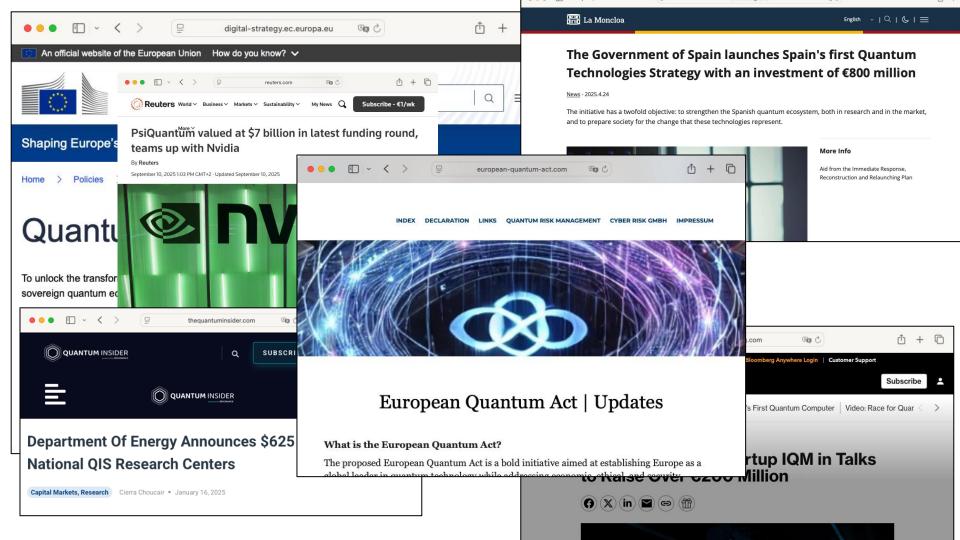
Quantum Software ante portas





Manuel Wimmer

Institute of Business Informatics -Software Engineering (BISE) manuel.wimmer@jku.at How to prepare for a new computing paradigm?



What can we <u>really</u> expect from QC?

(unfortunately) Nothing New!

But...

Every QC-solvable problem can be solved on a **classical machine** (with enough time).

... for **some problems**, certain quantum algorithms have **exponentially better** runtime complexity.

Actually, we currently simulate QC.

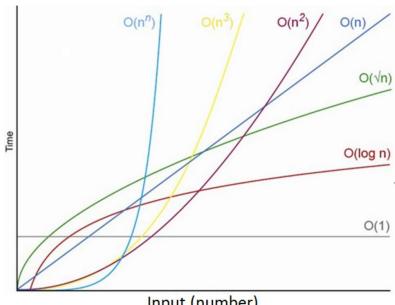
These algorithms are hard to find:

"quantum computers are very difficult to reason about using classical intuition"



The Potential of QC

- Many complex problems are **intractable** for classical computing
 - **Exponentially growing** search spaces
- Classical computers are reaching physical **limitations**
- Which problems can quantum computers solve faster than classical computers can?
- Aim: QC algorithms which provide polynomial/exponential speedup



Input (number)

Source: Hidary (2019). Quantum Computing: An Applied Approach, Springer 2021



Where QC is expected to excel?

Quantum Simulation: Natural modeling of quantum systems (chemistry, materials, molecular reactions) by following Feynman's original motivation.

Optimization Problems: Variational quantum algorithms (VQE, QAOA) and annealers tackle combinatorial or NP-hard problems.

Search and Sampling: Quadratic speed-up in unstructured search (Grover's algorithm); quantum Monte Carlo for complex distributions.

Cryptanalysis: Factoring and discrete logarithms (Shor's algorithm) → impact on RSA.

Machine Learning & Pattern Discovery: Quantum kernel methods, amplitude encoding, and quantum feature spaces for high-dimensional data.

Hybrid Workflows: Acceleration of subroutines (e.g., optimization or linear algebra) inside classical pipelines.



