QUASIM: Quantum computing enhanced service ecosystem for simulation in manufacturing

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Abstract

Machining is a key manufacturing technology, representing one of the most significant German economic sectors. To ensure required high-quality assurance and prevent manufacturing errors, process simulations based on digital twins can be applied. However, the current digitization and simulation models face limitations in terms of computational requirements and expert knowledge. As a consequence, important physical effects in industrial practice are either neglected or roughly approximated, resulting in compromised decision-making and economic disadvantages. Since quantum computing (QC) has shown promising benefits in solving numerous algorithmic problems and simulations, the QUASIM research project aims to use QC to improve simulations in manufacturing, reduce modeling efforts and error rates, and develop innovative solutions.

Keywords

Quantum Computing, Machine Learning, Conceptual Modeling, Quantum Computing Applications, Simulations in Manufacturing

1. Introduction

Metalworking is the largest industrial sector in the European Union [1] and holds critical importance in the manufacturing and machining landscape. To ensure the highest quality standards, simulations based on digital twins [2, 3, 4] have emerged as a key procedure, enabling the optimization of production with an emphasis on high-quality requirements and reducing high costs for errors [5]. These technology-specific simulation models mainly come from the categories of analytics (e.g., Euler-Bernoulli bending beam model), numerics (e.g., Dexel-based meshing simulation), and increasingly also from the field of machine learning (ML) (e.g., neural networks) [6]. In particular, the models from the numerics (e.g., Finite-Element Method) and ML categories (e.g., Neural Networks) regularly take even powerful digital infrastructures to their limits, as they are still based on conventional computers [7, 8, 9]. The resulting lengthy calculation times, erroneous calculation results, or unsolvable simulation issues hamper to transfer Industry 4.0 framework models to practical industrial applications. In addition, the

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required expert knowledge to apply is often lacking in the industry. These shortcomings require new approaches for performing efficient and reliable simulations in manufacturing.

Early investigations show that quantum mechanical functional principles have decisive advantages in solving numerous algorithmic problems, resulting in significant accelerations in numerical procedures, primarily through "Quantum Machine Learning" based approaches [10, 11]. Within the research project "Quantum Computing Enhanced Service Ecosystem for Simulation in Manufacturing (QUASIM)," we investigate how Quantum Computing (QC) combined with Machine Learning (ML) and QC combined with numerics can accelerate simulations in manufacturing. The project addresses critical simulation challenges in manufacturing, offering seamless integration into Industry 4.0 frameworks as "Quantum-as-a-Service (QaaS)." QUASIM brings together a diverse composition of project partners (cf. 1) that ensures the availability of necessary expertise to: a) correctly understand problem statements through industry experts, b) perform requirements engineering process, c) research and evaluate different QC and ML-based approaches, and d) provide efficient solutions to industrial end users in the form of a service. QUASIM seeks to accelerate simulations using QC, creating competitive advantages such as enhanced manufacturing quality, economic benefits, acceleration of the manufacturing process, and potential for new products and services.

Next, we will present descriptive project information, describe the project in more detail (section 2) and provide an overview of the current state of the project (section 3). We conclude the paper by elaborating on limitations, challenges and future work in the project.

1.1. Descriptive project information and partners

Table 1 provides descriptive information about the project QUASIM. The partners of the consortium project consist of leading institutions with expertise in AI, QC, manufacturing, and simulation. The consortium is composed of users from manufacturing (TRUMPF and IPT), research institutions (DFKI, FZJ, and IPT), as well as system providers (MW).

2. Project description

2.1. Project objectives

The objective of QUASIM is to develop and advance QC-driven approaches that can address critical simulation challenges in manufacturing. QUASIM aims to systematically integrate these QC methodologies into Industry 4.0 frameworks as QaaS solutions, facilitating a seamless transition from problem statements to simplified representations of actual manufacturing systems. Using different QC algorithms and methodologies, QUASIM will explore the acceleration and optimization of manufacturing processes through QC-based simulations. The project's aim includes reducing the economic disadvantages by improving the manufacturing quality and reducing complexities in the simulation. Collaboration with project partners allows the utilization of expert knowledge in exploring hardware capabilities and their limits, ensuring practical quantum adaptation for real-world industrial applications. The project strives to facilitate knowledge transfer for production-oriented simulation based on QC. Results and basic application possibilities of QC are communicated to mechanical engineering companies via the

Table 1
Descriptive information about the project QUASIM.

