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Quantum Computing in Industrial Applications

Four Domains – Four Case Studies

Imprint

Quantum Computing in Industrial Applications
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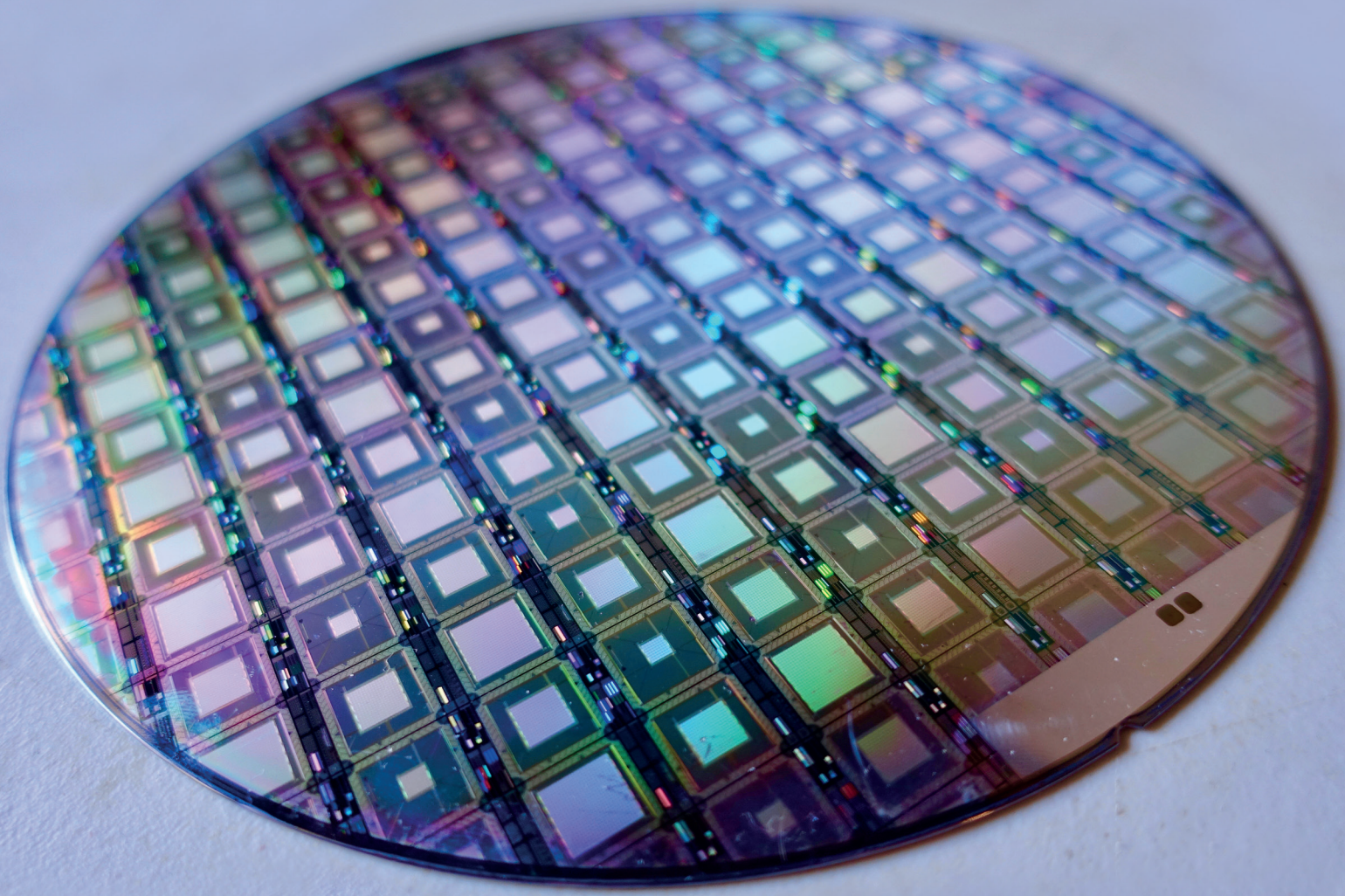

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1 Introduction

As industries navigate an increasingly complex and data-driven landscape, the demand for innovative solutions that optimize operations and enhance decision-making has reached remarkable heights. While traditional computing methods are effective, they often struggle to keep up with the increasing intricacies of modern challenges.

Excitingly, quantum computing is on the horizon, and although its practical applications in industry are still developing, theoretical research indicates that we are approaching a pivotal moment where quantum computers will become essential and indispensable tools across various domains. Quantum computing has the potential to revolutionize industries by solving complex problems beyond the capabilities of classical computers, enabling breakthroughs in various fields.

To ensure that industries are well-equipped to leverage this groundbreaking technology as it matures, early adoption and exploration of quantum solutions become increasingly relevant. Thus, applied quantum research is vital, connecting theoretical research and real-world implementation.

In this context, the virtual organization **"Fraunhofer Industrial Application Center Quantum Computing Hamburg (Fraunhofer IQHH)"** was founded by the Hamburg **Fraunhofer Institutes (CML, IAP, IAPT and ITMP)**. Within IQHH, four relevant industrial applications have been formalized, and suitable quantum algorithms have been successfully implemented and executed on simulators and real quantum computers.

The four use cases belong to four different business domains:

- **Maritime Logistics** (Chapter 4)
  A complex routing problem was formalized as a mathematical optimization problem and solved using a quantum annealer.

- **Catalyst Research** (Chapter 5)
  This project explores quantum computing for simulating platinum catalysts by reducing problem size with active space methods and ZX calculus.

- **Additive Manufacturing** (Chapter 6)
  In this project, a pipeline was deployed that uses in-situ sensor data and a quantum-enhanced Convolutional Neural Network for the challenging classification task of detecting defects in components.

- **Drug Discovery** (Chapter 7)
  This project aims to accelerate core stages of the drug discovery process. A quantum annealing-based approach to enhance Support Vector Machines is used to tackle this challenge.

We invite you to delve into the following chapters, which begin with a brief overview of quantum computing's potential and current state. This foundation is followed by detailed discussions of our four use cases, highlighting the applied methods and the advancements made.

2 Quantum Computing: Introduction and Potential

Quantum computing (QC) has been identified by the central scientific organizations in Germany, Europe and worldwide as one of the key technologies of the future. QC will allow us to tackle central societal and technological challenges such as energy transition and sustainability, transportation and mobility as well as biotechnology and life sciences with completely new disruptive tools, methods and concepts. Accordingly, companies from all sectors of industry are looking at this topic from the perspective of being able to deal with complex operational problems, where current computing resources reach their limits. QC enables competitive advantages and leaps in innovation for companies. The time scales of QC and its applications are long-term (10 years).

In contrast to a classical computer, a quantum computer does not work based on macroscopic states of electronic circuits, but on quantum mechanical states of suitable systems. This makes it possible to generate superposition states and quantum entanglement during the calculation, both of which are crucial for information processing in quantum computers. Superposition states are responsible for the ability of the quantum bits (qubits) to take on many other states in addition to the states 0 and 1, which allows a high expressibility within the quantum domain. In addition, states can be dependent on each other (so-called entanglement). This allows a fast computation of highly correlated states, which is computationally expensive in classical computation. Therefore, quantum entanglement is the reason for the anticipated quantum advantage.

There are currently no quantum computers that demonstrate a quantum advantage for industrial applications. However, there are already some important publications that demonstrate a fundamental quantum advantage for (a) applications that are neither scientific nor industrial [1, 22] and even (b) a quantum advantage for scientific applications [18]. This means that we are approaching a quantum advantage for industrial applications.

Algorithms have been identified that cannot be solved with current high-performance computing (HPC) systems or can only be solved in disproportionately long periods of time, which are polynomially or even exponentially accelerated with QC, e.g. by Shor [19], Grover [9], Harrow, Haddifim & Lloyd [10] , Babai, Beals & Seress [2] and Bennet, Bernstein, Brassad & Vazirani [3]. Not all these algorithms can currently be successfully implemented due to the limits of today's QC hardware. While these algorithms refer to perfect, fault-tolerant quantum computers, we are currently in the Noisy Intermediate Scale Quantum (NISQ) era. This means that today's available QC hardware is characterized by a

	NISQ	Perfect fault-tolerant Quantum Computers
Number of physical qubits	Several hundred	Millions
Error Correction	No error correction, however a mitigation of errors	Automatic error correction
Algorithms	Hybrid algorithms which are optimized iteratively	Direct algorithms
Readout of the results	Many measurements to determine results statistically	Results can be readout binary
Length of the quantum circuits	Short (hundreds to thousands of quantum gates)	Long (billions of quantum gates)
Quantum advantage	Not yet mathematical proven	Proven mathematically for certain problems
Availability	First prototypes exist	End of decade at the earliest

Table 1: Comparison of Noisy Intermediate Scale Quantum (NISQ) computers and perfect fault-tolerant quantum computers.

limited number of qubits (~less than 1000) and no or only minor error correction. We are approaching fault-tolerance fast and there are first demonstrations of error correction in real devices [4]. These showcase only a small number of logical qubits which possess smaller but still existing errors. Thus, these advances are not yet allowing to run algorithms for fault-tolerant QCs. Some of the differences between the NISQ and fault-tolerant quantum computers are listed in Table 1. As a result, hybrid algorithms (QC and classical) need to be used to limit the processing on a quantum computer and not accumulate too many errors. On a gate-based quantum computer, this means that the length of a quantum circuit is limited.

