance).

A quantum computing solution could potentially be developed as an alternative or complement to classical machine learning algorithms for the prediction of new mixes. The key goal would be to obtain higher-quality mixes with fewer experimentation-learning cycles, as the number of cycles involves expensive on-demand experiments.

A roadmap to impact

A quantum machine learning (QML) algorithm could replace the standard machine learning algorithms. This quantum approach consists of parametrized quantum circuits¹⁹. The quantum circuit operates on quantum bits which can be in superposition states and can therefore access an exponentially large space as compared to the classical bits in the traditional machine learning setup. This opens the possibility that the parametrized quantum circuit can provide a better (more accurate or shorter) representation of the true

¹⁵ Coates, AR., Halls, G., and Hu, Y., 2011, *Novel classes of antibiotics or more of the same*? Br J Pharmacol, <u>https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3085877/</u> (accessed 15 September 2023)

¹⁶ GARDP, Revive, *Natural products.*, <u>https://revive.gardp.org/resource/natural-products/?cf=encyclopaedia</u> (accessed 15 September 2023)

ⁱ⁷ Baiardi, A., Ch^ristandl, M., Reiher, M., 2023, *Quantum Computing for Molecular Biology*, <u>https://doi.org/10.1002/cbic.202300120</u> (accessed 15 September 2023)

¹⁸ Alphanosos, *Alphanosos website.*, <u>https://www.alphanosos.com/</u> (accessed 15 September 2023)

¹⁹ Cerezo, M., Verdon, G., Huang, HY. *et al. Challenges and opportunities in quantum machine learning. Nat Comput Sci* **2**, 567–576 (2022). <u>https://doi.org/10.1038/s43588-022-00311-3</u> (accessed 15 September 2023)



input/output relation (now seen as a "quantum-matrix") than what standard machine learning can provide. Ultimately it would lead to improved mixes which can be tested experimentally, resulting in an iterative quantum computing/biological experiment workflow with faster convergence and higher-qualitative final samples.

This solution falls into the class of quantum-adjacent methods, in which quantum machine learning is applied to classical data. Such an approach may not necessarily provide computational speed-up. Rather, it is about the generative quality of sampling from different distributions than the ones of generative AI that would bring advantage. The structure of parameterized quantum circuits being very varied, but above all fundamentally different from traditional machine learning methods, this actually opens up new possibilities.

In addition, quantum effects in the interaction of the chemical compound with the biological target could be taken into account. Since the compounds are both organic, the interactions are typically of a non-covalent nature. Accurate modelling requires a quantum chemical treatment within an effective classical description²⁰. The data underlying chemical compound/bacteria interaction is therefore at least to a small part based on a quantum mechanical model that could benefit from quantum computing.

While quantum chemistry approach would most likely require fault-tolerant quantum computers with a very large number of qubits that will only be available in many years, quantum machine learning approach could be tested and implemented in the short terms with the current "noisy" quantum computers. This short-term solution could provide insight into whether faster convergence to higher quality samples with fewer iterations could be reached in the future, and therefore contribute to the response to the alarming AMR situation.

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²⁰ Baiardi, A., Christandl, M., Reiher, M., 2023, *Quantum Computing for Molecular Biology*, <u>https://doi.org/10.1002/cbic.202300120</u> (accessed 15 September 2023)



Sustainable Food Systems or Global Food Security

SDG 2

Short Summary:

Improving sustainability of global food systems by making them more resilient to climate change through a quantum optimization solution to produce more nutritious food locally in less land, and by lowering costs and emissions of food transport.

Context

According to the Food and Agriculture Organization (FAO), global hunger has risen to 9.2% of the world population in 2022, compared with 7.9% in 2019²¹. Conflict and insecurity, economic shocks, and extreme weather events are the main drivers of acute food insecurity. To achieve Sustainable Development Goal (SDG) 2²², the FAO affirms that a better understanding of food systems requires a local-to-global perspective.

Food systems are complex networks of activities, actors, resources, and environments encompassing the production, processing, distribution, consumption, and disposal of food products. Comprehending these networks is arduous as they are constantly evolving, and are interconnected with broader social, economic and policy systems.

Climate change has a very strong impact on food systems, exacerbating hunger and malnutrition issues, especially in regions that are already vulnerable. It triggers extreme weather events, the emergence and spread of pests and diseases, and it compromises the adaptation of traditionally grown foods, resulting in reduced crop yields²³. Current projections indicate a necessary increase of food production per hectare by almost 60 percent by 2050 to meet the needs of the projected global population of 10 billion – assuming a static agricultural land²⁴. In this context, increasing productivity of agricultural land is not sufficient to address the core human need for food. Even now, countries with low and middle incomes, diets are known to be lacking in micro-nutrients including iron, zinc, folate, vitamin A, Calcium, and vitamin B12. As populations continue to grow, innovative solutions are much needed to devise sustainable agricultural practice that provide for more nutritious diets, while respecting planetary boundaries.