Description	Details
Name	QUASIM: Quantum computing enhanced service ecosystem for simulation in manufacturing.
Duration	01/01/2022 – 12/31/2024
Participants and partners	German Research Center for Artificial Intelligence GmbH (DFKI) (Saarbrücken), Jülich Research Center (FZJ) (Jülich), Fraunhofer Institute for Production Technology (IPT) (Aachen), ModuleWorks GmbH (MW) (Aachen), TRUMPF Machine Tools GmbH + Co. KG (Ditzingen)
Associated partners	Ford-Werke GmbH (Cologne), MTU Aero Engines (Munich)
Funding	QUASIM is funded by the German Federal Ministry of Economics and Climate Protection (BMWK) within the funding program "Quantum Computing - Applications for Industry", managed by the project management agency German Aerospace Center (DLR)
Project volume	approx. 5.2 million €
Website	https://www.quasim-project.de/

industry networks of the partners within workshops, symposia and fairs. Overall, QUASIM aims to transform manufacturing and machining operations and build the foundation for QC's broader adaptation in the industrial landscape. The project team focuses on two use cases. Within the first use case, whose results are described exemplarily for the project, the target is to improve simulations in the context of laser-cutting. During the cutting process, the heat influence of the laser can lead to unwanted expansion of the material, resulting in an unsuccessful cutting process and machine downtime. We aim to provide QC-based approaches (QC + ML) to improve current simulations and better capture potential thermal expansion in advance of the cutting process. The second use case deals with the development of QC + numerics methods to capture vibrations in the simulation of blade integrated disks (blisks) milling.

Figure 1 represents the target image for the QUASIM project capturing the key components of the system: the Hardware Layer supporting the QC and ML infrastructure, the Platform Layer having platforms to facilitate the AI and QC algorithms, the Algorithmic Layer with classical and quantum-based approaches along with its evaluation, the Data Layer handling simulation input and output data assets, the Service Layer representing the service on the user end where the solutions will be integrated as QaaS, and the Organizational Layer consisting of the stakeholders. Users interact with the system through the Service Layer to request simulations (thermal expansions), which utilize simulation input data (geometry, material properties, etc.) and run QC and classical ML algorithms in the Algorithmic Layer. The results are then handed to the Data Layer and made available to users through the Service Layer.

2.2. Work packages

Table 2 presents the division of the project into different work packages (WP), including the leading institutions of the WP. Each WP is conducted with at least three to four of the project partners. WP1 and WP9 are complementary WPs, ensuring appropriate project management

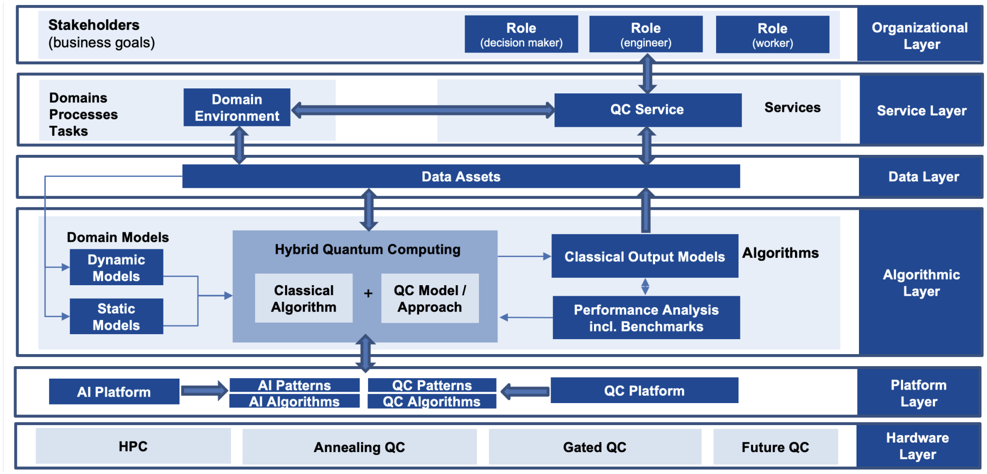

Figure 1: Representation of QUASIM target image.