Example: Quantum Combinatorial Optimization

- QCO aims to find the set of discrete decision variables that minimize a certain constrained or unconstrained optimization function.
- Problems are usually non-convex (causing many local optima) and are often characterized by an exponentially growing search space

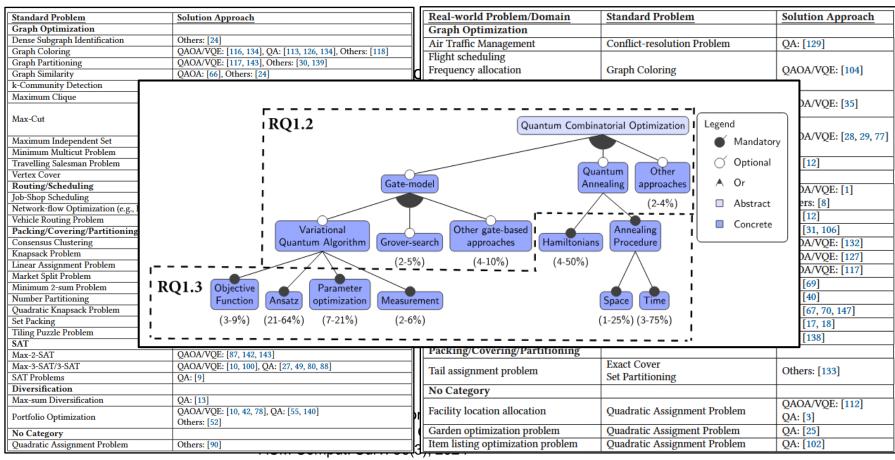


Example: Quantum Combinatorial Optimization

Standard Problem	Solution Approach	
Graph Optimization		
Dense Subgraph Identification	Others: [24]	
Graph Coloring	QAOA/VQE: [116, 134], QA: [113, 126, 134], Others: [118]	
Graph Partitioning	QAOA/VQE: [117, 143], Others: [30, 139]	
Graph Similarity	QAOA: [66], Others: [24]	
k-Community Detection	QAOA/VQE: [89, 123], QA: [101, 115], Others: [74, 124, 139]	
Maximum Clique	QA: [103, 110], Others: [24]	
	OAOA/VOE: [5, 33, 48, 56, 60, 65, 81, 84, 92, 100, 121, 142, 154],	
Max-Cut	[6, 10, 22, 23, 42, 51, 75, 76, 78, 125, 131, 137, 155]	
	QA: [72], Others: [83, 94, 97, 151],	
Maximum Independent Set	QAOA/VQE: [10, 100, 119, 120], QA: [148]	
Minimum Multicut Problem	QA: [34]	
Travelling Salesman Problem	QAOA/VQE: [96, 100], QA: [12, 45, 108, 109]	
Vertex Cover	QAOA/VQE: [95, 96, 117]	
Routing/Scheduling		
Job-Shop Scheduling	QA: [2, 156]	
Network-flow Optimization (e.g., Routing)	QAOA/VQE: [153]	
Vehicle Routing Problem	QAOA/VQE: [14, 61], QA: [2, 45, 59, 73]	
Packing/Covering/Partitioning		
Consensus Clustering	QA: [32]	
Knapsack Problem	QA: [45]	
Linear Assignment Problem	QAOA/VQE: [112]	
Market Split Problem	QAOA/VQE: [10, 100]	
Minimum 2-sum Problem	Others: [90]	
Number Partitioning	QAOA/VQE: [10, 78, 100]	
Quadratic Knapsack Problem	QA: [149]	
Set Packing	QAOA/VQE: [117]	
Tiling Puzzle Problem	QA: [41]	
SAT		
Max-2-SAT	QAOA/VQE: [87, 142, 143]	
Max-3-SAT/3-SAT	QAOA/VQE: [10, 100], QA: [27, 49, 80, 88]	
SAT Problems	QA: [9]	
Diversification		
Max-sum Diversification	QA: [13]	
Portfolio Optimization	QAOA/VQE: [10, 42, 78], QA: [55, 140] Others: [52]	
No Category	Outers, [32]	
Quadratic Assignment Problem	Others: [90]	
Zuantane Ussikiinieni i tonieni	Outco. [70]	

