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GESDA Solutions

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Solution Idea

Open Quantum Institute - SDG Use Cases

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In collaboration with:

Quantum for SDG Use Cases

Quantum computers, which are expected to be fully operational within 10 to 15 years, will have a transformative impact on our society and our planet, by solving currently insoluble problems. With its global community of academics, governments, and industry leaders, GESDA is convinced that action must be taken to anticipate the maturity of this technology and therefore proposed the idea of an "Open Quantum Institute".

One of the core missions of the Open Quantum Institute is to harness quantum computing to tackle the UN's Sustainable Development Goals (SDGs)[1]. Over the coming years we will be working with researchers, technology developers, UN stakeholders, diplomats, and policymakers from across the globe to come up with new use cases for the technology that can help solve some of the world's most pressing challenges.

To help our partners better understand the kind of solutions we are hoping to develop, we have started investigating directions in which quantum computing could contribute towards the SDGs. This was done by bringing together partners in UN and international organizations responsible for spurring progress on the SDGs and quantum scientists working at the cutting-edge of the field.

GESDAs science diplomacy community believes it is essential to anticipate the readiness of quantum computers and propose future SDG benefitting use cases for quantum R&D-ers to start exploring now. While quantum computers are still under development to ensure reliable and scalable devices to be put in production in the next 5-10-25 years, solutions to SDG relevant use cases can already start to be shaped today using currently available quantum simulators. The latter are more resilient to noise and, for some hard problems, can already provide practical quantum advantage[2] . This will help the R&D community to focus on where there is the best potential concretely contribute to the UN 2030 Agenda for sustainable development.

The initial use cases presented below are the result of collective exploratory work conducted from April to September 2022. They have been selected based on their potential impact on the SDGs and the likelihood that quantum computing can accelerate progress in these areas. This is a very first step and we will refine, deepen and expand this work in the coming months so that the Open Quantum Institute gradually becomes the centre of expertise on the SDGs

GESDA would like to thank the contributors to this experiment for their willingness to step out of their comfort zone, their openness to share their experiences and their enthusiasm for anticipatory science diplomacy.

Quantum Simulation Use Cases

Simulation of the quantum nature of quantum systems is the most direct application of quantum computers. Simulating the quantum mechanics of large systems relevant to chemical and biological processes is one of the most difficult computational problems. Quantum computers will offer exponential speedup over what is intractable with classical computers to solve these problems. To perform these quantum simulations, we will require scalable fault-tolerant quantum computers, which are still under development.

Three examples of quantum simulations application are presented below.

New Carbon Capture Materials

There is growing recognition that if the world is to avoid the worst effects of climate change, simply reducing greenhouse gas emissions will not be enough. Carbon capture technology will be essential if we want atmospheric CO_2 to return to a safe level[3].

Carbon captures relies on using specially designed materials to pull CO_2 directly out of the air, or from the exhaust gasses of power stations and other carbon-emitting facilities like cement plants or steel works[4]. The CO_2 can then either be stored deep underground or potentially reused to create fuels or valuable chemicals.

But while technically feasible today, current carbon capture technology is still far too expensive to be practical. One of the major challenges is finding new materials that are cheap, efficient at capturing CO_2 and require little energy to do their job. Solving this problem will be essential if we want to fulfill the SDGs related to climate action.

How quantum could help

A major challenge when designing new carbon capture technologies is the fact that today's computational models can only predict the behavior of simple materials. They are incapable of capturing the complex electronic dynamics involved in the relevant chemical reactions, and as a result, most work in this area relies on time-consuming experimentation to discover new materials.

This problem is a natural fit for quantum computing because simulating physical systems is one of the most promising applications for the technology. Emerging quantum algorithms could be used to predict the performance of candidate carbon capture materials, as well as potential chemical instabilities that could limit the ability to produce or use them in practical settings.

A roadmap to impact

One of the most promising materials for this application is a class of small molecules called metal-organic frameworks that have exceptional capacity for CO_2 adsorption[5]. But today's classical models struggle to accurately simulate their interactions with CO_2, limiting efforts to design new materials in this class.

One way round this involves using machine learning to generate a rich database of hypothetical structures of metal-organic compounds[6]. The computational cost of this approach means there is currently a trade-off between finding structures that can be easily synthesized in the laboratory and exploring more unusual structures. Quantum machine learning could potentially side-step this compromise to accelerate the design of new compounds that are both novel and practical to produce at scale[7].

