

Quantum Computing and its potentials for the pharmaceutical industry

Making product development and production more efficient through Quantum Computing.

Quantum computers operate on the principles of quantum mechanics: While classical computers store data in terms of bits, which can take the values 0 and 1, a quantum bit (qubit) is a superposition of 0 and 1. These qubits can interact with each other, which allows to perform certain computational tasks significantly faster and solve highly complex problems. Read more on our [website](#).

Quantum Computing: Use cases in pharma and our approach

Simulation of quantum mechanical systems

In the simulation of quantum mechanical systems, like molecules, numerical methods quickly reach their limitations if the systems consist of too many particles. Being of quantum-mechanical nature themselves, quantum computers are ideal to perform such simulations. Different hybrid quantum algorithms have been proposed which may already be beneficial using near-term quantum computers. At IKS, we will evaluate the performance of the latest available algorithms in this area.

Quantum machine learning

In the development of new drugs, machine learning algorithms are used to predict the chemical properties of molecules. Compared to classical methods, quantum-based algorithms may lead to more efficient learning rates. At IKS, we are investigating the potential benefit of quantum convolutional neural networks for imaging. Furthermore, we will study quantum reinforcement learning algorithms for drug discovery.

Optimization problems

Quantum computing has the potential to speed up optimization processes, which can have use cases in a variety of fields, such as in logistics, industrial IoT automatizations and drug development. In the latter, the description of protein structures requires the minimization of highly complex mathematical functions. The research focus of IKS in this area lies on the development and evaluation of hybrid algorithms, which can be executed on near-term quantum computers.

Business benefits

The improvements from quantum computers may allow to save both time and computing resources, which can lead to faster product development processes and reduce their costs. Thereby also very low drug production volumes may become economically profitable.

Why working with IKS?

Our vision of Quantum Computing: Providing easy access to reliable QC-assisted solutions for industrial end-users, ensuring the efficient use of available Quantum Computing hardware.

1. Our Technology

- **Software** development of quantum algorithms in Pharma and Medical & software tools and services for industrial end users
- **Hardware:** Access to powerful quantum computing services of IBM Q System One in Ehningen, IQM-Hardware, the hardware being developed within the Munich Quantum Valley (MQV) & to high-performance computing simulators of the Leibnitz-Rechenzentrum (LRZ)

2. Our QC network

- **Co-lead** of application part in **Munich Quantum Valley (MQV)** with partners in academia, QC solutioning, business and other associated companies (a.o. TUM, LMU, IQM, Infineon, Roche, Novicos)
- **Part of Bavarian Competence Center** for Quantum Security and Data Science (BayQS)

3. Our Ressources

- **QC research projects**
 - Two research topics within BayQS: quantum-computing-assisted verification of classical neural networks & efficiency improvement of AI-based medical diagnoses using quantum convolutional neural networks.
 - Additional quantum computing projects in the areas of simulation, quantum machine learning and optimization are in the planning stage and the corresponding scientific proposals are currently in the review process.
- **Expertise**
 - Dedicated research team for the BayQS-activities at the Fraunhofer IKS and further expanding
 - Fraunhofer IKS research knowledge in safety of classical AI methods can easily be transferred to also assess the reliability of quantum algorithms

About Fraunhofer IKS

The Fraunhofer Institute for Cognitive Systems IKS conducts applied research into the topics of tomorrow: artificial intelligence, cognitive systems and intelligent software architectures for autonomous systems. Our primary focus is safety-critical applications in the areas of Mobility, Production, MedTech and Smart Farming providing »Safe Intelligence«.

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