Guest editorial

Selected extended papers from the Quantum Software Architecture Workshop at IEEE International Conference on Software Architecture 2021 (ICSA 2021)

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At a fast pace, applications of quantum algorithms are being built by industrial and academic users to gain experiences with this quickly evolving technology. The more these endeavours are shifting from an experimental stage towards solving real practical problems, it becomes clear that a systematic approach is needed to develop the corresponding quantum applications. This need is based on the fact that software that involves quantum computers is very different from classical software. Such a systematic approach for building quantum software must especially consider the early phases of the corresponding development process addressing the architecture of quantum software.

Guidelines for successful quantum software architecture are missing and research in this domain has just begun. Questions to be answered include, for example, which architectural style should be followed, or whether there are already established best practices? Real-world quantum software is most often hybrid—that is, a quantum application consists of quantum circuits as well as classical programs. This implies that building a quantum application means having to solve a corresponding integration problem. For decades, such integration problems are addressed by workflow technology, implying a first architectural style for building hybrid quantum software. A quantum circuit that processes data expects this data as quantum states. Such states can be prepared by using any of a multitude of approaches each having pros and cons. The knowledge about these solutions can be presented as patterns, indicating the relevance of architectural pattern languages for hybrid quantum applications.

Running individual circuits is appropriate for initial experiments with quantum algorithms. But when quantum software is used in production, issues such as scalability, availability, or security, for example, appear. Furthermore, it should not be assumed that all quantum software is developed from scratch. Instead, existing applications should be reused as much as possible to accelerate benefitting from potential speedups or enhanced precision of quantum algorithms. For this purpose, methods for re-factoring existing applications, for example, are needed.

The articles in this special issue are partly based on contributions of the *1st Workshop on Quantum Software Architecture*. The goal of this workshop was to bring together researchers and practitioners from different areas of quantum computing and (classical) software architecture to help shaping a quantum software community and to discuss problems and solutions for hybrid quantum software like the ones mentioned above.

The workshop also proposed solutions to several questions of a lifecycle for developing hybrid quantum software on how to test implemented quantum software, how to migrate from proof of concepts to productive systems, how to automate the deployment of hybrid quantum software, and how to specify KPIs for measuring the quality of solutions. Two keynotes delivered by industry leaders completed the program and kicked off further discussions.

CONTRIBUTIONS

Four papers have been selected for this special issue. Three of them are extended versions of the workshop submissions adding further insights into the original publication.

‘Encoding Patterns For Quantum Algorithms’ by Manuela Weigold and Marie Salm. Extensions of a quantum computing pattern language under construction are suggested by the first paper. Additional data encoding patterns for quantum algorithms are described. This supports an understanding of the (potentially severe) consequences of state preparation circuits on the overall algorithm that may diminish a potential quantum speedup.

‘Analysis of a Hybrid Quantum Network for classification tasks’ by Gerhard Hellstern. A hybrid quantum-classical neural network for the classification of finance and MNIST data is presented in the second article. Compared to a pure classical neural network, the author reports performance advantages but observes, at the same time, overfitting in the hybrid quantum-classical neural net.

‘QuaSiMo: A Composable Library to Program Hybrid Workflows for Quantum Simulation’ by Thien Nguyen et al. A composable programming scheme for hybrid quantum-classical algorithms as well as hybrid workflows for quantum simulations are proposed in the next contribution. For this purpose, an expressive set of data structures is constructed accompanied by new methods enabling the development of complex hybrid applications.

'QProv: A Provenance System for Quantum Computing' by Benjamin Weder et al. The final paper focusses on provenance: it identifies information that is relevant when building a hybrid quantum application on concrete devices. A provenance system for quantum computing is sketched that automatically collects the identified information and prepares it in a uniform manner in a special provenance database.

CONFLICT OF INTEREST

There is no conflict of interest.

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Johanna Barzen leads the Quantum Computing and Digital Humanities research area at the Institute of Architecture of Application Systems (IAAS). Her research lies in the intersection of computer science, media science, digital humanities, and quantum computing. Thereby, she applies pattern languages, data analytics, and machine learning. Since 2012, she has been working on digital humanities projects and developed the MUSE method along with a supporting tool chain to identify costume pattern languages in films. Her interdisciplinary approach of combining research on digital humanities with the potentials of quantum computing coined the term Quantum Humanities. Ongoing research on (quantum) machine learning is currently determining the potentials of quantum approaches in contrast to classical approaches. Currently, she is also a visiting scientist at the Business Informatics Group of the TU-Wien bridging the research area's model-driven development and digital humanities.

Sebastian Feld is an assistant professor at Delft University of Technology, The Netherlands. He is a part of Quantum & Computer Engineering department, where he and his group are working on Quantum Machine Learning. The overall goal is to investigate how quantum technology might help creating near-term quantum applications and also how machine learning techniques may assist in developing scalable quantum devices. Before, he was the head of Quantum Applications and Research Laboratory (QAR-Lab) at LMU Munich. His main focus as a post-doctoral researcher was on optimisation problems and the application of quantum-assisted artificial intelligence. He earned his doctorate from LMU Munich working on planning of alternative routes, time series analysis and geospatial trajectories.

Frank Leymann is a full professor of computer science and the founder of the Institute of Architecture of Application Systems (IAAS) at the University of Stuttgart, Germany. His research interests include architecture of large systems, middleware, pattern languages, and quantum computing. The projects he is working on are funded by the European Union, the German Government, or directly by industry partners. Frank is the co-author of about 500 peer-reviewed papers, more than 70 granted patents, and several industry standards. Before moving to university, he served as a Distinguished Engineer at IBM.

Karoline Wild received the Master of Science degree in Information Systems from the University of Stuttgart and the University of Hohenheim in 2016. Currently, she works as a research associate at the Institute of Architecture of Application Systems (IAAS) at the University of Stuttgart, Germany. Her research interests are in the area of multi-cloud deployment and management, focussing on the distribution of application fragments and their cross-cloud communication behaviour.