The first NISQ quantum computers are in operation and commercially available for industrial users. While we are probably a decade away from the advent of perfect fault-tolerant quantum computers, there are few real backends that can already use error correction albeit on a small number of qubits. It is widely accepted that a quantum computer with several hundred error corrected qubits will reach quantum advantage for industrial applications.

3 Quantum Computing: State of the Art

In the domain of quantum computing, two architectures stand out: gate-based and annealing. Gate-based quantum computers manipulate qubits with the help of quantum gates. This offers flexibility in algorithm design and means that all calculations that can be done on classical systems are also possible on gate-based quantum computers, albeit not necessarily with an acceleration. Quantum annealers (QA) solve mathematical problems that can be formulated as a quadratic unconstrained binary optimization (QUBO) problem. The minimum of such a function can be found with the help of annealing using quantum mechanical effects such as tunneling. While gate-based quantum computers can solve any problem that can be solved on classical computers and therefore pose a bigger potential than quantum annealers, they are not yet as mature. I.e. for now, they can solve smaller problems with a longer time-to-solution compared to quantum annealers. In this white paper we demonstrate algorithms for both types of machines.

Current quantum computers are prone to considerable error rates and limited in size by the number of qubits in the system. This is called NISQ era. In the NISQ era, the computer architectures QA and gate-based universal computers are used. While QUBOs can be solved natively on a quantum annealer; robust, iterative algorithms based on the variation principle are used on the gate-based computers. These solve the computationally intensive part on the quantum computer and rely on classical resources to provide guidance towards the optimum. An example of such algorithm, the variational quantum Eigensolver (VQE) is particularly suitable for determining the energy states of molecules on a gate based quantum machine. It's functionality principle is outlined in Figure 2. Generally, in this document algorithms for the NISQ era are examined.

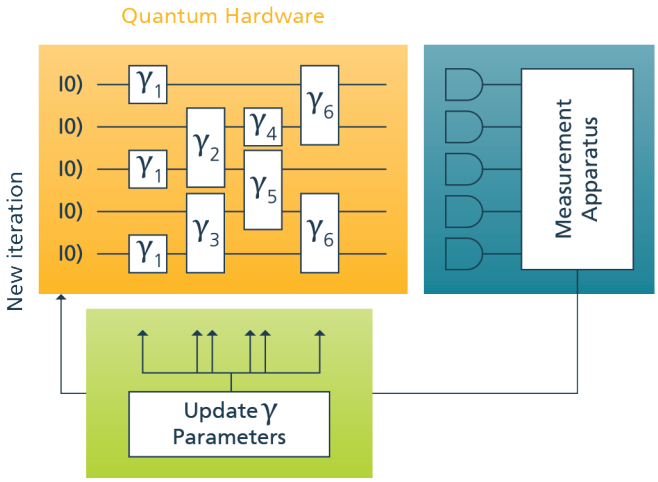

Figure 2: Principle of the VQE algorithm.

Algorithms for fault-tolerant QCs are completely different in nature. These include algorithms for search problems, quantum Fourier transforms, the solution of linear systems of equations as well as the prime factor search. Compared to the NISQ era, this opens up new accelerated applications such as computational fluid dynamics, algorithms for image processing and the breaking of RSA encryptions. A quantum advantage is expected, once hardware exist that enables larger simulations. As depicted in Figure 3, for a potential algorithm with exponential scaling, a quantum scaling advantage will be only visible for larger problem sizes.

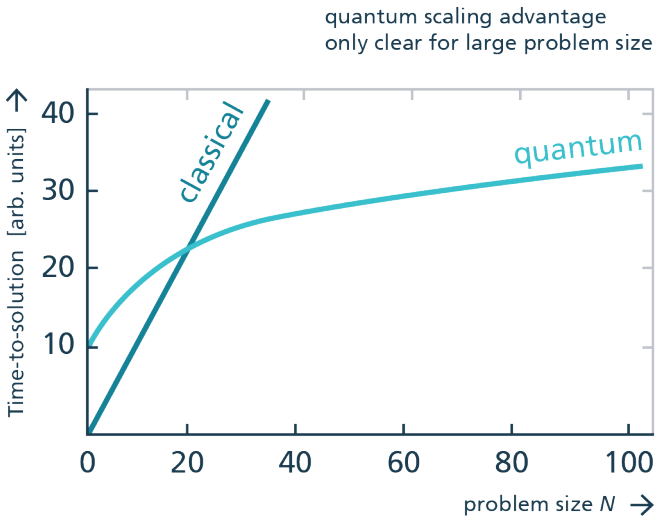

Figure 3: Example of scaling behaviours of classical and quantum algorithms and corresponding break-even points after which a quantum advantage can be reached.

In this white paper, we look at different application areas (from additive manufacturing, drug discovery, chemistry and maritime

logistics) and adapt algorithms to consider the specifics of these applications and improve their scalability even on current systems to be prepared for quantum advantage. The applications can be methodically traced back to three domains:

- **Optimization** deals with finding optimal solutions for problems in logistics, production planning, financial markets, etc.. In this white paper we present the maritime inventory routing problem, a problem for maritime logistics. Such problems can quickly get computationally intractable and classical methods often employ heuristics. The corresponding potential of quantum algorithms is that the solution of large optimization problems can be accelerated in the future.

- **Quantum Chemistry** simulates the behavior and reactions of molecules. Exact classical methods are limited to small molecules. In most cases an approximation (such as Density Functional Theory) is being used quite successfully. However, such approximations do not hold if molecules are highly correlated, i.e. when the atoms in the molecule influence each others behavior. Here the feature of entanglement makes quantum computers the ideal platform to simulate quantum mechanical systems such as molecules and can moreover be a game changer for the chemical and pharmaceutical industry, once larger quantum computers become available on the market.

- **Quantum Machine Learning** is a field that is currently quite unexplored. There is a plethora of methods already available classically. Many of them lack a reasonable explainability of the results (e.g. in the case of Deep Learning). Quantum Machine Learning builds on these approaches. In particular, it is possible to adapt computationally elaborate parts of the classical methods to the quantum world. In the scope of this white paper two methods are presented: A Quantum Support Vector Machine for drug discovery and Quantum Kernels for Convolutional Neural Networks to detect defects in additive manufacturing.

Thus, all areas in which quantum computing is currently expected to have an advantage for in the NISQ era are being investigated. Even though quantum computers are still limited in the size of the computational problems they can solve and fundamental research is still being carried out, developments are progressing rapidly. This white paper is therefore a call to get to grips with the topic today.

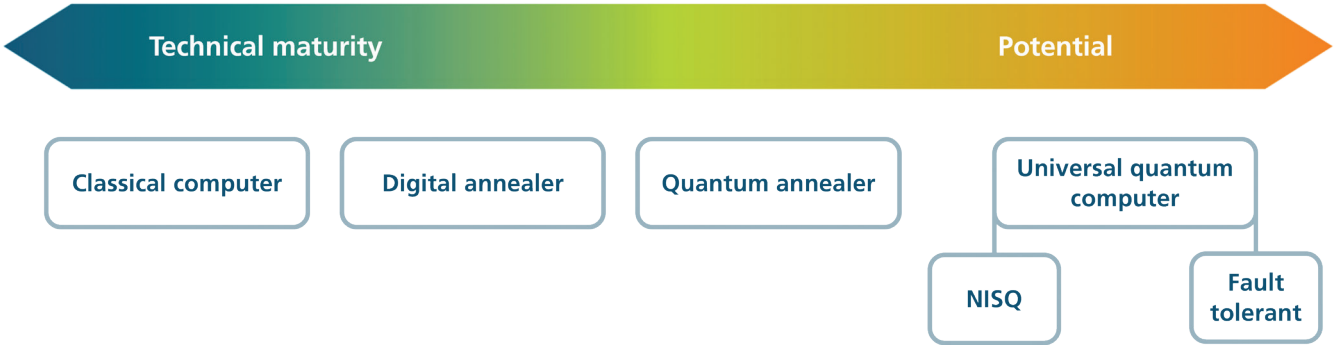

Figure 4: Overview of classical and quantum hardware.

4 Maritime Inventory Routing

4.1 Problem Definition

As shipping volumes grow with the economy, it becomes increasingly important to find better shipping routes and schedules, because even marginally more efficient operation can save large amounts of resources. In addition, further requirements on efficiency are posed by the tightening environmental regulations. Formalizing logistic operations as mathematical optimization problems and using their solution as guidance in action not only tackles the above-mentioned challenges of the required increase in efficiency but also automatizes the planning process. This opens the door for repeated short-notice planning with possible adaptations. Quite often, however, the time it takes to find optimal solutions using classical methods scales unfavorably with the problem size. One alternative is to employ so-called "heuristics" to look for good (but possibly not optimal) solutions in less time. Next to existing classical approaches, quantum algorithms have great potential in that regard and are expected to outperform their classical counterparts in the future. As an example of a maritime optimization problem, we here consider the Maritime Inventory Routing Problem (MIRP), which aims to optimize the sea trade of bulk products. It is relevant for shipping companies which are not only responsible for organizing the shipping routes and schedules of a fleet of vessels, but also for the inventory management at the storage facilities visited along the routes. This interplay between routing and inventory optimization makes it especially challenging to solve, even for small instances with only few vessels, ports and products. In the following we outline the Maritime Inventory Routing Problem (MIRP) setting but restricted to one type of product. A given amount of vessels is able to travel between a given set of ports to load and unload cargo (see Figure 5). Both the vessels and ports have limited capacities for storage. In order to simulate supply and demand, it is assumed that at some ports the product is produced (pick-up points) while at others it is consumed (drop-off points), i.e. the inventory levels either steadily rise or decline. To ensure that the ports do not run full or empty, the fleet of vessels must handle the distribution of the product accordingly. In particular, the aim/objective is to maximize the total revenue generated by the trade, under consideration of the aforementioned factors. This is done by balancing the earnings from product sales with travel and berthing costs.

