Software and Quantum Computing

Executive summary

This position paper is an analysis by NESSI[1] of issues concerning software technology in quantum computing.

Advances in the development of quantum computing hardware need to be accompanied by advances on the software side to make quantum computing a reality. While the technological progress on the hardware side has been exponential in the past, progress on the software side has been slower. This experience, and the fact that quantum computing requires radically new thinking about developing algorithms and programming them, suggest that software will hamper the uptake of quantum computing. Therefore NESSI is proposing to put more emphasis on quantum software research, including the following.

- Extend the European Quantum Research Agenda with items focusing on software.
- Increase education and training to develop expertise and skills required for European leadership in quantum technology.
- Foster interdisciplinary research into developing quantum algorithms.
- Investigate hybrid systems combining classical computing with quantum computing.
- Create a new software engineering branch covering the methodology and technologies required for managing the full lifecycle of quantum software.
- Support building industry-led initiatives and ecosystems addressing the opportunities offered by quantum software.

What is quantum computing about?

Quantum computers operate on qubits which can represent a combination of both zero and one at the same time by exploiting the quantum phenomenon of superposition. Combining qubits into a larger system enables quantum computers to perform multiple calculations with multiple inputs simultaneously. In addition to superposition and quantum parallelism, there are other quantum effects such as entanglement and hidden information of quantum states which can be used during calculations. Moreover, distributed quantum computing benefits from significant lower communication overhead compared to classical computers. All these effects contribute to an enormous - in some cases exponential - speed-up in executing certain algorithms for solving specific problems. For example, multivariable problems could be solved in a significantly more efficient way in quantum computers than in classical computers, in applications such as complex optimization, weather forecasting, large system simulations, and quantum machine learning.

Today's commercially available quantum computing services, offered for example by Amazon, Google, IBM, and Microsoft, still have limitations on the number of qubits and on the types of problem they can solve. Nevertheless, users of these services gain early experience about which problems could best be solved by quantum computers and how the algorithms need to be designed for solving these problems. However, to process business-relevant algorithms, today's quantum computers must scale up by a factor of 10,000.[2] To achieve this, significant physical challenges still need to be addressed in the design of quantum computing

[1] NESSI (Networked European Software and Services Initiative), the European association promoting research, development and innovation in the field of software, data and digital services; http://www.nessi.eu/
[2] https://blog.softwareag.com/quantum-computing

circuits, in controlling the interaction of qubits, and in correcting errors caused by the environmental interference the qubits are exposed to. Different technologies and architectures are being explored to overcome these obstacles and to increase the number of qubits that can be integrated into a single computer. These technologies include superconducting systems, trapped ions, gate-based methods, and quantum annealing. Significant R&D&I funding[3,4] is being invested in such technologies, and we can expect major advances over the next ten years.

Quantum computing from a software, services and data point of view

A quantum computation usually consists of preparing the quantum states, running the algorithm and measuring the results. Quantum algorithms make use of quantum superposition or entanglement and perform operations on qubits that change their quantum state. A major difference to classical computing is that the calculation performed by a quantum computer returns a range of possible results together with an estimate about how probable the different results are. Measuring and reading out the results introduces unwanted errors caused by environmental interference, known as 'noise'. A quantum computer is therefore inherently noisy, which leads to errors in the calculations that are to be performed. In addition, these errors build up over time, resulting in only a small time-window for calculations before all information is ultimately lost. Therefore, proper post-processing is required to mitigate the effect of errors and to do error correction.

