Pharmaceuticals & Medical Products Practice

Recalculating the future of drug development with quantum computing

Two experts discuss how quantum computing can help solve intractable problems in drug discovery and development.

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Quantum computing (QC) is a fundamentally different computing approach based on the laws of quantum mechanics, which allows certain computations to be performed far more quickly and efficiently than traditional computing does and therefore holds enormous potential for the pharmaceutical industry. Recognizing the game-changing nature of this approach, leading pharma companies are setting up quantum task forces and investing significant sums to explore the application of quantum computers and software to chemistry and biology. McKinsey's Anna Katharina Heid and Ivan Ostojic asked Chad Edwards, product lead at Cambridge Quantum Computing (CQC), and Lucas Siow, CEO and cofounder of biotech company ProteinQure, to share their insights into how specialist start-ups like theirs are working with pharma companies.

McKinsey: What kinds of problems is quantum computing best suited to addressing in the pharma industry?

Chad Edwards: In the computer-aided drug-design (CADD) process, increasing the accuracy of molecular simulations incurs a punishing exponential increase in computational cost. Quantum computing could transform the way we think about the simulation of solids, molecules, atoms, nuclei, and subatomic particles. It could help overcome the scaling limitations of classical computational methods and allow for numerically exact solutions to the Schrödinger equation for larger and more complex molecular systems.

As quantum hardware continues to mature in both quantum bit (qubit) quality, count, and quantum volume—we expect quantum computing to affect all phases of the drug-development pipeline. Fault-tolerant quantum devices are still at least a decade away, but NISQ[1] devices and variational algorithms are permitting the early adoption and commercialization of quantum chemistry and QML,[2] priming pharma to be one of the greatest beneficiaries of the technology.

Lucas Siow: At ProteinQure, we believe that quantum computing will be applicable to many of the workflows in computer-aided drug discovery. We currently focus on molecular similarity, protein-structure prediction, and protein design, but QC would also be relevant to quantum chemistry, QSAR[3] models, and molecule docking. Most of our near-term applications are concerned with reframing problems in drug discovery as energy-minimization problems and using a quantum device to solve computational bottlenecks. The algorithms involved tend to be quantum–classical hybrids.

McKinsey: Where will quantum computing deliver the most value for pharma companies?

Chad Edwards: There's little doubt it has the potential to disrupt drug discovery. Today's drug-discovery and development process is notoriously expensive and time inefficient—a new chemical entity takes, on average, about $2 billion and ten years to reach the market. While classical machine-learning technologies are already starting to show great promise in reducing both time and cost to market, quantum processing could truly revolutionize the process. Once quantum computing is mature enough, we will probably see the greatest value being realized in the preclinical and clinical stages, where failure rates are currently over 90 percent.

Lucas Siow: Our hope is that in the long term, quantum computing will enable computational tools for antibody design. Large proteins, mostly in the form of antibody therapeutics, are a market worth close to $200 billion. That market was created 30 or 40 years ago with the development of new experimental techniques that made it

[1] Noisy intermediate-scale quantum.
[2] Quantum machine learning.
[3] Quantitative structure–activity relationship.

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–Chad Edwards

possible to make therapeutics out of antibodies. If there was a great computational tool for designing and developing antibodies, it would help create another set of novel antibody structures and motifs for addressing undruggable targets.

McKinsey: How do you go about integrating quantum technologies with classical computing to meet the needs of pharma companies?

Chad Edwards: At present, all our work is focused on variational quantum/classical algorithms, which are well suited to the NISQ devices available today and allow us to exploit the best of the classical and current quantum computational worlds. As for the future, we can foresee a time when a pharma company, or any other company for that matter, looks at a problem and then looks at its tool set—CPU,[4] FPGA,[5] GPU,[6] and QPU[7]—to decide which tool or combination of tools is best suited to solving it. Integration happens naturally as we use our expertise in HPC and computer architecture to strategize on how to solve a problem by taking advantage of the different architectures.

Lucas Siow: Our work at ProteinQure focuses on the design and optimization of protein therapeutics, and we've invested heavily in classical algorithms and approaches. Our tools work on classical cloud computing scaled to thousands of CPUs and GPUs. The quantum devices available today aren't yet ready to add value, so ProteinQure has built an automated platform where QC can be combined with many other computational tools to solve commercial problems. We believe hybrid algorithms and approaches are likely to be relevant soonest. When NISQ devices are ready, they'll become another computational module to be included, just as we combine computational modules[8] on the cloud today.

McKinsey: How big a technological gap will pharma companies have to bridge to integrate quantum computing into their operations?

Chad Edwards: The current technological gap is quite large, as off-the-shelf quantum tools are not yet available for application by nonspecialists. The primary challenge is for the pharma industry to start viewing problems in a quantum way and to understand where quantum algorithms can be employed. Today the industry assumes that the best answer to any problem can be found through employing classical methods and tools, and we need to change that assumption. It is the role of quantum computing start-ups and incumbents to assist and accelerate this. I do, however, foresee this gap closing quickly, as across the pharma industry we see rapid adoption, which is predicted to reach 60 to 70 percent by 2021.[9]

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[4] Central processing units.
[5] Field-programmable gate array.
[6] Graphics processing units.
[7] Quantum processing unit.
[8] For instance, machine learning, molecular dynamics, and bioinformatics.
[9] "Almost one third of life science companies set to begin quantum computing evaluation this year," July 14, 2020, pistoiaalliance.org.

McKinsey: How do start-ups connect with pharma companies about applying QC, and who takes the lead in identifying demand and matching offerings?