A solution to the problem is specified and can vary based on the vessel routes, berth occupation, inventory levels, production and consumption rates of the product, and turnover volumes of cargo. Next to variable-defining constraints, which we do not specifically mention here, the following problem-specific constraints apply:

- Port and vessel inventories are bounded by their capacities
- Berth places are limited
- Port production and consumption rates are bounded
- Loading rates are bounded
- Vessels enter the system at a specified time-period and location

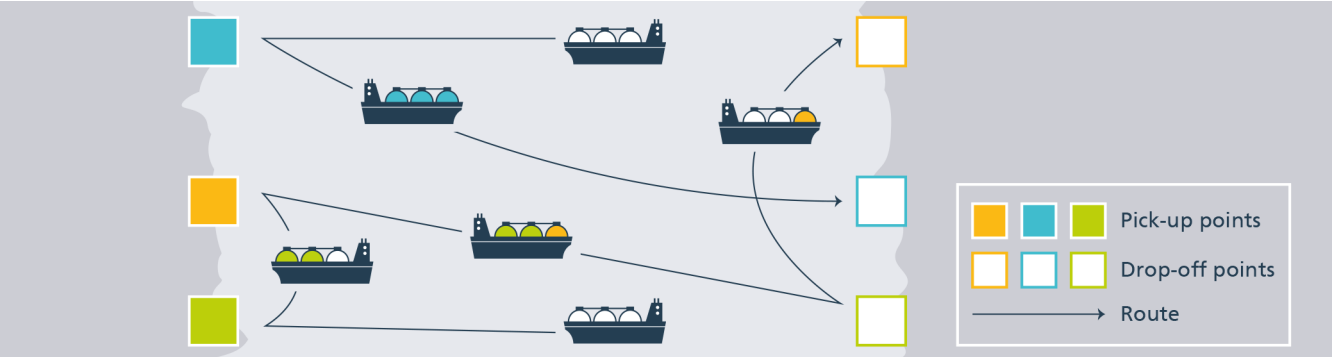

Figure 5: Sketch of the maritime inventory routing problem with different pick-up and drop-off points and several ships that can transport between these points.

4.2 Solution approach

In order to solve an optimization problem algorithmically (on classical or quantum hardware), it must first be modeled mathematically. As with many other optimization problems, it is common to model the MIRP as a Mixed Integer Linear Program (MILP)[8]. Thus, linear expressions for the objective function (the revenue, to be maximized) and the constraints must be found, all in terms of discrete and continuous variables. Larger problem instances, i.e. with more ports, vessels and/or a larger time scale (periods), typically result in larger models with more variables, which are harder to solve algorithmically. Below in Figure 6 we present some instances chosen for a benchmark comparing classical and hybrid (quantum-classical) solution methods.

	Ports	Vessels	Periods
A2	3	2	10
A3	3	2	15
A4	3	2	20
A5	3	2	25
B5	4	3	10
B6	4	3	12
B7	4	3	14
B8	4	3	16
B9	4	3	18

Figure 6: Specified parameters of MIRP benchmark instances.

For the classical side of the benchmark, we ran the model on the generic state-of-the-art MILP solver CPLEX, which can either return exact optimal solutions after a possibly long time span, or, as a heuristic, the best solution found within a given shorter time span. The underlying solution method is based on the so-called branch-and-cut algorithm, together with the simplex algorithm for continuous problems [7]. We employed both the exact solver and the time-based heuristic, for the following reasons. While the latter is more common state of the art, as it can give near optimal solutions in little computation time, we still wanted to know how close to optimality those solutions can get. Thus, we had to restrict to relatively small problem sizes which can be solved exactly in a reasonable amount of time. The other side of the benchmark, a hybrid algorithm, is a time-based heuristic as well, hence by also limiting the computation time of CPLEX, we allow for a fair benchmark.

The requirement to keep track of the inventory levels makes the MIRP difficult to embed on quantum computers, as these in their current state do not excel at representing real variables. Rather it may be favorable to split Mixed Integer Problems into discrete and continuous parts and run the prior with quantum algorithms while reverting to classical methods for the latter. This is common practice with hybrid algorithms. We used the "Leap Hybrid Solver" by D-Wave for the benchmark, which is a combination of a quantum annealer and high-performance classical resources. As a downside being one of the largest-capacity hybrid solvers currently existing, the description of the algorithm running on it is not public. Hence, we can benchmark its performance but not analyze its inner workings . As with quantum annealers, the solver is probabilistic and returns a large sample of solutions varying in quality. We compared the best one to the classical solution.

It is possible to submit the MILP model of the MIRP to the D-Wave hybrid solver and run it, but there is no guarantee to receive the optimal solution. However, the hybrid solver can actually handle more general problem types as well, while CPLEX is optimized for and somewhat restricted to linear models. To fully utilize D-Wave's capacities, the MILP model of the MIRP was modified to a Mixed Integer Quadratic Program (MIQP) by employing quadratic terms in the objective. The main benefit is that the MIQP formulation requires fewer variables than the MILP formulation because it encodes the solution more efficiently. As a comparison of the models, Figure 7 presents the numbers of variables of the instances of Figure 6 formulated linearly as MILP and quadratically as MIQP. The grey diagonal represents equal number of variables. Notice that the instances starting with 'A' and 'B' are aligned with their peers. This is because the scaling advantage of the MIQP in the number of variables roughly depends on and increases with the number of ports, which does not vary within these groups.

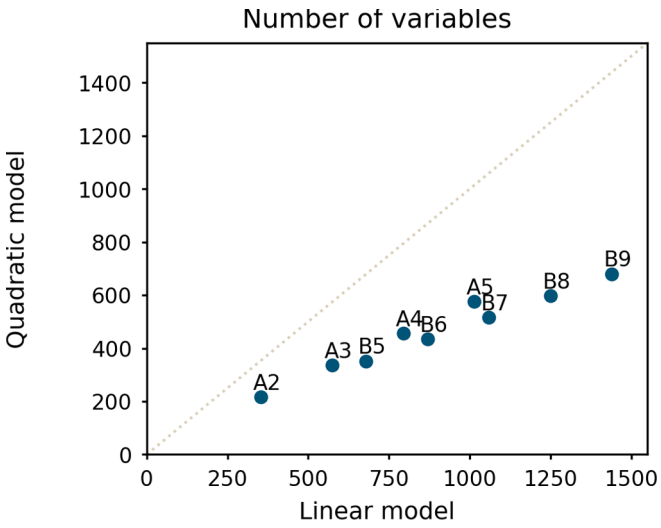

Figure 7: Number of variables in the MILP model vs. the MIQP model of the benchmark instances from Figure 6.

4.3 Results

For the benchmark, we computed solutions of the MIRP problem instances from Figure 6 in three different ways. Running CPLEX on an ordinary laptop, the problem instances were solved to optimality, yielding the optimal objective values and the corresponding computation times. Then, both on the same device (as a MILP) and the D-Wave hybrid solver (as a MIQP), we searched for the best solutions within a computation time limit of 5, 10 and 20 seconds. For smaller problem instances, CPLEX already found the optimal solution during those time spans, while for larger instances, it only found near optimal solutions. The results are visualized in Figure 8 and Figure 9 below.

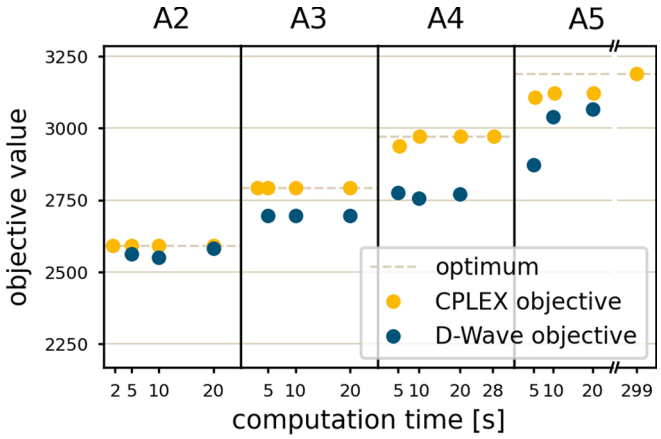

Figure 8: Benchmark results of the D-Wave hybrid solver vs. CPLEX on benchmark instances A. Higher values mean better solutions.