As quantum computers scale up, new quantum chemistry models will also dramatically improve our ability to predict how materials interact with CO_2, allowing for more directed design. This will likely take many years to yield results though, as quantum chemistry simulations will require fault-tolerant quantum computers with many thousands of qubits.

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Tackling Antibiotics in Wastewater

Antibiotics revolutionized healthcare in the second half of the 21st Century, but excessive use of these vital drugs is threatening both human health and the environment.

Global consumption of antibiotics rose by 46% between 2000 and 2018, and as much as 76% in low income countries, thanks to over-prescription in humans and increasing use in livestock farming and aquaculture[8]. This has led to growing antibiotic resistance (AMR) in disease causing pathogens, but also rising levels of antibiotic pollution in wastewater. This presents serious threats to human health and can significantly disrupt downstream ecosystems.

Finding a way to efficiently remove antibiotics from wastewater could help tackle SDGs related to improving water quality, reducing deaths from toxic chemicals and restoring aquatic ecosystems. In March 2022 the Global Leaders Group on Antimicrobial Resistance called for action to protect the environment from antimicrobial pollution through improved discharge management and R&D to find new ways to remove antimicrobial residues[9].

How quantum could help

Traditional water treatment plants are not designed to deal with antibiotics[10]. Several technologies for the degradation and removal of these drugs exist, including physical adsorption, chemical oxidation, photodegradation, and biodegradation[11]. However, their performance is still unsatisfactory, and none have been implemented at scale.

Quantum computing could help by designing new materials and chemicals to remove antibiotics from wastewater. The performance of these materials is determined by their chemical structure and chemical interactions, which can be well-described by various quantum chemistry models.

A number of quantum algorithms are under development that should enable these models to run at far greater speed and scale than on today's classical computers[12]. These quantum simulations could help to create novel water filters that can chemically capture or degrade antibiotics in water.

A roadmap to impact

An important first step will be to analyze current antibiotic use to determine which of these drugs it is most imperative to design solutions for. Once that is done, quantum computers can be used to simulate how new materials interact with these molecules.

Simulations are only the first step in the process though. Material scientists would then need to work out how to engineer these materials and experts in wastewater treatment would have to provide feedback on the scalability and potential risks presented by proposed solutions. It will likely take few years to develop a first blueprint solution, after which a small pilot in close proximity to human hospitals or aquaculture farms could help to validate the proposal.

Eco-friendly Fertilizer Production

Fertilizers play a crucial role in feeding the world's population and we use about 200 million metric tonnes globally every year[13]. But the processes used to manufacture these crucial chemicals are incredibly power-hungry, accounting for approximately 1-2% of global energy use[14] and use a similar fractional of global natural gas production in the reaction.

Most fertilizers today are created using the Haber-Bosch process, which involves combining nitrogen from the atmosphere with hydrogen gas at high temperatures and pressures. This method requires huge amounts of energy, which means fertilizer has to be produced in large centralized facilities that contribute significantly to climate change.

Despite the fact that the current approach is more than 100 years old we've yet to find a more efficient way to produce fertilizers in local small-scale facilities. Doing so could go a long way to tackling SDGs around climate change and might allow us to democratize the process of producing these vital agricultural inputs. This would have major social and economic impact for the local communities.

How quantum could help

We know that better approaches exist, because bacteria naturally fix nitrogen from the atmosphere using a fraction of the energy. But we have yet to crack the complex biochemistry that allows them to do so[15].

That's partly because the interplay of different enzymes and cellular processes involved are difficult to simulate on classical computers. But quantum computers are expected to excel at simulating chemical reaction pathways and enzymatic behavior of this sort[16-18].

In principle, this should make it possible to model critical aspects of the natural nitrogen fixation pathway, which could dramatically improve our understanding of the process. This could help us design novel catalysts or even new biochemical process that could allow us to produce fertilizers using considerably less energy.

A roadmap to impact

The heart of this biochemistry problem relies on chemistry simulations that are quantum native problems for which quantum computers will provide substantial speedup and accuracy advantage. Different quantum chemistry algorithms are currently being developed by researchers. To reach the level of simulation accuracy needed to deeply understand the catalyst and biochemical processes, such as nitrogenase enzymes found in cyanobacteria, more reliable and powerful quantum computers with a very large number of qubits are necessary. Given that today's leading processors feature just hundreds, we are unlikely to have the hardware to perform such calculations until the end of this decade, but the goal appears within reach.