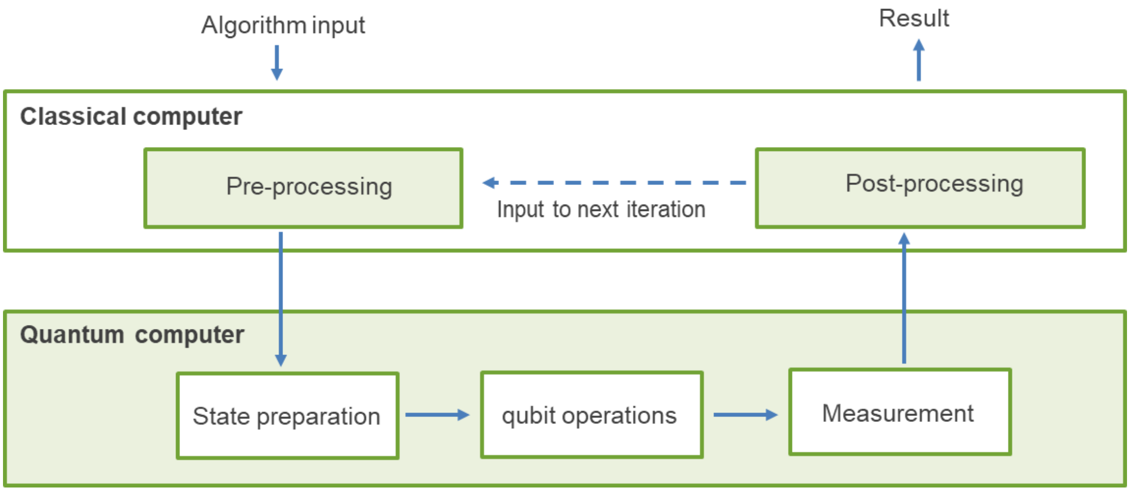

Figure 1 Quantum Computing workflow

An entire new branch of software engineering is expected to emerge over the next few years to develop the new programming paradigms required for quantum computers and to address the related software challenges. A new branch of AI making use of quantum computing will also emerge. The related quantum software research challenges are many-fold.

- A basic prerequisite is a sound understanding of the fundamental quantum effects and how they can be combined into efficient quantum algorithms. It requires thinking that is radically different to classical digital computing.
- In addition to knowing about the basic quantum effects, designing quantum algorithms requires an understanding of which problems quantum computers can solve in an efficient way, and it requires knowledge about the problem domain (e.g. chemistry, telecommunication networks, logistics, etc.).

[3] Report on National Quantum Strategies Covers 46 Countries Plus the European Union - Quantum Computing Report
[4] https://qureca.com/overview-on-quantum-initiatives-worldwide-update-mid-2021/

As an example,[5] chemistry researchers together with quantum computing experts have developed an algorithm combing classical and quantum computation for calculating ground state energies of molecules. The algorithm – a quantum Monte Carlo simulation for calculating probabilities in a system with many random unknown variables – deploys a quantum computer only for the most computationally complex part.

- Today's quantum computers are based on different hardware solutions. On the one side, it would be desirable to hide the details of the hardware from the programmer. On the other side, the class of problems that can be solved depends very much on the specifics of the available hardware, and the algorithms must be tailored to the hardware in order to be most efficient. The challenge is to find approaches that make it unnecessary to need to know hardware details whilst benefiting from the power of specific hardware.
- Quantum computers and classical computers will coexist, and hybrid algorithms utilize both. More general, classical computing will be required for the pre- and postprocessing of a quantum computation, addressing the effect that data cannot be stored on a quantum computer for a longer duration than the computation. Quantum computing and classical computing resources will be accessible from the cloud and should be usable in an integrated way, similar to the way today's High Performance Computing (HPC) is used.
- As part of the post-processing, quantum error correction needs to be done faster than the errors occur. For gate-based quantum computers this is theoretically guaranteed by the quantum threshold theorem. If the error is below a certain threshold, information on several physical qubits can be combined to create a logical qubit. The number of physical qubits depends on the error rate; the lower the error rate, the fewer physical qubits are needed. It is estimated that the first logical qubit will need hundreds or thousands of qubits. It is still an open research field to find optimal 'codes', i.e. ways to encode the information, depending on the features of the underlying physical qubits. In addition, the codes must be created in such a way that they also allow for computation. The correction algorithm repeatedly a) performs certain measurements, b) solves optimization problems to find out which error has occurred, and c) corrects those errors. Error correction creates immense amounts of data and optimization problems which need to be solved with very short latency. There are important theoretical and software challenges present (in addition to the hardware challenges) which need to be overcome.
- Error mitigation improves the accuracy of the obtained results but does not help with the small time-window. An example application where this is very helpful is energy calculations within quantum chemistry. There are different types of noise, which can be treated in different ways. As a first step one needs to characterize the type of noise. This in itself is an active research field. This is needed to create good and relevant noise models. Finally, efficient error mitigation methods need to be created, tailored to the quantum device at hand, balancing accuracy and computational overhead. Overall, the challenge is to create practical algorithms which extend the state of the art and scale well with increasing number of qubits.
- The full software lifecycle and software stack for quantum computers are different to those in classical computing. At the lowest machine level, qubits and their interfacing need to be controlled and optimized. At the next level up the software stack, it is about the coding of the algorithm by quantum circuits combing multiple qubits. On top of the stack, the algorithm execution is integrated with other parts of the application software. Simulation of qubits and quantum circuits as well as testing and debugging adds further challenges.

