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https://www.gesundheitsindustrie-bw.de/en/article/news/hqs-quantum-simulations-for-industrial-quantum-mechanics-applications

Company profile

HQS Quantum Simulations for industrial quantum mechanics applications

The door to the quantum world is opening wider and wider. Behind it is a whole new view of materials and molecules. Quantum mechanics applications not only benefit science, they also offer huge economic potential. The Karlsruhe start-up HQS Quantum Simulations is playing a pioneering role in quantum simulations for the chemical and pharmaceutical industries.

Amongst other things, HQS Quantum Simulations has access to IBM's quantum system. IBM's 50-qubit quantum computer at the IBM Q lab in Yorktown Heights, New York is protected from overheating using a special cooling device (IBM Q cryostat).
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Researchers are penetrating the microcosm and the nanocosm with increasingly sophisticated and more precise methods. However, conventional methods of investigation alone do not suffice to understand unimaginably small materials and molecules at the much deeper quantum level where the physical laws are quite different to those in our relatively coarsely knit macrocosm. Mathematics has provided a solution: physicists and mathematicians have been working for years on algorithms that can be used to fathom and describe the quantum world.

The quantum computer is a result of this effort. It goes beyond simple binary states, i.e. either-or-decisions encoded into binary digits (0 and 1), like a "normal" computer, and uses so-called quantum bits or qubits. These qubits can represent the simultaneous existence of basis states, known as the state of superposition, which have certain probabilities attached to them that can be calculated. The result is a highly complex and high-performance data processing tool – perfect for managing the rapidly growing data piles produced in academic and industrial research and development settings.

Field of application has been carefully defined in dialogue with industry

As scientific progress in quantum computing is continuing, more and more commercial applications are emerging. "In 2012 it became clear that quantum computers can actually be built. Since then, we've been thinking about how to develop products," says Thomas Marthaler, physicist, CEO and co-founder of HQS Quantum Simulations. Marthaler had worked as a postdoc and group leader at the Institute for Theoretical Solid State Physics at the Karlsruhe Institute of Technology (KIT) for ten years before he and three of his colleagues decided to establish HQS Quantum Simulations in November 2017. The team was supported by "upCAT", the start-up catalyst at the KIT.

"Prior to establishing our company, we had many in-depth discussions with potential industrial clients, including companies from the chemical and pharmaceutical sectors, where we were looking at the application of quantum computing in material and molecule simulations. Basically, we can deal with all issues that cannot be solved with conventional computing," says Marthaler, mentioning as examples processes in chemical and biochemical catalysis, and issues related to the optical excitation of molecules and to magnetism, for example in memory components. The future objective is to optimize related industrial processes using quantum computing.

However, despite all the progress that has been made, quantum computers available for companies to purchase are not yet available on the market. The HQS Quantum Simulations team is therefore testing its algorithms on cloud-based platforms provided by developers of quantum computers. "We have access to Rigetti Computing in Berkeley, USA, and the IBM quantum system," says Marthaler. In addition, the start-up initially implements its methods on normal computers. This involves developing algorithms and multiscale simulations that can be used to study processes of several orders of magnitude down to the molecular level and beyond. This enables the scientists to zoom deeper into chemical and biochemical processes over several steps. The very last step into the quantum level and thus to a more detailed analysis can be added relatively easily once quantum computers become more widely available, says Marthaler. He expects that quantum technology will be available

for the first commercial niche applications in the cloud in the early to mid-2020s.

Developing simulations for tomorrow today

Calicheamicins are enzymes from the bacterium Micromonospora echinospora that cause DNA double-strand breaks. The strong cell toxin is used in cancer therapy, amongst other things. Multi-scale simulations like those developed by HQS Quantum Simulations help to decipher the exact mode of action of such enzymes.
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Future commercial applications in the chemical and pharmaceutical industries aim to optimize processes for the production of valuable materials and active pharmaceutical ingredients. Some initial examples already exist. Marthaler cites as an example the quantum mechanical simulation of calicheamicin, a bacterial toxin, which is used, inter alia, in cancer therapy. As substances and their interactions with other molecules are increasingly studied and understood down to the quantum level, the possibility of developing targeted and even personalized therapies also increases. All in all, quantum computing opens up new, unforeseen opportunities for the life sciences whose effects cannot yet be anticipated.

Since quantum computing is an extremely forward-looking topic, the question arises as to whether HQS Quantum Simulations is currently able to make money with it. "Our software developments already enable our customers to fully exploit the possibilities of multiscale simulations and accordingly generate value. The value gain will become even greater when they are able to add quantum simulations in the foreseeable future. We are helping our customers prepare optimally for this. In addition, we offer our clients comprehensive consulting services for molecular and material simulations," says Marthaler outlining the business model of the seven-member company team. As momentum around the quantum computing hype grows, it is safe to say that HQS Quantum Simulations will be ready with its expertise for further industrial implementation.

Article

09-Jan-2019
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Data mining: new opportunities for medicine and public health



Big data - the big promise of the new digitised world



The quantum revolution in the healthcare industry

bioinformatics | pharma | database | chemical biology | data mining | big data