On the other hand, food systems also contribute significantly to climate change. While the production of food is a large contributor, greenhouse gas emissions associated with food transport also keep increasing²⁵. Both the UNFCCC and the FAO are working not only towards climate-resilient and low-emission agricultural practices, but also acknowledge

²¹ FAO, Putting a number on hunger: different measures for different

purposes., <u>https://www.fao.org/interactive/state-of-food-security-nutrition/en/</u> (accessed 15 September) ²² U.N, Sustainable Development

Goals, SDG2: Zero Hunger, https://www.un.org/sustainabledevelopment/hunger/ (accessed 15 September 2023) ²³ IPCC: Mbow C., Rosenzweig, C., Barioni, L.G., et al., 2019, Food Security. In: Climate Change and Land: an IPCC special report on climate change, desertification, land degradation, sustainable land management, food security, and greenhouse gas fluxes in terrestrial ecosystems https://www.ipcc.ch/srccl/chapter/chapter-5/ (accessed 15 September 2023)

²⁴ GESDA, 2023, *GESDA Radar Breakthrough*, <u>https://radar.gesda.global/sub-topics/resilient-farming</u> (accessed 28 September 2023)

²⁵ Pradhan, P., 2022, *Food transport emissions matter*. *Nat Food* **3**, 406–407., <u>https://doi.org/10.1038/s43016-022-00524-9</u> (accessed 28 September 2023)



the considerable potential to maximise co-benefits of adaptation and mitigation of food global supply chains²⁶.

Recent large-scale disruptions like the Panama Canal drought have reinforced awareness of the vulnerability of the global food supply chains²⁷, in critical chokepoints represented by maritime corridors such as straits and canals, and coastal and inland transport infrastructures in major crop importing-exporting regions.

Accurate modelling of food systems will help provide the basis for improving our ability to produce nutritious food sustainably and foster resilience and respond to unforeseeable food systems disruptions.

The OQI addresses the interconnection between food and nutrition security and climate change from two angles. A first use case focuses on Food Production, i.e.: on how to produce enough affordable, nutritious food for a growing population without exceeding planetary limits. A second use case looks at food distribution, i.e.: how to improve the resilience of the global food supply chain against potential disruptions.

How could quantum help

a) Nutritious Food

GAIN (Global Alliance for Improved Nutrition) has launched multiple initiatives to strengthen and support the implementation of country food system pathways that can accelerate improvements in the consumption of safe and nutritious food for all, especially the most vulnerable, produced in a sustainable way. One new programme is to develop a new food rating system and use the obtained scores as functional units to conduct nutritional Life Cycle Assessments in Indonesia and Bangladesh. The nutritional value scores will consider nutrient density, as well as dietary factors related to non-communicable diseases (NCDs), such as fibre and nutrient ratios, to account for the double burden of malnutrition (i.e., coexistence of overnutrition and undernutrition) that low- and middle-income countries are currently facing. The methodology developed will be adaptable and applicable to other countries and regions worldwide²⁸

Ultimately, the global food system needs to be mapped and optimized. This means to incorporate additional factors, such as societal, environmental, and economic factors. Amongst critical objectives to optimize are: (i) Maximizing nutrition/public health outcomes, ii) Minimize environmental impact (beyond waste iii) Maximize supply chain profits (economic); (ii) (iii) Minimize unsatisfied demand; (iv) maximize shelf live and food safety; (v) Maximize affordability; (vi) Maximize desirability with cultural context, vii) Maximize impact of food policies and innovations, etc.

b) Resilient Food Supply

The FAO, in its report "The State of Food Security and Nutrition", states that bottlenecks in food supply chains is an important factor of increases in food prices and therefore calls for addressing inefficiencies and problems in transportation²⁹. It identifies digital technology

²⁶ FAO, 2022, FAO Strategy on Climate Change, 2022-2031., <u>https://www.fao.org/3/cc2274en/cc2274en.pdf</u> (accessed 28 September 2023)

²⁷ Nelson, A., de By, R., Thomas, T., Girgin, S., Brussel, M., Venus, V. & Ohuru, R. ,2021, *The resilience of domestic transport networks in the context of food security – A multi-country analysis. Background paper for The State of Food and Agriculture 2021*. FAO Agricultural Development Economics Technical Study No. 14. Rome, FAO, https://doi.org/10.4060/cb7757en (accessed 27 September 2023)

²⁸ GAIN, *GAIN website.*, <u>https://www.gainhealth.org/</u> (accessed 15 September)

²⁹ FAO, IFAD, UNICEF, WFP and WHO, 2023, *The State of Food Security and Nutrition in the World 2023. Urbanization, agrifood systems transformation and healthy diets across the rural–urban continuum.* Rome, FAO. <u>https://doi.org/10.4060/cc3017en</u> (accessed 15 September 2023)



as a lever to make supply chains technically and economically efficient with strong storage, processing, and transportation infrastructure³⁰.