Quantum Inspired Optimization Use cases

Optimization is another class of where Quantum research is already creating value today. By thinking radically differently on how to solve a problem, quantum researchers have generated novel ideas which led to the development of new powerful algorithms for combinatorial optimization. Until now, however, these algorithms have been "quantum inspired" which means that researchers ultimately found out that some of them can be effectively run on classical computers.

Two examples of optimization problems are presented below.

Sustainable and Nutritious Food Production

Growing populations and poor access to nutritious food in much of the world mean that crop production needs to increase by 60% by 2050[19]. But intensification of agriculture can have serious knock-on effects on the environment.

Agricultural yields rose by 44% between 1965 and 2010 thanks largely to increasing use of fertilizers, pesticides, mechanization and irrigation[20]. There is growing recognition that those tools are reaching the limits of their usefulness and could in fact be doing irreparable harm to critical ecosystems and the soil farmers rely on[21].

This is leading to growing efforts to find sustainable approaches to agriculture that can boost nutritious food production while protecting the environment. One of the most promising ways of achieving this is to grow crops appropriate for the local climate and culture rather than taking a cookie cutter approach. Finding a solution to this problem could go a long way towards solving SDGs related to ending world hunger and protecting nature.

How quantum could help

A central problem for sustainable agriculture is working out what food to produce where, so that we can meet the world's nutritional needs without damaging the environment. This involves considering everything from environmental conditions, to demographics, to local dietary traditions, to indigenous agricultural practices, to the nutritional make up of different crops.

This is an optimization problem, which refers to situations where you have to find the best solution from a large number of possible solutions. This can also be expressed as a predictive problem, in which, given specific local constraints and food characteristics, one needs to identify which selection of food crop can maximize the nutritious outcomes to the population. Problems with many variables, and therefore many potential solutions, quickly become too complex for even the most advanced supercomputers.

Research into quantum algorithms has uncovered a new class of quantum-inspired algorithms that we can run today on classical computers to tackle complex optimization problems[22].

A roadmap to impact

A significant challenge in this area is collecting data on key variables affecting optimal nutritious and sustainable food production. At present much of this has to be done by hand in the field, even if there are a growing number of global datasets that can be leveraged.

The Periodic Table of Food Initiative is developing standardized ways to represent nutritional data for different foods alongside metadata covering environmental, economic, and socio-cultural metrics. The hope is that this will help compile an open database on the world's most important foods[23]. Elsewhere, the World Soil Information Service is providing an ever-expanding repository of standardized soil profile data from around the world[24]. Leveraging these complex sets of data will not only help optimization the food production in a sustainable manner, it provides the opportunity to predict how to magnify the nutritious outcomes of given food in a given environment.

This is one area where quantum approaches on classical hardware could provide significant value today. The next level will be to put in production such enhanced solutions, linking them to existing, although currently disjointed, crop models, livestock models, climate models, and nutritional models[25-27]. Validating the output of these calculations will still require extensive experimentation on farms around the world, which will likely take years.

Optimizing Vaccine Distribution

The Covid-19 pandemic highlighted that simply developing new vaccines can't solve a global health crisis. Actually, getting them to patients all over the world can be just as crucial for determining the success of the public health response.

While wealthy countries rolled out new vaccines quickly, efforts to ensure equitable distribution around the world were less successful. While this was partly a political problem, it was also a logistical one.

The COVAX vaccine sharing program has managed to distribute 1.72 billion doses to 146 countries[28]. According to UNICEF, which has been responsible for delivery, allocating them efficiently has been challenging[29]. Smarter ways to optimize vaccine distribution could improve responses to future health emergency's and help tackle SDGs around access to health services.

How quantum could help

The process of distributing vaccines efficiently involves complex interactions between many different players and processes. At the most fundamental level, it involves accurately forecasting both manufacturers ability to supply new doses and the ability of various national health systems around the world to make use of them before they expire[30].

On top of that, it's necessary to take account of the state of the logistics networks used to connect this supply and demand, which can be in constant flux. A host of other factors, including national export rules, insurance requirements, and transport costs all need to be considered too.

Current vaccine distribution schemes use optimization algorithms to balance these competing priorities. Classical approaches quickly become intractable as the number of parameters grows, and shortcuts often have to be taken. Future quantum inspired algorithms on the other hand are expected to be able to deal with far more parameters, making them a promising candidate for logistics optimization problems like this[31].

A roadmap to impact

The complex logistics of vaccine distribution can be mapped into a combinatorial optimization problem. The overall objective is to minimize inequality, and prevent further inequality, in population over time, taking into account a set of constraints. Quantum inspired algorithms to combinatorial optimization could provide substantial speedup over existing methods.

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