Real-world Problem/Domain	Standard Problem	Solution Approach
Graph Optimization		
Air Traffic Management	Conflict-resolution Problem	QA: [129]
Flight scheduling		
Frequency allocation	Graph Coloring	QAOA/VQE: [104]
Register allocation		
Smart charging electric vehicles	Max-k-Cut	QAOA/VQE: [35]
	Maximum Independent Set	QAOA/ VQE. [55]
Cluster head selection		
Wireless scheduling	Maximum Weighted Independent Set	QAOA/VQE: [28, 29, 77]
Satellite scheduling		
Satellite sub-constellation assignment	Weighted k-Clique Problem	QA: [12]
Routing/Scheduling		
Social workers problem	Combination of Vehicle Routing	QAOA/VQE: [1]
Social workers problem	Problem and Scheduling Problem	Others: [8]
Military maintenance	Job-Shop Scheduling	QA: [12]
Robot routing	Routing	QA: [31, 106]
Binary paint shop problem	Scheduling	QAOA/VQE: [132]
Flight-gate assignment problem	Scheduling	QAOA/VQE: [127]
Multiple processor scheduling	Scheduling	QAOA/VQE: [117]
Nurse scheduling	Scheduling	QA: [69]
Railway dispatching problem	Scheduling	QA: [40]
Traffic flow optimization	Scheduling	QA: [67, 70, 147]
Transaction scheduling	Scheduling	QA: [17, 18]
Workflow scheduling	Scheduling	QA: [138]
Packing/Covering/Partitioning		
Tail assignment problem	Exact Cover	Others: [133]
	Set Partitioning	Oulers, [155]
No Category		
Facility location allocation	Quadratic Assignment Problem	QAOA/VQE: [112]
		QA: [3]
Garden optimization problem	Quadratic Assigment Problem	QA: [25]
Item listing optimization problem	Quadratic Assignment Problem	QA: [102]

Example: Quantum Combinatorial Optimization



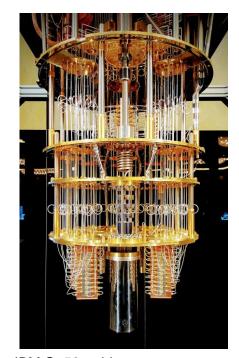
However...

Current Quantum Computers are...

- Room-filling machines
- Expensive
- Prone to error

Software running on these machines is...

- Often hardware-specific
- Low-level and complex
- Usually developed by physicists or mathematicians.



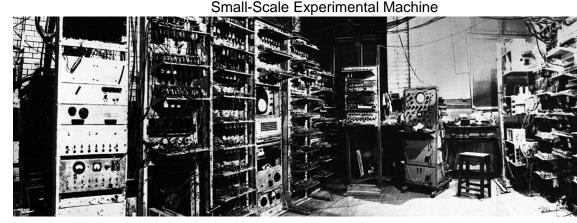
IBM Q: 50-qubit quantum computer (photo © Lars Plougman)



However...

Early computers were:s.are...

- Room-filling machines
- Expensive
- Prone to error.



https://www.cs.manchester.ac.uk/about/history-and-heritage/

Software running on these machines was...

- Often hardware-specific
- Low-level and complex
- Usually developed by physicists or mathematicians.



We've been there before!

- QC faces similar challenges classical computing faced in the mid of the last century
- Back then, a new profession emerged to solve these challenges
- People built abstractions & languages, invented techniques & tools
 - Software engineering discipline
- QC is coming with fundamentally different working principles.
 - Let's prepare for it!



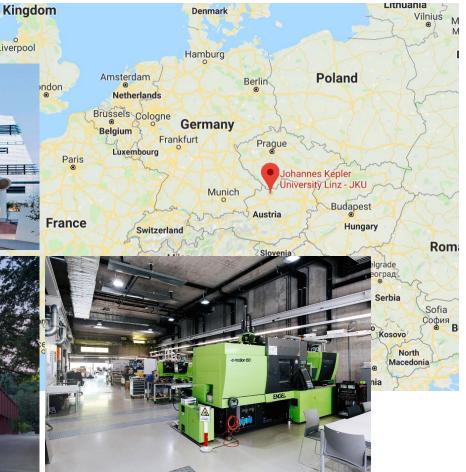
BISE @ JKU Linz





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Starting Point 2019







Manuel Wimmer Head of Institute



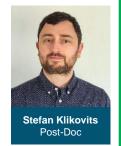
Birgit Breitschopf Administration



Dominik Lamprecht Software Technician



















University Assistant

Sabine Sint



Johannes Sametinger Associate Professor **Assistant Professor**



Reinhold Plösch Associate Professor



Honorary Professor







LIT Secure



BISE @ JKU Linz

Foundations

- Languages: UML, SysML, AutomationML, DSMLs, ...
- Methods: MDSE, DSM, MPM,
- Techniques: transformation, code generation, tracing, ...
- Management: evolution, versioning, variants, ...
- Tools: editors, repositories, validators, engines, Alware, ...