and dissemination of results, e.g., through developing demonstrators, and priming of future users of QC in manufacturing and scientific publishing. In WP2 the needs of the future users are analyzed and requirements for QC-supported services for industrial production are specified. WP2 aims to create conceptual models to create abstract representations of the system. It starts in parallel with the technical modeling (WP3) and the development of the QC+ML and QC+numerical approaches (WP4 and WP5). Semantic and structural data modeling using ontologies [12] to describe the content and structure of the input and result variables of the submodels is achieved in WP3. WP6 comprises the technical development and provision of the relevant service use cases derived in WP2 concerning the thematized data and software assets on a GAIA-X-compliant hyper-scaler [13] in a prototypical form. The proof of concepts of QC+numerics and QC+ML approaches developed in WP4 and 5 are incorporated here. The developed services will be evaluated internally and externally, including benchmarking experiments in WP7. In WP8, economic and financial analyses of the use cases are performed, including business model development and specifying perspectives for QC use in other domains.

Table 2
Individual work packages with their respective lead among project partners.

Work packages	Description	Lead
WP1	Project management	DFKI
WP2	Requirements analysis and conceptual modeling	DFKI
WP3	Technical modeling	FZJ
WP4	Development of QC+numerics approach	IPT
WP5	Development of QC+ML approach	FZJ
WP6	Services: Conception and reference implementation	DFKI
WP7	Evaluation and benchmarking	MW
WP8	Profitability analysis	IPT
WP9	Knowledge transfer and communication	MW

2.3. Conceptual modeling

Conceptual models attempt to capture requirements to create a shared understanding among various individuals during the design of a project within the boundaries of the application domain or an organization [14]. For information systems based on programming and machine learning approaches, conceptual models are used as requirements for implementations [15]. In QUASIM, we use conceptual modeling in several contexts. First, we use it in requirements engineering in order to capture the as-is situation in our use cases and to conceptualize the envisioned service system. In addition, we make use of ontologies for representing the data, e.g., in the laser-cutting use case. Therefore, we built on existing ontologies to develop a focused ontology in our project. Furthermore, we incorporate technical modeling for data generation.

3. Current state of the project

In this section, we will explore and describe various aspects of the laser-cutting use case. We will discuss requirements engineering and conceptual modeling, as well as the process of generating synthetic data and data representation. Additionally, we will investigate and evaluate different concepts and approaches used for predicting heat flow and thermal expansion. Lastly, we will provide an overview of the current prototype of QUASIM.

3.1. Requirements and service design

The project team followed a thorough requirements engineering process with four steps: (1) Analysis of manufacturing and simulation processes, (2) identification and prioritization of problem spaces, (3) formulation of potential solutions, and (4) derivation of requirements [16]. In the context of (1), we first represented the current service in the as-is situation (see Figure 2) and extended the service design based on the gathered requirements. This conceptual model helps visualize user interactions and corresponding backend actions. It illustrates various user input options like geometry, material properties, and simulation model choices, as well as outputs such as visualization of predicted simulation, and evaluation of model performance. The conceptual model played a crucial role in QUASIM by providing a clear representation of the system, enabling effective communication and informed decision-making, guiding design and development, identifying challenges, and facilitating seamless integration of QC technologies for enhanced simulation capabilities in the manufacturing process.

3.2. Data generation

TRUMPF is currently working on generating real laser-cutting process samples by placing thermal cameras on their machines to gather heat flow information during the laser-cutting process. However, to make preliminary studies, we generate synthetic simulations of heat flow during a laser-cutting process using Finite Element Method (FEM) [8, 17] to solve Partial Differential Equations (PDE), particularly the heat equation in the 3-D case:

$$\frac{\delta u}{\delta t} = a\left(\frac{\delta^2 u}{\delta x} + \frac{\delta^2 u}{\delta y} + \frac{\delta^2 u}{\delta z}\right)$$