This implies developing a global-scale supply flow optimization that takes a spatially refined approach to make sure that risks can be quantified spatially. Performing optimization on such large domains is challenging, in particular given that data limitations can make it hard to constrain the solutions.

The Oxford Programme for Sustainable Infrastructure Systems³¹ studies resilience of the global food supply. In particular, it looks at large-scale freight allocation models. While some of these models work on simple "all-of-nothing" allocation schemes (simple shortest paths), others work with greedy search algorithms³², yet all of them must take several simplifications. The lack of detailed models currently limits the ability to capture the complexity of food supply from field to consumer. In fact, most of the global analyses do not even do any form of transport flow optimization³³. A common approach to resilience analysis is the percolation method, where one removes one or multiple route segments or nodes (e.g., ports) from a model and re-runs the analysis. Obviously doing this on a global scale is very challenging³⁴. In short, none of the global freight flow allocation models can solve multiple objectives within a common framework.

In both approaches to a) nutritious food and b) resilient food supply, they relate to a class of optimization problems known as *mixed-integer linear programming*. Classical algorithms to find approximate solutions (heuristics) to this class of problems exist and are commercially available. However, this class of problems is in general computationally hard, making large-scale optimization (e.g., many crops, many farmers, many processing options, many ports, various tariffs, many consumer segments, many objectives, etc.) challenging with classical computers and algorithms, as they would require exceedingly long computational time to reach a good approximate solution. Quantum algorithms hold promise to significantly enhance the quality of the solution to these optimization problems and represent therefore an ideal use case. Quantum computing could therefore potentially help navigate these challenges by providing a more detailed and real-time understanding of food systems.

A roadmap to impact

The most representative and studied quantum optimization algorithm is the Quantum Approximate Optimization Algorithm (QAOA). QAOA has the promise to lead to a practical advantage over classical optimization algorithms³⁵. QAOA was developed to optimize a class of problems known as Quadratically Binary Unconstrained Optimization (QUBO)

³⁰ FAO. 2023. Guidelines to increase the resilience of agricultural supply chains. Rome. <u>https://doi.org/10.4060/cc5481en</u>

³¹ Oxford Programme for Sustainable Infrastructure Systems, *OPSIS website*, <u>https://opsis.eci.ox.ac.uk/</u> (accessed 27 September 2023)

³² Tavasszy, L., Minderhoud, M., Perrin, J-F., Notteboom, T., 2011, *A strategic network choice model for global container flows: specification, estimation and application., Journal of Transport Geography*, Volume 19, Issue 6, 2011, Pages 1163-1172, <u>https://doi.org/10.1016/j.jtrangeo.2011.05.005</u> (accessed 27 September 2023)

³³ Kinnunen, P., Guillaume, J.H.A., Taka, M. et al., 2020, Local food crop production can fulfil demand for less than one-third of the population., Nat Food **1**, 229–237, <u>https://doi.org/10.1038/s43016-020-0060-7</u> (accessed 27 September 2023)

³⁴ Colon, C., Hallegatte, S. & Rozenberg, J., 2021, *Criticality analysis of a country's transport network via an agent*based supply chain model., Nat Sustain **4**, 209–215, <u>https://doi.org/10.1038/s41893-020-00649-4</u> (accessed 27 September 2023); Karakoc, D.B., Konar, M., Puma, M.J. et al., 2023, *Structural chokepoints determine the resilience of agri-food supply chains in the United States. Nat Food* **4**, 607–615, <u>https://doi.org/10.1038/s43016-</u> <u>023-00793-y</u> (accessed 27 September 2023)

³⁵ Zhou, L., Wang, S., Choi, S., et al., 2019, *Quantum Approximate Optimization Algorithm: Performance, Mechanism, and Implementation on Near-Term Devices.*, <u>https://arxiv.org/pdf/1812.01041.pdf</u> (accessed 15 September 2023)



problems. QUBO are characterized by a quadratic objective function of many binary variables and do not have constraints. There is however a well-established scheme to efficiently map mixed-integer linear programming to QUBO.

With the expected size of this optimization problem, only future large-scale quantum computers will be suitable to host it. Alternatively, the same optimization problem may be tackled using advanced physically-inspired and even quantum-inspired optimization algorithms run on conventional large-scale computers. New quantum-inspired algorithms in particular have shown evidence of practical advantage over the best conventional algorithmic strategies. The use of physical- and quantum-inspired algorithms will likely be an efficient alternative strategy to address the optimization of food systems in the short- to mid-terms.

Efficiently solving these optimization problems related to the global food system instances can lead to significant cost savings, reduced environmental impact, and improved resource allocation.

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