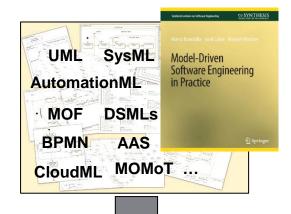
Applications

- Software: Web, Cloud, Databases, Workflows, IoT, ...
- Systems: Industry 4.0/5.0, BIM, Tunneling, ...
- Emerging Paradigms: Al, Digital Twins, Quantum Computing

Quantum Computing

- Applications of QC (k-community detection, graph matching, ...)
- Quantum Software Engineering (read SE 4 QC)





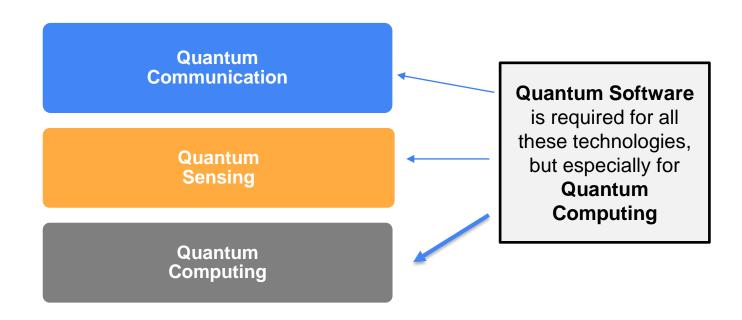


What to expect from the rest of this talk?

- Quick outline of QC
 - How does the technology work?
 - What can it do?
- Quantum Software in addition to Classical Software
 - Where are we?
 - Current challenges
- How to approach Quantum Software research?
 - Some insights how we approach this area
- What's next?



Quantum Technologies: What are we speaking about?





What is Quantum Computing?

Quantum computers process information using the **laws of quantum physics**, not classical Boolean logic.

While a classical computer is in one of 2^N states at a time (where N is number of bits), a quantum computer is in probability distribution of 2^N states.

Programming a QC is not about transforming one state through operations a computer can perform faster than a human. It is about manipulating a **distribution over all possible solutions** to a problem in a meaningful way.



Basic Concepts - Superposition

Classic bits: two states (0, 1)

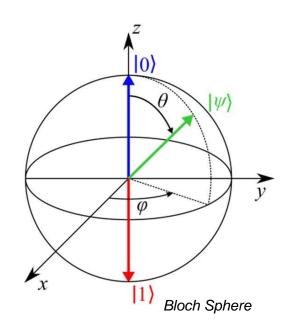
Quantum bits (Qubits): represent a probability distribution between 0 and 1

$$|\psi\rangle = \alpha * |0\rangle + \beta * |1\rangle$$
, where $|\alpha|^2 + |\beta|^2 = 1$

Similar to classical bit $0,1 \rightarrow |0\rangle$, $|1\rangle$

Can also be a mixture → superposition

Upon measurement, states collapse to 0 or 1





Basic Concepts - Entanglement

Correlation between probability distributions of qubits

Probabilities of two qubits can be entangled

E.g.,: **Bell States** (completely entangled):

50% probability of measuring
$$|00\rangle$$

 $|\Psi_{+}\rangle = \frac{1}{\sqrt{2}}|\mathbf{00}\rangle + \frac{1}{\sqrt{2}}|\mathbf{11}\rangle$ 50% probability of measuring $|11\rangle$
0% probability of measuring $|01\rangle$ or $|10\rangle$

When one qubit is measured, the shared superposition collapses.
 Right after measurement, both qubits have the same value

Entanglement is an important building block for achieving speed-ups in quantum algorithms
Side-note: Linking two quantum computers through entanglement gives exponential speedup

Basic Concepts - Quantum Parallelism

Because our system is in a **multitude of states** at **once** (superposition), a **single operation** can **affect all** of these **states** at **once**.

There is no free lunch!

Due to the laws of quantum physics, quantum operations have to be reversible.

Most operations from **classical computing** are **not reversible** (e.g., AND, OR, ...), and therefore, cannot directly be executed on a QC.