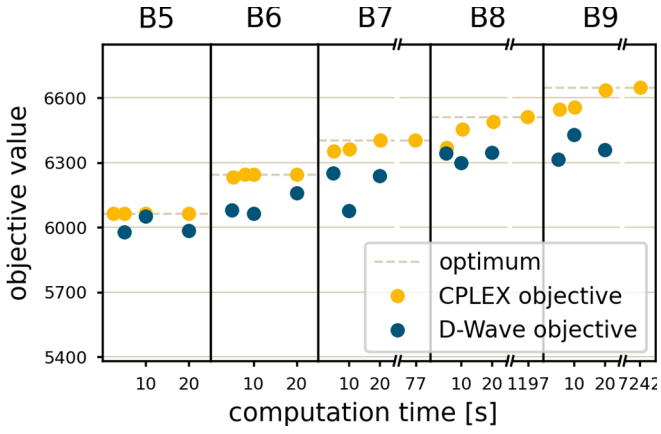

Figure 9: Benchmark results of the D-Wave hybrid solver vs. CPLEX on benchmark instances B. Higher values mean better solutions.

In those plots the achieved objective function values on the vertical axis with respect to the calculation time on the horizontal axis for both CPLEX on the linear formulations (red) and D-Wave on the quadratic formulations (blue) of the MIRP instances (see Figure 6) are displayed. The optimal objective function values are represented by the dashed lines. Thus, the closer a value is to the dashed line, the better. Remember that in context of the considered logistical problem, the objective function corresponds to the revenue generated by operational decisions encoded in a solution.

While the heuristic solutions of the classical solver did outperform the respective solutions of the hybrid solver, it is important to note that the latter does not perform badly at all as its reaching 96.5% of the optimal objective on average. At worst, the D-Wave objective reaches 90% of the optimal objective and 92% of the respective CPLEX objective for the same computation time. Hence, the outcome of the benchmark suggests that while we did not achieve a computational advantage with the tested hybrid solution method, its results are not far from the state of the art.

The current weakness of the hybrid solver lies in the regime of large instances, where the number of variables exceeds the capacity on the D-Wave quantum annealer. However, with future improvements in connectivity, error resilience and qubit count, it may be able to match or even surpass the generic linear solver in that regime.

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Fraunhofer CML used its deep understanding of maritime logistics and optimization to establish the use case and successfully solved it through its expertise in quantum computing.

5 Catalyst Research

5.1 Problem definition

The chemical industry relies on high-performance catalysts across numerous processes. These catalysts not only save energy by allowing reactions to run at lower temperatures and lower pressure but also enable a faster conversion of educts to products, as depicted in Figure 10. The use of catalysts therefore also plays an important role when it comes to sustainability. In addition, catalysts enable a wide range of innovations and secure the supply of many basic materials that are used in products in our daily lives. The development of new, improved catalysts is important for the chemical industry. Of special interest, of course, is the enhancement of catalysts which consists of rare and expensive precious metals like platinum and iridium. These are needed for applications in the new hydrogen economy.

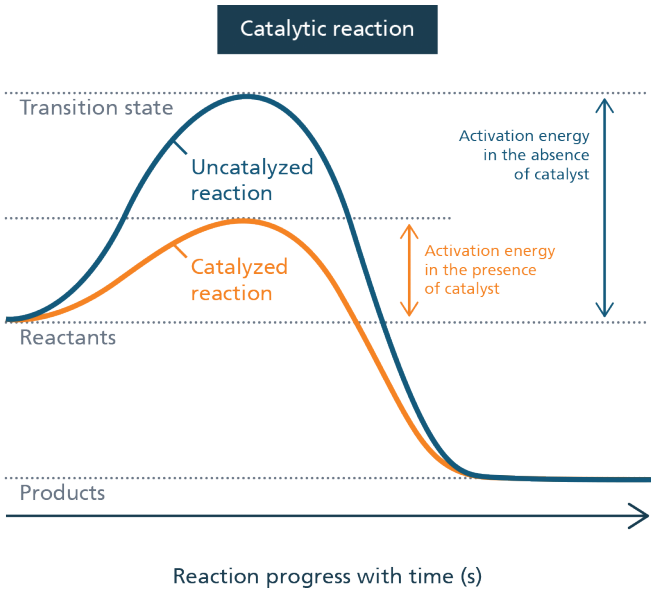

Figure 10: Energy profile of an uncatalysed (blue) and a catalysed (red) reaction. The catalysed reaction is much more energy efficient.

Until now, the task of engineering new and more active catalysts has relied on experience, knowledge and a lot of testing. This development process takes a long time, is very cost-intensive and possibly the best solution will be overlooked.

To enhance the performance of a catalyst, the adsorption and desorption energies of the involved chemical species on the surface of the catalytic material have to be optimized to reduce the so-called activation energy as much as possible.

A typical material used in catalysis is platinum. As a noble metal, it has outstanding catalytical properties but at the same time is rather expensive and considered a scarce resource or so-called critical material. It is therefore of great benefit to select the most energetically favorable particle shape for the respective reaction.

The underlying mathematical calculations are highly complex and time-consuming. This is where classical computer-based methods often reach their limits and quantum computing can potentially provide a remedy without losing the precision of the calculations or increasing the computing time immeasurably. Based on the results of the theoretical calculations, the catalysts can be specifically produced in the laboratory and tested with partners and customers. In this way, lengthy "trial and error" test series can be avoided or at least significantly shortened.

A typical approach is to synthesize a specific catalyst in the lab, characterizing it using different analytical methods and then testing it. For highly specific reactions needing multielement catalysts, this can take days until a comprehensive assessment of its performance has been executed. If the performance is lacking, the whole cycle starts anew.

5.2 Solution approach

Strongly correlated systems, such as transition metal compounds, which are used as catalysts in nature and in industry, are difficult to simulate on classical computers and it is hoped that the use of quantum computers will offer initial advantages. The variational algorithm VQE (Variational Quantum Eigensolver) is used, which outsources the computationally intensive part of the calculation to the quantum computer and approximates the result iteratively on a classical computer.

The ab initio electronic structure problem in quantum chemistry is concerned with the determination of the eigenstates of the Hamiltonian of an atom or a molecule for a given set of nuclei

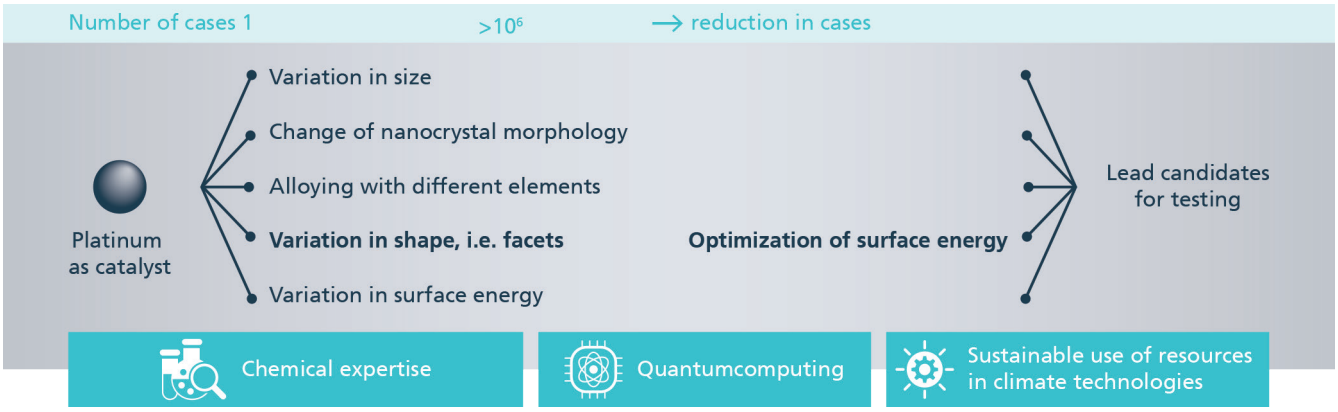

Figure 11: Schematic of combining chemical expertise and quantum computing in order to harness the mulitude of possible routes for optimization in material development.

positions. VQE starts from an Ansatz comprised of some educated guess for an initial state and a unitary circuit defined by a set of classical variational parameters.

The ground state energy is estimated by applying this circuit to the initial state, with this output the variational parameters are optimized to lower the energy of the Ansatz state, and the procedure is repeated until reaching the desired convergence. The qubit representation of the Hamiltonian and the states is the first step in a VQE simulation. Starting from the discretized electronic Hamiltonian, the quantum simulation algorithm requires the encoding of the fermionic degrees of freedom into qubits.

There are different classes of variational quantum Ansatz, mainly distinguished by the circuit complexity and the problem to be solved. Thus, e.g., the unitary variant of coupled cluster theory is an Ansatz very well suited to quantum chemistry applications. Once the expectation values of the Hamiltonian are estimated by the actual quantum hardware for a given set of parameters this information is fed into the classical optimizer.

Due to the exponential complexity of the Hilbert space of electrons, the configuration space of molecules, a quantum chemistry simulation for classical computers scales at least polynomially for approximate solutions. On quantum computers it is already possible to outperform algorithms from classical computers with a three-digit number of qubits in case that they work perfectly.