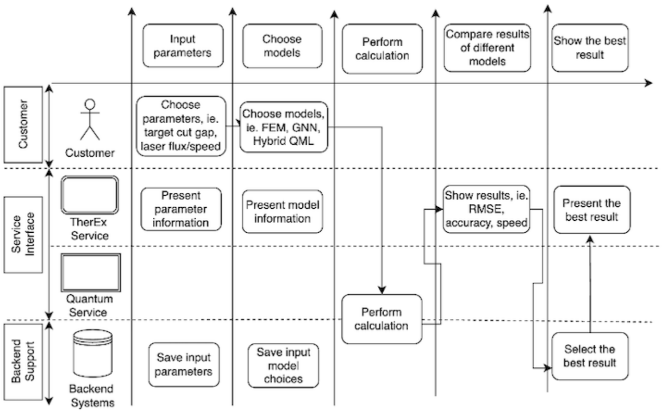

Figure 2: Service design for the laser-cutting use case. Here, TherEx refers to an application used by TRUMPF where simulation solutions will be provided as a service.

Here, $u(x, y, z, t)$ describes the temperature at point (x, y, z) at time t in a material with thermal conductivity of a. The goal is to recover the values of the function $u(x, y, z, t)$ which satisfy the conditions of the above PDE. First, we start by modeling the metal sheet geometry in 2-D as a 10cm ×10cm square as seen in Figure 3 (a). Now, we set parameters that are varied throughout the dataset to determine the exact cut geometry i.e. the width of the cutting gap in m (w_{cut}), the height of the cut in m (h_{cut}), the number of steps into which the cut is discretized (n_{cut}). Next, a third dimension is added by turning all 2-D faces into 3-D cuboids with Z-dimension parameterized by depth d. Once this 3-D geometry (see Figure 3 (b)) has been obtained, the Matlab meshing algorithm creates a mesh from it (see Figure 3 (c)). Let the mesh have N nodes which are connected by the adjacency matrix $A \in \mathbb{R}^{N\times N}$ and have D features; $X \in \mathbb{R}^{N\times D}$. The goal is to train a model which predicts the nodal temperature at a timestep $t + 1$: $T(t + 1) \in \mathbb{R}^N$ given input features such as coordinates and temperature at time t. Figure 3 (d) shows the simulated temperature on the mesh during laser-cutting, using predictions of a hybrid QML GNN (cf. section 3.4).

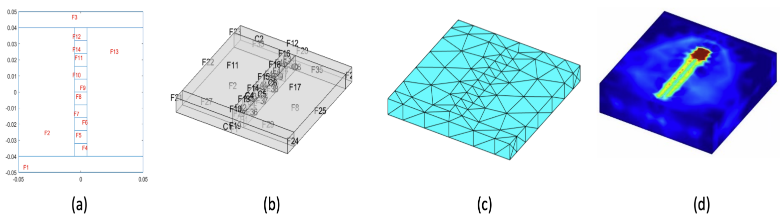

Figure 3: From geometry to simulation on a mesh. Steps involved in simulating laser-cutting.

For preliminary analysis, we created a large dataset '$LASER - LARGE$' [18], containing 36 geometries with varying cut widths, heights, and sheet diameters. There are 20 timestamps each per simulation yielding a total of 720 graphs with 800 nodes and 2600 edges on average. In addition, we created a smaller version of this dataset, referred to as '$LASER - SMALL$' [18], to allow reasonable training times for quantum-based models. $LASER - SMALL$ contains 4 geometries with 15 timesteps each, having on average 900 nodes connected by about 3000 edges.

3.3. Ontology for data representation

A sub-goal in QUASIM was to develop an approach to represent the data used in the project. We aimed for a semantic description in the sense of an ontology to capture explicit and implicit knowledge, analyze and share the domain knowledge, and enable a clear data representation. We analyzed a multitude of existing ontologies in manufacturing, production, and industry domains, representing a mid-level or domain ontology. Due to its fitting with the domain, generalizability, and rich ontology environment, we chose SAREF [1] as a basic ontology to be extended for QUASIM. We extended SAREF by the classes of "Data Dimension," "Programmatical Representation," "Pictures," "Simulation Backend," "Classical Backend," "io" - standing for Input and Output, as well as "Graph," "Edge," "Adjacency Matrix," "Geometries," "Laser" and "Metal". An overview of the extended ontology for QUASIM can be found in our GitHub [2].