Basic Concepts - Measurement

Measurement destroys superposition

Non-reversible quantum operation

Intermediate states of the quantum system are not accessible

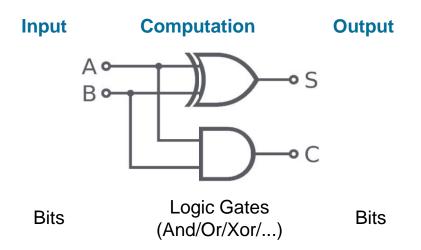
Copying is not possible, see no-cloning theorem

• To reproduce states, repeated state computation and measurement required



What does a quantum program look like?

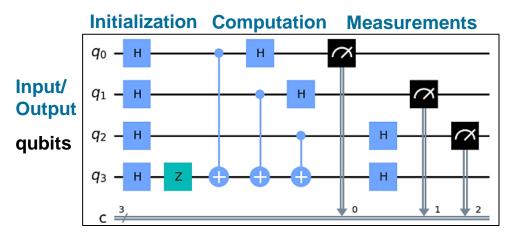
Recall: Classical Logic Circuit Diagram





What does a quantum program look like?

Current Status: Quantum Circuit



Quantum Operations Gate Set {X, Z, H, ...}

Quantum Gate

actions on the qubits

- X (Pauli-X): bit flip
- Z (Pauli-Z): phase flip
- H (Hadamard): creates superposition
- ...

A **unitary matrix** U acting on a qubit $|\psi'\rangle = U|\psi\rangle$

Gates are <u>reversible</u> (important property)

Typical Problem:

"Create a circuit that does ..."

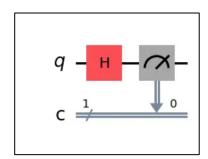


What does a quantum program look like?

Current Status: Quantum Circuit

Initialization Computation Measurements

Input/ Output qubits



Quantum Operations Gate Set {X, Z, H, ...}

Quantum Gate

actions on the qubits

- X (Pauli-X): bit flip
- Z (Pauli-Z): phase flip
- H (Hadamard): creates superposition
- ...

A **unitary matrix** U acting on a qubit $|\psi'\rangle = U|\psi\rangle$

Gates are <u>reversible</u> (important property)

Typical Problem:

"Create a circuit that does ..."



Current Limitations of Quantum Computing

Multitude of technical challenges

- Fragile qubits
- Inaccuracy of quantum operations
- 0 ...

Main paradigms

- Noisy Intermediate Scale Quantum (NISQ-era)
- Fault-tolerant Quantum Computing



Current Era: NISQ "Noisy Intermediate-Scale Quantum"

NISQ = *Noisy Intermediate-Scale Quantum* (term coined by John Preskill, 2018).

Size 50-1000 physical qubits;

Error-prone, short coherence times; no full error correction

Goal: Demonstrate *quantum advantage* for specialized tasks before large-scale fault-tolerant systems exist

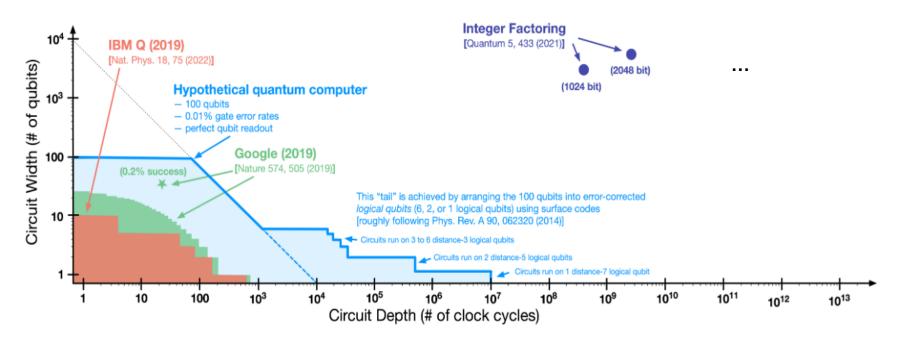
Approach: Use hybrid algorithms (VQE, QAOA, HQCC) — classical optimization controlling quantum circuits

Limitations: Noise limits circuit depth; results are probabilistic and hardware-specific

Software Challenge: Optimize and mitigate errors through compilation, calibration, and classical post-processing



Quantum Computing: Where are we?