At present, only small chemical systems can be simulated exactly on classical computers. Molecules such as platinum, which - as described above - are important catalysts, cannot yet be calculated on quantum computers due to the size and errors of current quantum computers. Therefore, we have applied some techniques to reduce the quantum circuits and the number of qubits necessary to simulate large molecules

We have been limiting the active space of the molecule that will be simulated. The active space is a type of classification of molecular orbitals. Spatial orbitals are classified as belonging to three classes:

- **core**, always hold two electrons
- **active**, partially occupied orbitals
- **virtual**, always hold zero electrons

Based on the freedom left for the occupation in the active orbitals, a certain number of electrons are allowed to populate all the active orbitals in appropriate combinations. The active classification can theoretically be extended to all the molecular orbitals, to obtain a full configuration interaction treatment. In practice, this choice is limited, due to the high computational cost needed to optimize a large complete active wavefunction on medium and large molecular systems.

A clever choice of an active space will allow NISQ quantum computers to simulate large molecules such as platinum. However, the choice of a sufficiently large active space is an art. In the scope of this white paper, we show how the quantum computing resources needed to simulate the possible active space configuration scale and showcase a possible method to reduce the quantum computing resources during compilation, i.e. mapping of gates to the quantum computer.

5.3 Results

For this study we are using the crenbl basis set which is based on [17] for the geometry of the dataset, the Bravyi Kitaev Mapper which maps fermions to qubits in a resource efficient way and the Unitary Coupled-Cluster Single and Double excitations variational form (UCCSD) which is a quantum variant of the gold standard in classical quantum chemistry, CCSD. The resulting quantum circuit generated with qiskit is imported in the pyzx package [11] and optimized by converting the circuit into a ZX diagram, simplifying the diagram and then converting it back into a circuit. ZX diagrams can be seen as a generalization of quantum circuit notation. For a given active space choice several

optimization methods have been compared. First, the quantum circuit has been generated using the qiskit framework, different optimization levels in the qiskit framework have been used, then additional methods available in pyzx have been applied to the circuit. As depicted in Figure 13 the basic optimization method of pyzx delivers the best results in terms of number of single gates and multiqubit gates, i.e. gates that encompass more than one qubit. This optimization method has been used in the rest of the study as it seems to be optimal for the use case. Figure 12 shows the optimized results for the number of gates, the number of multi-gates which involve more than one qubit and the number of qubits depending on the number of active orbitals. While the number of qubits grows linearly with the number of active orbitals, the number of gates grows very quickly and reaches numbers that are not achievable with current QC devices for a low number of active orbitals. This is not yet considering topologies of real quantum devices which might increase the gate count even more.

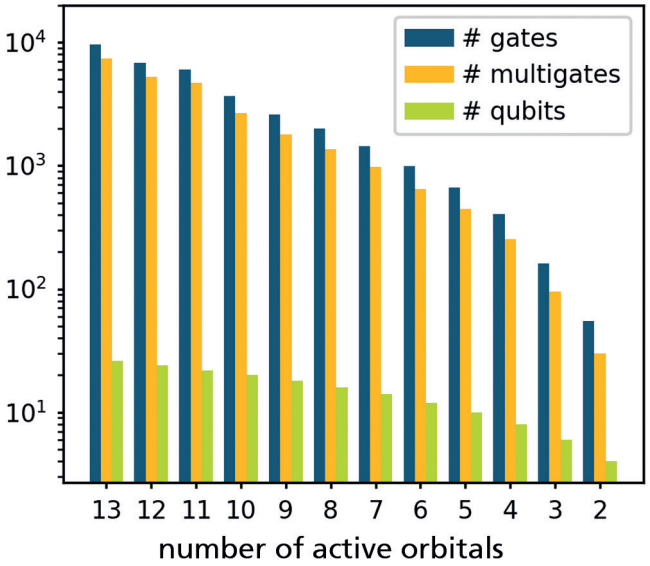

Figure 12: QC resources needed for different sizes of active spaces.

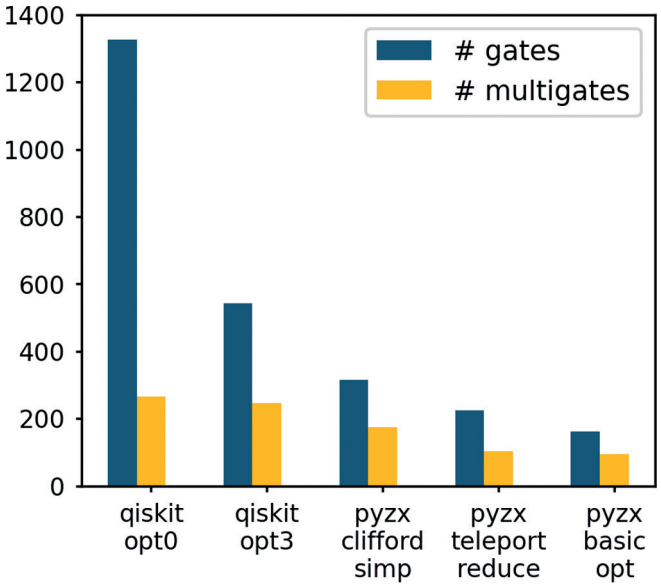

Figure 13: Quantum circuit characteristics of different optimization methods for an active space of 3 orbitals (qiskit framework and additional optimizations available in pyzx).

This study optimizes some of the parameters available in the quantum computing algorithm and gives a hint on the resources needed to simulate a platinum atom. Thus, the catalyst use case is not yet feasible on real quantum computers, however quantum chemistry on quantum computers is an active field of research where a lot of developments are expected in the coming years.

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Fraunhofer IAP provides the industrial use case. The division for applied nanotechnology CAN has profound expertise in the production and characterization of material.

Fraunhofer CML provides the quantum computing knowledge and has worked on optimizing quantum circuits for quantum chemistry problems.

6 Additive Manufacturing

6.1 Problem definition

Laser Powder Bed Fusion (LPBF) is an advanced and widely utilized additive manufacturing (AM) process, particularly valued for its ability to produce geometrically complex metal components for industries such as aerospace, automotive, medical implants and tooling. This process functions by selectively melting thin layers of metal powder using a high-energy laser (Figure 14).

Next to its high material-efficiency, a key advantage of LPBF is given by its ability to allow the fabrication of parts with complex designs that would be difficult, if not impossible, to achieve using conventional manufacturing methods. In addition, LPBF is able to produce highly customized parts directly from CAD models, eliminating the need for specialized tooling, significantly reducing lead times and enabling rapid prototyping and iterative design improvements. In the aerospace sector, for example, LPBF is particularly beneficial due to its capacity to produce lightweight, high-strength components with complex geometries. Parts with intricate internal cooling channels or weight-optimized structures contribute to enhanced fuel efficiency, reduced emissions, and overall improvements in aircraft performance. In the medical industry, LPBF is invaluable for the production of patient-specific implants, prosthetics, and surgical instruments.

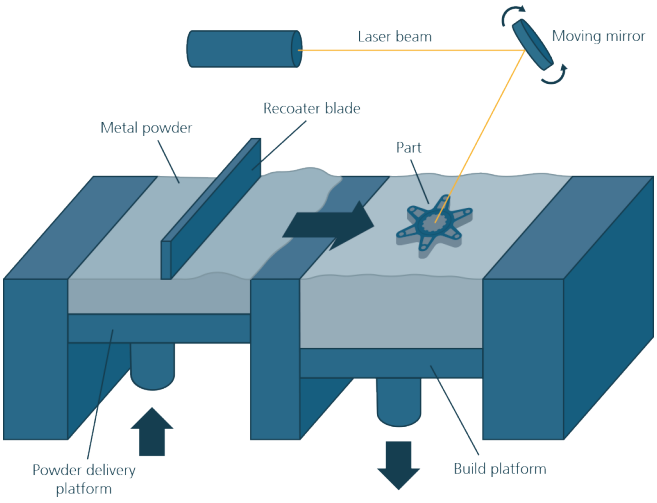

Figure 14 shows a schematic representation of the Laser Powder Bed Fusion (LPBF) process.

For instance, LPBF-implants benefit from highly customized components tailored to an individual's anatomical features and in addition mimic the natural bone architecture, which helps the bone and implant fuse together for long-term stability.

One of the major challenges in LPBF is the formation of defects in the form of too large pores within the manufactured components (Figure 15). The presence of these pores can compromise the structural integrity of the part, potentially leading to premature failure. Pores arise from mechanisms such as Lack of Fusion (insufficient energy to melt powder), Gas Porosity (trapped gas during processing), and Keyhole Pores (localized vaporization due to excessive laser power). Detecting defects before deploying parts in critical applications is essential for ensuring component reliability and safety. Various approaches are utilized for quality assurance in LPBF, where one distinguishes between destructive testing (DT) and nondestructive testing (NDT).

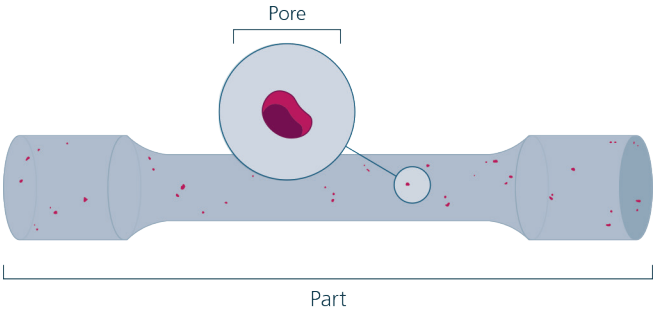

Figure 15 shows a transparent LPBF Part with visible pores in red.

