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QCi QuantiCoM

Press Release

DLR commissions d-fine with water simulation on quantum computers

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- d-fine has been selected by the German Aerospace Centre (DLR) to advance the development of algorithms for atomistic simulations in the field of statics and dynamics of water and hydrogen in the QuantiCoM H2Q project of the DLR Quantum Computing Initiative.
- d-fine is realising the project together with planqc and Molecular Quantum Solutions (MQS).
- Quantum computers are considered a disruptive technology that enable much faster calculations and simulations in a variety of application areas such as the behaviour of water-based and hydrogen-based mixtures of substances in interaction with periodic materials such as alloys (e.g. metal hydrides).
- The DLR Quantum Computing Initiative (DLR QCI) involves start-ups, industry and research to jointly develop quantum computers, software and applications and the necessary enabling technologies.
- d-fine is a European consultancy specialising in technically and analytically challenging topics with 1,500 experts with a scientific background.
- MQS was founded in 2019 with headquarters in Søborg (Denmark) and develops a cloud-based platform for the simulation of chemicals and molecular structures.
- planqc is located in Munich's Quantum Valley and was founded in 2022 by scientists from the Max Planck Institute of Quantum Optics and the Ludwig Maximilian University of Munich, and is the first purely German company to build and commercialise highly scalable room-temperature quantum computers based on atoms in optical lattices.
- Keywords: quantum technology, quantum algorithms, material simulation, drug development, quantum computing, water, hydrogen

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Frankfurt, November 9th, 2023 – In the QuantiCoM H2Q project, d-fine, together with the German Aerospace Centre (DLR), will use the possibilities of quantum computing to identify and solve problems in the field of material simulation. plancq and MQS will contribute additional expertise.

As pioneers in their respective fields, planqc, MQS and d-fine are pooling their expertise to jointly develop and evaluate quantum computing algorithms for atomistic simulations of water and hydrogen as part of the DLR Quantum Computing Initiative (DLR QCI) with researchers at the DLR Institutes of Materials Research, Materials Physics in Space and Engineering Thermodynamics in the QuantiCoM H2Q project.

With its DLR QCI project QuantiCoM (Quantum Computing for Materials Science and Engineering), DLR is pursuing the goal of pushing the development of advanced methods using quantum computers for materials science, materials engineering and industry in order to enable faster materials development in the future. The sub-project „QuantiCoM H2Q" includes the development of algorithms for atomistic simulations in the field of statics and dynamics of water and hydrogen, based on classical calculations aiming at optimisation for quantum hardware.

The simulation of water offers an excellent opportunity to test the capabilities and limitations of material simulation, to develop and validate new methods, and to investigate fundamental relationships between the structure, dynamics and other properties of materials. Since water and hydrogen are ubiquitous in many technical and biological processes, a more precise prediction of the dynamics and reaction mechanisms of these molecules can directly advance many research areas and industrial applications. Examples are the understanding of degradation processes or optimal operating parameters of electrolysers, the material simulation of alloys in contact with hydrogen and the more efficient simulation of drug candidates for drug development. Many of the basic physical principles and modelling approaches used in the simulation of water can also be applied to other liquids, solutions or complex materials.

The challenging task of simulating water and its various forms, taking into account larger systems and multi-scale effects, pushes classical methods and known ab initio methods to their limits. This is due to the exponential increase in complexity and thus the computing time required as the number of particles increases. The use of quantum computers (QC) promises a revolution in this field thanks to the improved scalability of simulations.

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However, current digital quantum computers are limited both by the number of qubits that can be used and by their gate quality. While the number of qubits limits the amount of information that can be processed, the limited gate quality inevitably leads to errors in the results of calculations, which is why they are referred to as NISQ computers (short for noisy intermediate-scale quantum). Variational quantum algorithms (VQA), such as the Variational Quantum Eigensolver (VQE) or the Quantum Approximative Optimisation Algorithm (QAOA), have found their way into the solution of quantum chemical models on a hybrid „classical+NISQ" architecture. They have the potential to achieve a (quantum) advantage over classical methods for specific molecules (e.g. correlated systems, quantum dynamic systems) in terms of the ratio between solution accuracy and required computing time.

The selection of d-fine to support this ambitious project confirms its activities and successes in the field of quantum computing. d-fine is a founding member of the PlanQK consortium, which was established in 2020 with funding from the German Federal Ministry for Economic Affairs and Climate Protection and develops and implements quantum applications for various use cases. The German start-up planqc was founded in April 2022 and develops quantum computing hardware as well as algorithms in hardware-software co-design. This is already the second DLR project for planqc and d-fine, following the commission to improve climate models using quantum machine learning. MQS is a Danish start-up founded in 2019 that is developing a cloud-based simulation platform to improve users' ability to determine material properties of chemicals and molecular structures. Together with planqc and MQS, d-fine damir is the ideal partner for DLR and the development of QC algorithms for atomistic simulations of water and hydrogen.

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About MQS

Molecular Quantum Solutions ApS (MQS) is a start-up founded in 2019. MQS is headquartered in Søborg outside Copenhagen (Denmark) in the Alfa Laval Innovation House. MQS was founded by two PhD graduates from the Technical University of Denmark (DTU): Mark Nicholas Jones and Lukasz Ruszczynski. The expertise of MQS is based on quantum chemical simulations for thermodynamic material properties and computational multiscale modelling. MQS is developing a cloud-based simulation platform to improve users' ability to determine material properties of chemicals and molecular structures.

Further information can be found at https://mqs.dk

About planqc

planqc builds quantum computers and stores quantum information in individual atoms – inherently the best qubits. The quantum information is processed by arranging these qubits in highly scalable registers and then manipulating them using precisely controlled laser pulses. planqc is characterized by a unique combination of quantum technologies that opens up the fastest path to quantum processors with thousands of qubits, thereby creating the necessary

prerequisites for an industry-relevant quantum advantage. planqc was founded in April 2022 by Alexander Glätzle, Sebastian Blatt, Johannes Zeiher, Lukas Reichsöllner together with Ann-Kristin Achleitner and Markus Wagner. planqc is based in Garching near Munich.

Further information can be found at https://www.planqc.eu

About d-fine

d-fine is a European consulting company with a focus on analytical and quantitative challenges and the development of sustainable technological solutions. The combination of over a thousand scientifically trained employees and many years of practical experience enables tailor-made, efficient and sustainable implementations for our more than two hundred customers from all sectors of the economy.

Further information can be found at https://www.d-fine.com/

About the DLR Quantencomputing-Initiative (DLR QCI) of the German Aerospace Center (DLR)

The DLR Quantum Computing Initiative (DLR QCI) involves start-ups, industry and research to jointly develop quantum computers, software and applications and the necessary enabling technologies. The Federal Ministry for Economic Affairs and Climate Protection (BMWK) provides the funds for this. This is how the economic and industrial basis for the quantum computing ecosystem is being created at the DLR innovation centers in Ulm and Hamburg.

Further information can be found at https://qci.dlr.de/