Example Technology Roadmap: IBM





The Challenges Ahead

Edsger Dijkstra on the early challenges of software:



(photo © Hamilton Richards)

"As long as there were **no machines**, **programming** was **no problem** at all; when we had a few **weak computers**, **programming** became a **mild problem**, And now we have **gigantic computers**, **programming** has become an **equally gigantic problem**."

(Excerpt from his 1972 Turing Award Lecture)



Complex Computing Infrastructure

How to specify?

Where can we find algorithms and guidelines how to select/realize them?

How to best program a QC?

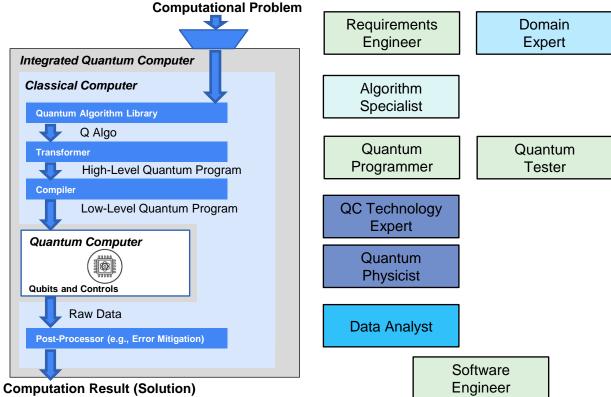
What is the best deployment?

What is the best QC for a given problem?

What is the quality of the computed solution?

How to integrate the results in a larger system?





Integrated Quantum Computer Illustration based on Proctor *et al.* Benchmarking quantum computers. *Nat Rev Phys* **7**, 105–118 (2025).

Abstraction levels

Classical Software

Models, No-Code, 4GL, 5GL, ...

Python + Frameworks

Java, ...: objects

C++: objects

C: arrays, data types, ...

Assembler Language

Machine language (00100101...)

Quantum Software

?Models, No-Code, 4GL, 5GL?

IBM Quantum Composer elubits)

Python + Fragan (1965)

...

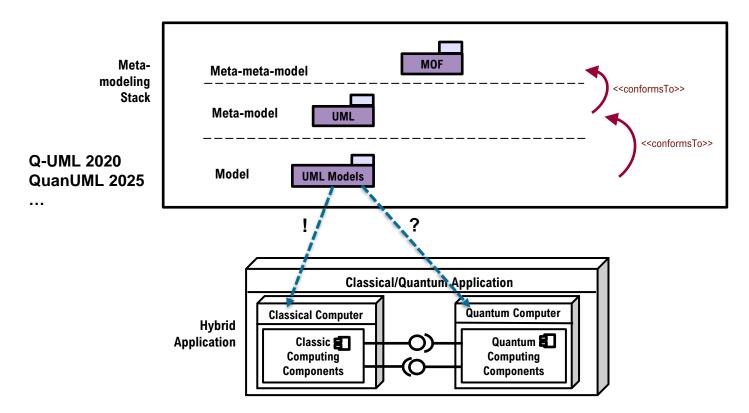
Circuits of transpilation (qubits)

Circuits (du transpilation (qubits))

Pulse-level, ...

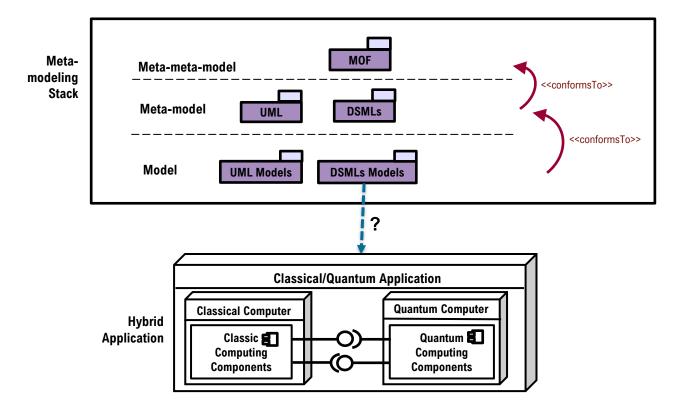


And what about Modeling Languages?