Although DT-methods provide the most detailed information about internal defects, they render the tested part unusable. Witness specimens are an alternative but consume extra material and time without directly assessing final part quality. In contrast, NDT techniques, such as micro-computed tomography (micro-CT), provide highly detailed insights into the internal structure and potential defects within the part without causing damage. However, the high cost and slow speed often limit their practicality for routine quality inspections in high-volume production environments. Developing faster and more cost-effective NDT solutions is crucial for maintaining consistent part quality in industrial applications.

6.2 Solution approach

To predict pore formation during the LPBF process, we have developed an innovative methodology that uses in-situ sensor data to train a convolutional neural network (CNN). The objective of this research is to investigate the potential of gate-based quantum computing in the form of hybrid quantum-classical convolutional neural networks (QCCNN), addressing this specific use case.

An advanced sensor system was integrated to monitor the melt pool during the LPBF process, enabling real-time observation through the laser beam. This system is designed to capture emissions across three distinct wavelengths, each offering critical data related to the melt pool's characteristics. As a result, the sensor system generates a three-dimensional dataset throughout the build process, providing detailed information on the entire part. The printed components were scanned using micro-CT to acquire high-resolution three-dimensional images of their internal structures, which allowed for the precise detection of pores within the components. By identifying and quantifying these internal features, the micro-CT images provided essential ground truth information for the classification task.

The sensor data and micro-CT scans were carefully aligned and processed through a comprehensive pipeline to ensure their appropriateness for model training, utilizing processed sensor data organized within specific samples. Using the pore locations identified in the micro-CT scans, the sensor data were labeled into two distinct classes: sensor data corresponding to regions containing detectable pores and sensor data representing defect-free material. Moreover, the dataset incorporates a voxelization technique that transforms the traditional X, Y, Z coordinate system of the sensor values. This transformation is crucial for aligning the data with the input requirements of the CNN resp. QCCNN.

CNNs are a widely used type of feed-forward neural network and especially known for their exceptional performance in classification tasks on image and audio data. In a CNN, the convolutional kernel, which functions as a small filter, is systematically applied to an input image or feature map to generate the output. This results in a feature map that highlights the detected patterns within the data. In the development of the hybrid QCCNN, a CNN architecture serves as the foundation, but a classical convolutional kernel is replaced by a quantum convolutional (quanvolutional) kernel.

In this study, rather than utilizing the conventional kernel computation, we flatten the segments of the kernel and employ them as input to a quantum circuit. The output generated by this circuit is utilized as the new feature representation, allowing for enhanced information extraction and potentially improving the performance of the CNN in classification tasks (Figure 16).

Inspired by preliminary studies on QCCNNs by Matic et al. [13] the quantum circuits were constructed as follows: An initial layer of single qubit rotations (RY gates), encoding the input data, is followed by a deeper layer of random gates, which entangles the qubits. The layer of random gates includes further single-qubit rotations, and more importantly some number of two-qubit gates (CNOT gates) to employ entanglement across multiple qubits. Different implementations of the random layer, varying the number of rotational gates and CNOT gates, were tested and the quantum circuits were executed on classical hardware with the PennyLane simulator analytically calculating the expectation values. As a non-linear function the quantum circuit potentially detects hidden structures in the data and could be a useful addition to a classical CNN architecture. Furthermore, the comparatively small number of qubits required makes this approach generally interesting for the NISQ era.

The initial layer of the CNN will be replaced with the quanvolutional layer. Instead of executing multiple computations for each sample over multiple epochs using the quanvolutional layer, we have integrated the quanvolutional layer as a preprocessing step applied to the data prior to feeding it into the CNN. This approach aims to streamline the computational process by transforming the input data with quantum-enhanced features before subsequent analysis. By leveraging both quantum computing

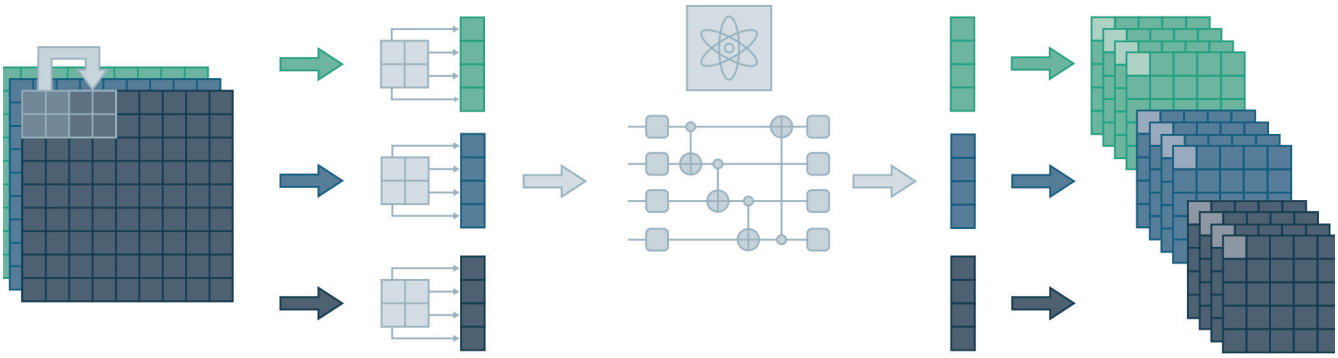

Figure 16 shows a simplified version of the quanvolution layer with a 2D input having 3 features., e.g. image with r, g, b values. The convolution used in this study builds up on a 3D input with more complex features.

capabilities and traditional CNN architectures, this method seeks to harness the strengths of both technologies to achieve superior performance in feature extraction and classification tasks.

6.3 Results

To draw a meaningful conclusion, a comparative analysis between an ordinary pure-classical CNN, a pure-classical CNN with a classical preprocessing layer (CNNP) and the hybrid (quantum-enhanced) QCCNN was conducted. Given that the preprocessing step used in the QCCNN is not typically implemented in classical CNN architectures, we designed the CNNP to match the configuration and structure of the QCCNN as closely as possible by using an initial convolutional layer with non-trainable parameters, followed by the same (classical) convolutional layers which are used in the QCCNN.

Several metrics (accuracy, precision, F1 score, loss-function and Cohen's kappa) were calculated and considered for the evaluation of the models' performances, both on the training data and on the validation data. The kappa value, due to its holistic definition and the fact that it respects the possibility of coincidental matches between ground truth values and predictions, was chosen as the key evaluation metric. The experimental results show strong performance across all models with a kappa value of more than 0.75 on the validation data already after a few epochs (Figure 17). The measured accuracies and precision were also very high, reaching 90% on the validation data and up to 95% on the training data. In all metrics, no significant differences between the performance of the QCCNN approach and the classical CNNs on the validation data were observed.

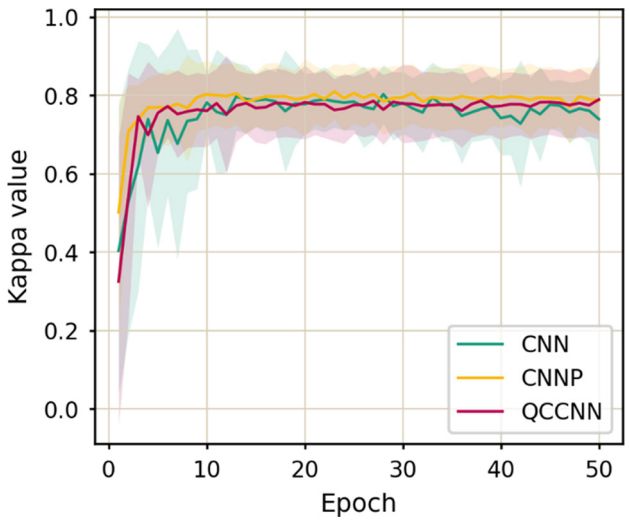

Figure 17 shows the kappa value of the different models on the validation/test data (higher kappa values meaning better model performance). The results are averaged over 20 runs, varying the training and validation splits to assess consistency across different data configurations. The standard deviations are represented by the shaded bands.

Based on the results obtained, we can draw two conclusions: Firstly, the findings indicate that our groundwork in preparing the data and establishing a robust pipeline – from the initial raw laser data to accurate pore prediction in components produced via the LPBF process utilizing CNNs – has proven to be effective. Secondly, the results show that, although no significant advantage was identified, we have successfully integrated quantum kernels into the classical CNN framework, resulting in a QCCNN that can be effectively utilized for pore detection. These findings motivate further exploration and continued research into their performance, and applicability to other complex problems. Future work could focus on incorporating a quanvolutional layer or a quantum fully connected layer as a trainable component of a QCCNN, while also investigating alternative data encoding techniques and optimizing quantum circuit hyperparameters (e.g. number of CNOT gates), through grid or Bayesian search methods. Furthermore, the potential of quantum algorithms for new hybrid deep learning architectures and the impact of utilizing real quantum hardware on the model's performance should be investigated.

Looking to the future, we are excited about the growing opportunities to solve real-world use cases with (hybrid) machine learning algorithms using quantum computing, building on our achievements to date.

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Fraunhofer IAPT is a leading institution in 3D printing technology transfer, specializing in research and development of additive manufacturing with a focus on digitization, process automation, and end-to-end solutions.