[5] https://scitechdaily.com/new-algorithm-helps-quantum-computer-crunch-chemistry-equations/

- Benchmarking, testing and debugging of quantum computation is a more challenging task than in classical computing. Performance depends not only on the number of qubits but also on the quality of the qubits, the error mitigation and correction, and the specific characteristics of the quantum hardware. That means that a given quantum algorithm will have different performance when running on different machines. Testing and debugging is extremely challenging because of the very large size and complexity of quantum states and because measuring these states is destructive.

Quantum research and standardization initiatives

Major research initiatives at EU and Member State level include the following.

- EU Quantum Flagship[6], a ten-year long-term research project launched in 2018 with a budget of at least €1 billion.
- European Quantum Industry Consortium[7].
- Finnish QuTI project[8], a three-year project launched in 2022with a total budget of €10 million.
- NordiQuEst project[9], a three-year project with the aim to build Nordic-Estonian quantum computing infrastructure uniting Nordic quantum computers and simulators.
- Norwegian centre for quantum technology[10].
- Quantum alliance[11], a German cluster of excellence

Notable quantum standardization activities are as follows.

- CEN/CENELEC Focus Group on Quantum Technologies[12].
- ITU-T Focus Group on Quantum Information Technology for Network[13].

Recommendations

To meet the challenges identified above, investment in software-related research is needed in Horizon Europe to support the following.

- Increased interdisciplinary research - including quantum information, computer science, physics, chemistry, and especially mathematics - to develop domain- and problem-specific quantum algorithms, and to improve the efficiency of existing ones. The problem categories that are suitable for quantum computers in various domains need to be better understood. Promising application areas include chemistry, combinatorial optimization problems in various sectors, and machine learning[14].
- Studies of classical continuous optimization for high dimensional and noisy target functions in the context of quantum computing.

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[6] https://qt.eu/
[7] https://www.euroquic.org/
[8] https://www.vttresearch.com/en/news-and-ideas/major-project-brings-together-finnish-industry-and-research-quantum-technology
[9] https://neic.no/nordiquest/
[10] https://www.quantumcomputing.no/
[11] https://www.quantum-alliance.de/
[12] https://www.cencenelec.eu/areas-of-work/cen-cenelec-topics/quantum-technologies/
[13] https://www.itu.int/en/ITU-T/focusgroups/qit4n/Pages/default.aspx
[14] https://www.globenewswire.com/news-release/2021/12/01/2344216/0/en/Rigetti-Enhances-Predictive-Weather-Modeling-with-Quantum-Machine-Learning.html

- Understanding what the best software technology stacks for quantum computers are.
- Research into the programming abstractions (e.g. abstract machines, compilers, libraries, programming languages, APIs, etc.) that facilitate the design of hardware-independent quantum programs which nonetheless benefit from the specific features of the underlying quantum hardware.
- Benchmarking, testing and debugging of quantum programs is still at a very early stage and needs to be explored at a fundamental level. Machine learning might provide highly valuable support in this area.
- More research emphasis on the integration and orchestration of classical and quantum computing. This includes the interplay at the level of algorithms and the lower level of pre- and post-processing of a quantum computing. It also should cover the access, orchestration and integration of quantum computing resources that are available as a service within a computing continuum.
- New processes and methodologies to engineer quantum software for business-relevant applications.
- Development of education and training programs in Europe to build up the skills, knowledge and qualifications essential for technology leadership in quantum computing. The programs should provide training at different levels of depth, including an easy-to-understand introduction into software aspects of quantum computing, with the aim of increasing the number and expertise of quantum software experts in Europe.
- Development of a strategic research and innovation agenda dedicated to quantum software which aligns activities across Europe and defines a roadmap for quantum software.