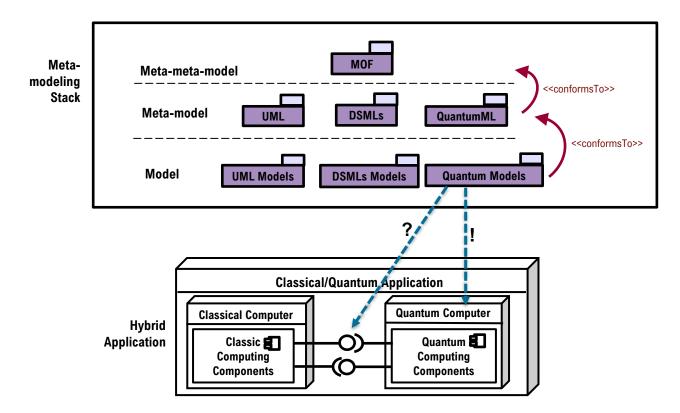


And what about Modeling Languages?





And what about Modeling Languages?





Reality Check: Multitude of Challenges/Opportunities

QC community focus

- More and better qubits (hardware)
- Demonstrating quantum advantage (algorithms)

However, software is the next bottleneck

- Abstraction gap: gate-level (like assembly!)
- No best practices: Testing, debugging, verification
- Tooling immaturity: Limited IDE support, e.g., profilers, debuggers, validators, ...
- **Skills gap**: Quantum physicists ≠ software engineers

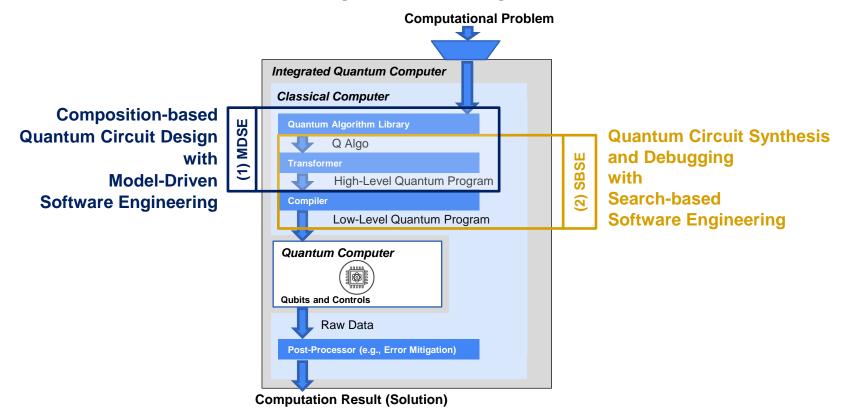
Opportunity for computer scientists

(Non-exhaustive List!)

- ✓ Model-driven engineering
- ✓ Search-based software engineering
- ✓ Testing and verification
- ✓ Software processes
- ✓ Service Oriented Computing
- ✓ Software Architecture
- Quantum AI



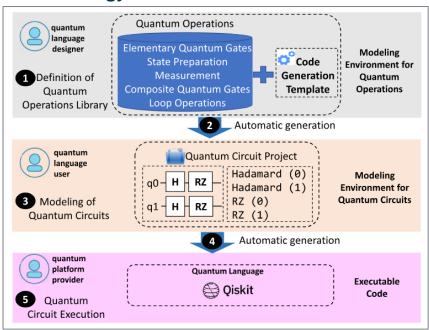
QSE Focus at BISE (JKU Linz)