Fraunhofer CML has deployed the quantum CNNs, simulated quantum computers and analysed the results.

7 Drug Discovery

7.1 Problem definition

The cost of developing a novel pharmaceutical drug has soared from millions to billions of Euros since the 1950s. While clinical studies of efficacy and safety in human patients constitute the most protracted and expensive phase of the process, preclinical drug discovery and development typically account for 30 to 40% of the total cost. The high attrition rate at every step from hit identification and lead optimization to the selection of clinical candidates requires the screening of large numbers of molecules in the early stages of the drug development process.

Highly automated sample preparation and analysis techniques for experimental studies of molecules (in-vitro screening) have been established over the past decades. These have been complemented by approaches to computer-aided drug discovery (in-silico screening) which aim to predict molecular properties such as its efficacy on a target, transport and metabolism in the body, and toxicity and safety profile. In-silico screening enables the assessment of much larger substance libraries, which cover a more diverse chemical space, and hence the discovery of more effective, accessible and safer drugs.

However, in-silico screening is computationally expensive: Large libraries of substances must be screened and complex molecular properties modelled and predicted for each substance. Quantum computing promises a significant acceleration by exploring a large solution space in parallel.

The study presented herein aims to assess the potential of today's quantum computing platforms to solve practical problems in in-silico drug discovery. Using three representative examples, we apply quantum-based classification algorithms to predict the following molecular properties:

- Blood-brain barrier penetration ability (Martins 2012 [12], 2030 compounds),
- P-Glycoprotein inhibition efficacy (Broccatelli 2011 [5], 1218 compounds),
- Aqueous solubility (Sun 2019 [20], 2456 compounds).

We aim to illustrate the capabilities of today's quantum computers and the limitations they may impose on problem scale and result quality.

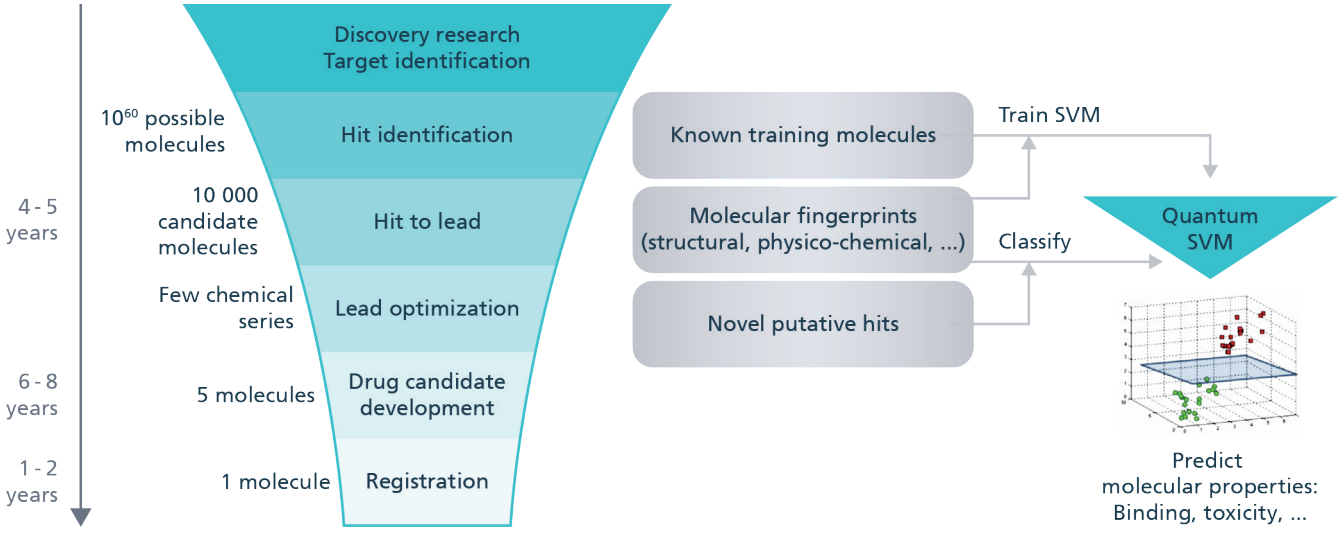

Figure 18: This case study explores the application of quantum computing-based Support Vector Machines to in silico screening, aiming to accelerate core stages of the drug discovery process.

7.2 Solution approach

Public Datasets

We selected three publicly available datasets for this study. The Polaris Hub [15] offers open access to biochemical datasets for use in machine learning benchmark studies. By using these data, we enable future performance comparisons with work from other research groups. The molecular structure of compounds in each dataset is described via SMILES strings. Morgan fingerprints [14] with 1024 bits were generated from the SMILES strings using the RDKit cheminformatics Python library (RDKit) and were used as the feature space in predicting the molecular properties. Datasets were divided into 50% training data and 50% test data in our machine learning study.

Quantum Annealing Platform

As discussed in Chapter 3, gate-based quantum computers and quantum annealers are the two fundamental architectures available. Gate-based designs offer flexibility in algorithm design, but current implementations are limited to tens to hundreds of qubits, which imposes tight limits on the tractable problem size. In contrast, quantum annealers can solve mathematical problems that can be formulated as a quadratic unconstrained binary optimization (QUBO) problem. But with up to 5000 qubits they can handle significantly larger problems. Since our focus in this study is on achieving results at a practical scale with today's quantum computers, we selected the commercially available D-Wave quantum annealer platform. The Advantage system with 5000 qubits was used via D-Wave's Leap cloud access.

Support Vector Machines

Support Vector Machines (SVMs) are a well-studied supervised machine learning model, developed in the 1990s by Cortes and Vapnik [6] . While SVMs are essentially linear classifiers, they can also perform non-linear classification by representing a set of high-dimensional data points through pairwise similarity measures, calculated using a kernel.

SVMs are well-suited for quantum computers with limited problem sizes, and particularly for implementation on quantum annealers: After training an SVM model on a manageable subset of molecules with known properties, it can be repeatedly applied to predict the properties of a large number of test molecules. Using a kernel enables non-linear classification while also significantly reducing problem dimensionality by converting high-dimensional data into scalar similarity measures. Furthermore, SVM training can be formulated as a QUBO problem, making it compatible with quantum annealers. A quantum annealer-based formulation of SVMs has been provided by Willsch et al. [21].

SVM implementations on classical computers are readily available, well-understood and provide robust and reproducible classification. They can hence serve as a benchmark for assessing quantum SVM performance in our study. Even with the relatively large capacity of the D-Wave Advantage quantum annealer, quantum SVMs cannot be trained with complete training data. A slice-based approach as outlined in Figure 19 was used. To isolate a potential performance impact of this size limitation in the comparison of quantum vs. classical SVMs, the effect of limited slice sizes on training performance was assessed for the classical SVM as well.

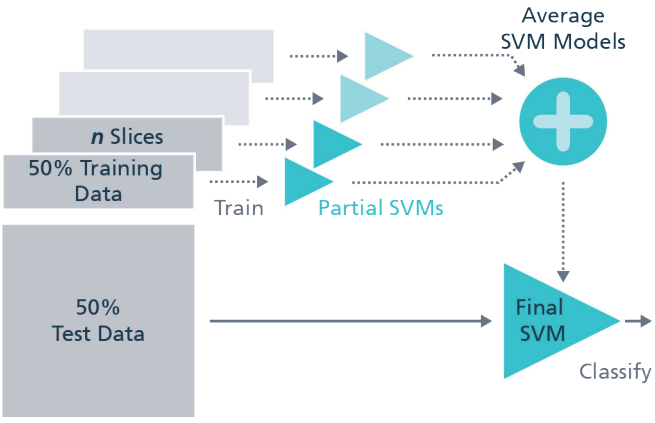

Figure 19: Data flow for the slice-wise training and test of Support Vector Machines.

7.3 Results

Size constraints and discretisation

Figure 20 shows how the classification performance of a classical SVM for our three datasets is impacted by the size of training data slices. Cohen's Kappa was used to quantify the agreement of classification results with known ground-truth properties of the test data. Classification accuracy generally deteriorates with smaller slice sizes, but the effect varies across the datasets.

Further analysis suggests that datasets where the molecular fingerprints show a pronounced bimodal distribution can be trained reliably even with small slice sizes – exemplified by Broccatelli's data for P-Glycoprotein inhibition. In contrast, Sun's solubility data, with a continuous distribution of molecular fingerprints in the parameter space, benefit from training the SVM with the largest possible slice sizes. Hence, whether quantum SVMs with their technical size limitation are suitable will be impacted by the data properties. The limited number of physical qubits further means that problem coefficients can be represented by a few bits only. Depending on the slice size, our implementation allows for only 1 to 4 bits to represent coefficients. To represent a larger dynamic range, a numeric base $B=10$ was evaluated in addition to the obvious choice of $B=2$.