Chad Edwards: In brief, I would say that there is a direct and indirect route to enabling collaboration between QC start-ups and pharma players. The direct route entails the two organizations bringing together their respective domain expertise to work on use cases of mutual interest and the potential for significant IP generation. The second and more indirect route is via industry consortia and not-for-profits, such as the Pistoia Alliance and the QuPharm Alliance, which promote precompetitive engagements between pharma players and the quantum community. In either instance, it is the duty of the QC players to meet the needs of the pharma players and ensure that QC tools augment the established pharmaceutical workflows.

Lucas Siow: We QC start-ups need to respect the drug-discovery workflows that drug companies have developed over the years. It's our obligation as the solution provider to build tools that address customer demand. Creative partners play an instrumental role in helping us identify novel ways to use our capabilities to solve challenges in drug discovery. We've built software, biology, and drug-discovery competencies and spoken to major biologics players to make sure we're not just building novel technologies but also creating tools that help solve the problems pharma faces today, like working on non-natural amino acids or engineering cell permeability.

McKinsey: What does a pharma company need to have in place to work with QC start-ups? Are there issues in data availability or expertise in HPC applications, for instance?

Chad Edwards: At present, we work with data scientists and teams from research, informatics, and modeling to identify and tackle the use cases that matter most to their companies. We don't expect all our clients to have quantum information theorists; that wouldn't be realistic at this stage. We work with these teams to reduce barriers to adoption and enable teams to use our software to tap into the capabilities of the devices they already have, with the goal of seamlessly integrating QC applications into their existing workflows.

Working with a start-up gives pharma companies the best way to bring QC expertise into their teams and move forward with adoption at lower risk. Given the short supply of QC expertise, tools, and hardware in the coming years, I expect this partnership model to be dominant for quite some time. A select number of pharma companies are currently integrating one or two quantum information theorists into their teams, but the majority will continue looking to external providers for core expertise and tool kits.

Lucas Siow: In many of our partnerships, what our collaborators bring is experimental and domain expertise in biologics drug discovery. The ability to generate data and synthesize novel chemistries helps them get the most out of our tools because those aren't capabilities we have. We don't need large amounts of data, machine-learning expertise, or HPC experience. The platform we've built doesn't require our partners to duplicate our strengths but rather allows them to take advantage of their own expertise. For instance, some of our partners have unique capabilities in certain types of synthetic chemistry. Computational tools can help them explore that novel space.

McKinsey: How would you advise pharma companies to approach quantum computing in terms of capability building, technology infrastructure, and partnerships?

Chad Edwards: The first step is to acknowledge that quantum computing is coming and will be a force in the industry. The next step is to get educated: go to conferences, talk to a start-up, or experiment with cloud quantum-computing platforms. From there, we believe that a company should draw up a plan for adopting the technology—a plan that includes capability building and partnerships with both academia and industry. Today's technology infrastructure is predominantly cloud-based, which is acceptable for most users.

Lucas Siow: Most pharma companies will have to decide whether to take a partner or build their own QC capabilities. Developing these skills internally will be a challenge on a scale similar to adopting world-class AI capabilities. I would expect big pharma companies to start the partnering process by understanding which problems in drug discovery are high value and can be addressed using computational methods. They could then engage in scientific conversations with potential partners, whether academics or start-ups. That stage would probably take a year or two to complete.

Pharma companies would then spend another couple of years working with their partners to understand whether the problems they've identified can be ported to QC and either building internal teams with QC experts or finding external partners that can bring value. Over the longer term, companies would start to understand hardware offerings, both on-premises and in the cloud.

McKinsey: Many QC players intend to deploy their offerings via the cloud. Does this pose any regulatory issues for the pharma industry?

Chad Edwards: Many countries have laws governing the use of patient data in the cloud and where that cloud is located. These laws will need to be addressed as quantum computing enters the mainstream. Security is another issue. As the capabilities of quantum hardware grow, current data-security measures will be broken or severely compromised, so every company will need to transition to a level of IT security that can withstand quantum technology.

Lucas Siow: There could be regulatory issues if the industry needs to start using QML on patient data. But for our purposes at ProteinQure, where we're modeling physical phenomena, we'll be fine with a cloud offering.

McKinsey: What kinds of use cases will pharma companies have for quantum computing, both in the near term and later on?

Chad Edwards: I foresee the most valuable use cases in the near term, three to five years, residing in the CADD process—for example, studying protein-ligand binding or modeling mechanisms for drug action. In recent years, DFT[10] has played a pivotal role in drug design as a quantum-mechanical method that can be applied to chemically and biologically significant

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>
> –Lucas Siow

[10] Density functional theory.

molecular systems at a fairly low computational overhead. I don't expect QC chemistry to displace or compete with DFT in this context but rather to augment it in tackling larger and more complex systems at greater levels of accuracy than are currently attainable. As the technology matures, I'd expect to see intractable problems being solved further down the drug-development pipeline—those associated with increased expenditures, preclinical and beyond, using larger-scale quantum chemistry and QML techniques.

Lucas Siow: In three to five years, I'd expect to see hybrid algorithms for protein design, structure prediction, and quantum value for prediction problems such as QSAR. In five to eight years, I'd expect quantum chemistry and QML and, after eight years or so, modeling for larger biological systems. I think in general we often overestimate what can be accomplished in the short term but underestimate the changes that can happen in the medium to long term.

McKinsey: What technological and economic leaps are needed for quantum computing to be successful in the pharma industry?

Chad Edwards: Though there's been huge progress on the hardware side, there are still many major bottlenecks in engineering and scaling better quality qubits. Quantum software players that focus on extracting maximum value from today's processors have devised clever solutions to working with the noise. These improved, and more noise-resilient algorithms are starting to be adopted more widely and to generate impact. As pharma and QC companies collaborate more deeply, we'll see greater creativity enabling solution development to take off.

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