3.4. Technical approaches and preliminary results

Inspired by MeshGraphNets [19], we use Graph Neural Networks (GNN) [20] as our base model architecture [18] given its ability to utilize the local neighborhood of a node to predict the next temperature making it well-suited for modeling heat diffusion spatially for diverse geometries. We use Multi-Layer Perceptrons (MLPs) [21, 22] to embed node features into a latent space and decode final output predictions. For the message passing block, we evaluate three different aggregation functions: a) GraphConvolutionalNetwork (GCN) [23], b) GraphConv [24], and c) Graph Attention Networks (GAT) [25]. To explore quantum advantages [10, 11] for efficient simulations generation, we develop a hybrid QML approach [18] by utilizing quantum embeddings instead of embeddings generated by MLP encoders in a GNN. First. feature vectors are represented in the Hilbert space H [26, 27] as angles on the R_Y rotations in 4 qubits embedding circuit. Next follows the variational circuit consisting of a parameterized R_X rotation followed by CNOT entanglement with the direct neighbors [28, 29, 30]. The processed quantum state is then measured with Z-measurement [31] on each qubit. In the end, one obtains a QML embedded latent node vector $x' \in \mathbb{R}^4$ which is now ready for further processing by the GNN. The QML model's high generalization capability along with low feature dimensionality per node requirement may produce a competent model with minimal parameters. Additionally, we explore Physics-Informed Neural Networks, particularly Thermodynamics-Informed GNN (TIGNN) [32] for enhanced heat flow simulations. In TIGNN, an additional loss is added alongside mean-squared error (MSE) loss to encourage learning based on thermodynamics principles. Furthermore, it will also be highly beneficial to research whether and how considerably QC-enhanced TIGNNs can outperform classical methods in the laser-cutting use case [33].

As first results, we show the comparison of the different encoding methods: Quantum-based encoding (f_{QML}) with $O(D)$ parameters and MLP-based encoding f_{ML-D} with $O(D^2)$ parameters and f_{ML-2^D} with $O(2^D)$ parameters for both datasets is shown in Table 3. We observe that the models with quantum embeddings (f_{QML}) exhibit the best performance with an MSE of

[1] https://saref.etsi.org/core/v3.1.1/
[2] https://github.com/InformationServiceSystems/quasim-project

0.21 on LAGER-SMALL. By using a QML-based approach instead of classical MLP, we achieve significantly lower errors with exponentially fewer parameters than competing models. This empirical evidence demonstrates the power of QML models, benefiting real-world applications.

Table 3
[Lower is better] MSE after 20 training epochs on $LASER-SMALL$ and $LASER-LARGE$ datasets [18]

	LASER-SMALL			LASER-LARGE
	$f_{\text{ML}-D}$	$f_{\text{ML}-2^D}$	f_{QML}	$f_{\text{ML}-2^D}$
GCN [23]	0.54	**0.50**	**0.50**	0.07
GraphConv [24]	0.56	0.55	**0.39**	0.07
GAT [25]	0.34	0.29	**0.21**	0.11

3.5. Protoype for QC-supported simulations in laser-cutting

We present a UI demonstrator that showcases heat flow simulations generated by our models during laser-cutting operations. The prototype allows users to select input parameters such as material properties and laser flux, and to visualize and compare predicted heat flow simulations among different models. A demo video of the QUASIM prototype can be found in the GitHub.[3]

4. Conclusion and future work

We presented QUASIM, a research project leveraging QC to address critical simulation challenges in manufacturing processes, offering QaaS solutions for integration into Industry 4.0 frameworks. By combining QC with ML, QUASIM seeks to significantly improve simulation accuracy and reduce computation times, leading to economic benefits, and faster manufacturing processes. The current work on laser-cutting simulations using hybrid QML models shows promising results. With QUASIM, manufacturing companies are introduced to how QC can be practically used to identify and implement competitive advantages, contributing to the future success of mechanical engineering. As the next steps, we plan to investigate fully quantum GNNs for faster and more efficient thermal simulations, as well as implementing and evaluating the TIGNN approach. Despite the challenges of QC's current state (hardware limitations, scalability, noisy estimations) [34, 35, 36], we are confident that QUASIM through its excellent consortium support and meticulous investigation will provide innovative solutions enhancing manufacturing quality. To overcome the challenges, we investigate how the developed solutions can be used with today's noisy hardware as well as with perfect simulators, representing the next quantum hardware generation.

Acknowledgement

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[3]https://github.com/InformationServiceSystems/quasim-project

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