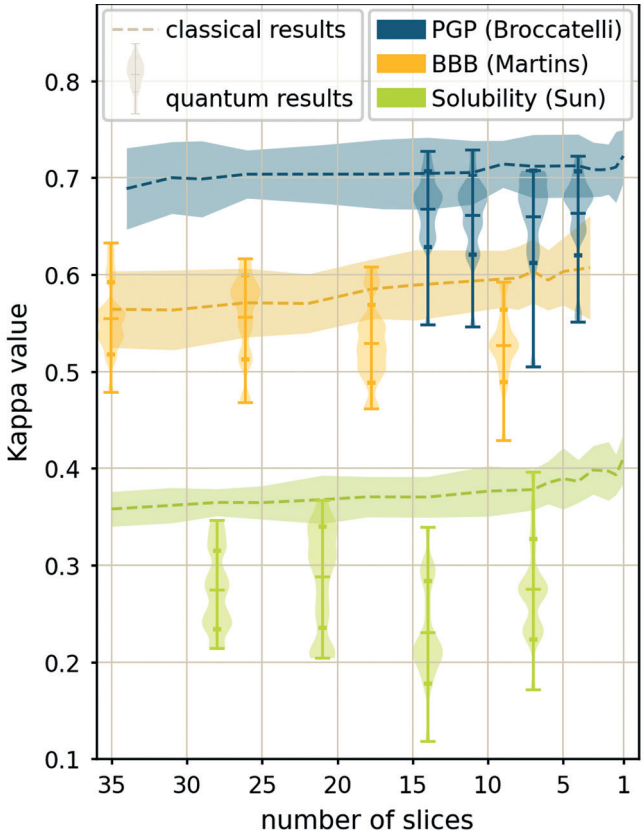

Figure 20: Classical and quantum SVM performance as a function of training slice size. These results are averaged over 18 different training and test sets. The standard deviations are represented by the shaded bands for the classical results and the small horizontal markers for the quantum results.

Choosing the optimal values for the numeric base and number of bits becomes part of the required hyperparameter optimization for the quantum SVM. Consequently, establishing optimal hyperparameters requires a search in a higher-dimensional parameter space than for the classical SVM. This introduces an additional computational overhead for the quantum approach.

We found that Bayesian search offers a computationally more efficient alternative to grid search and produces equally valid results. It was employed for both approaches with the number of iterations adapted to the respective parameter spaces.

Quantum vs. classical SVM performance

Comparison of the classification performance of quantum vs. classical SVMs (Figure 20) shows two pronounced differences: Quantum SVMs provide lower classification accuracy in general, and do not show the expected increase in classification accuracy with increasing size of the training data slices. We assume that both effects are due to the qubit and coupler noise in the quantum processing unit (QPU). The transition to larger slice size requires the use of increasingly large sections of the QPU, up to full capacity. This may drive increased sensitivity to errors, since long indirect coupling chains via intermediate qubits are required to connect all logical qubits.

This assumption is supported by results we obtained from simulated annealing, i.e. classical simulations of an error-free annealer. While computationally very expensive, these simulations provide classification results on par with classical SVMs.

Conclusions

Support Vector Machines (SVMs) lend themselves well to an implementation on limited-size quantum annealers: A QUBO formulation is possible; after training with limited datasets SVMs can efficiently classify large numbers of unknown compounds; slice-based training can enhance the training quality with limited machine size. But the size constraints and remaining error rate still limit quantum SVM performance. Further progress in quantum annealer design – increasing the number of qubits and couplers and decreasing noise – will be required to make quantum annealers an attractive platform for this approach.

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Fraunhofer ITMP has provided the use case and prepared the data. The Fraunhofer Institute for Translational Medicine and Pharmacology investigates and develops innovative ways of early detection, diagnosis and treatment of diseases resulting from impaired function of the immune system.

Fraunhofer CML provides the quantum computing knowledge and has worked on quantum support vector machines, run the resulting algorithms on D-Wave quantum annealers and analyzed the results.

8 Recommendations and Collaboration Opportunities

We are in an era where QC technology is reaching a tipping point and first algorithms show a quantum advantage. With further evolving technology, QC will quickly gain in importance for companies. However, the disruptive nature of this new technology will make it difficult to switch to it without prior knowledge. We therefore offer support in building up in-house expertise in companies for the use and application of quantum computers. At Hamburg's Fraunhofer institutes your company will find a thrilling combination of quantum computing and domain expertise, so that we can accompany your business from problem definition to solution.

In this white paper, we have outlined four industrial application examples on which the Hamburg-based Fraunhofer Institutes have worked on together to advance the field. We are looking forward to doing the same for your business use case.

In addition, the Fraunhofer Society as a whole, naturally has a broader domain knowledge. Cooperation partners from industry can benefit from the combined expertise of the Fraunhofer Institutes. We are happy to establish contacts with experts from other institutes that are relevant to the industrial partner.

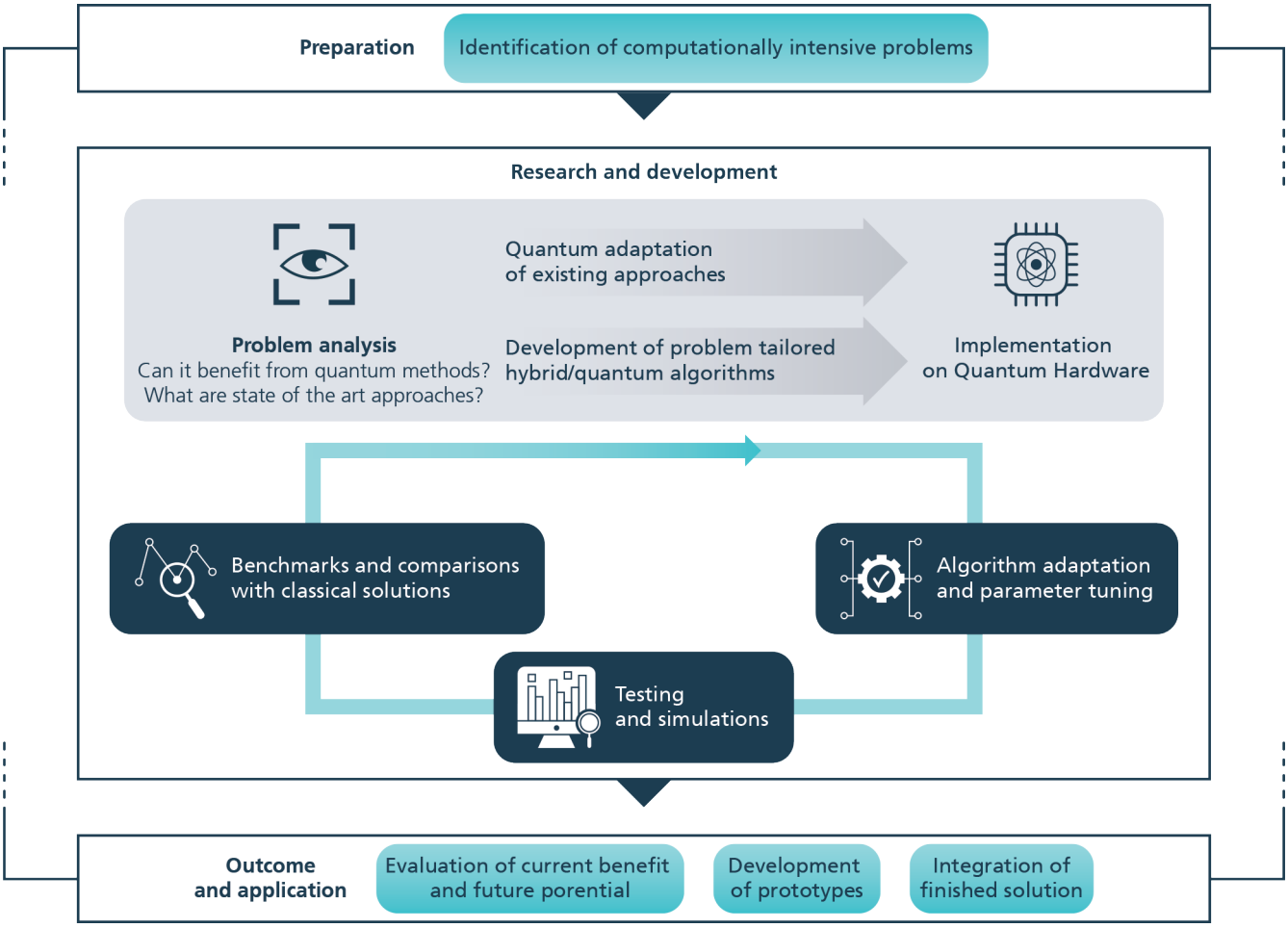

Figure 21: The typical cooperation process.

For further details, please feel free to contact us – we are happy to help.

Fraunhofer CML

Fraunhofer CML used its deep understanding of maritime logistics and optimization to define a maritime use case and successfully solved it through its expertise in quantum computing. The quantum computing realization of all other use cases was supported by specialists from Fraunhofer CML.

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Fraunhofer IAP provides the industrial use case materials and catalyst research. The division for applied nanotechnology CAN has profound expertise in the production and characterization of material.

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Fraunhofer IAPT is a leading institution in additive manufacturing technology transfer with a focus on digitalization, process automation, and end-to-end solutions to empower industrial series production and sustainable innovations across industry sectors.

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Fraunhofer ITMP

Fraunhofer ITMP works on the early detection, diagnosis and treatment of diseases resulting from impaired function of the immune system. The Discovery Research ScreeningPort facility in Hamburg supports industry and academic partners with comprehensive expertise in high-throughput drug discovery and medical data science.

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