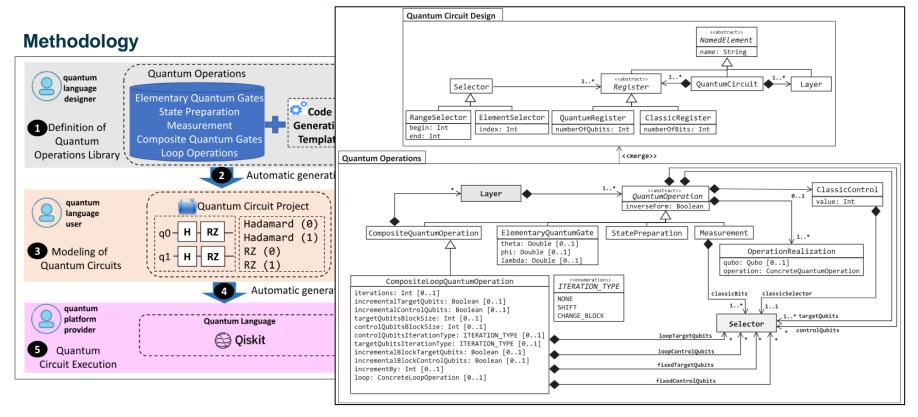
Area #1: MDSE 4 QSE

Methodology



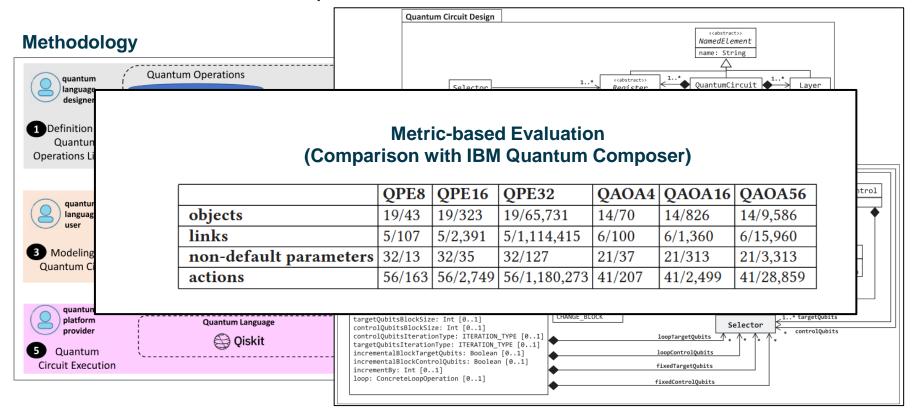
Area #1: MDSE 4 QSE

Metamodel for Quantum Circuits



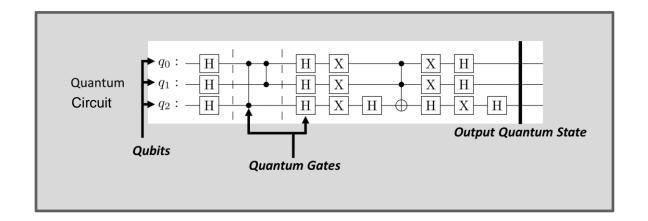
Area #1: MDSE 4 QSE

Metamodel for Quantum Circuits



Area #2: Quantum Circuit Synthesis (QCS)

Goal: Find a quantum circuit that implements a desired behavior.





QCS comes in many different flavors...

Compilation and Circuit Mapping

Abstract Algorithm →
Concrete Circuit
⊢ hardware constraints

Quantum Architecture Search

Unitary → Variational QC (+ parameters)

Quantum Algorithm Discovery

Unitaries/Cases → Abstract Algorithm

State Preparation

Target State → Concrete Circuit

Challenges

- Vast design space
- Precision vs. computational cost
- NISQ: Errors, Probabilistic Nature, Hardware Specifics

→ We treat QCS as a Search Problem!



QCS as a Search Problem

SBSE has been used for classical software for more than two decades [Harman, Jones 2001]

Goal: Find a software system / program that optimizes a given fitness function

Advantages:

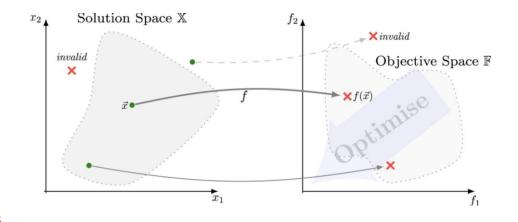
Automated exploration by

Meta-heuristic searchers

• Genetic Programming (GP), ...

Challenges: Finding a good

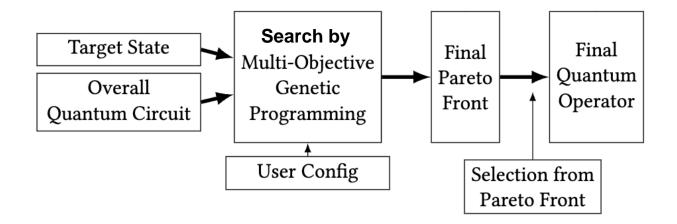
- 1. Program encoding
- 2. Fitness function + evaluation capabilities





Our Approach: Search Scheme using GP

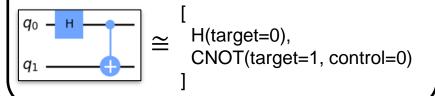
Multi-Objective Optimization allows to deal with NISQ characteristics





Typical GP Setup for Quantum Circuits

Encoding: gate vector



Fitness

behaviour: accuracy/fidelity/distance, and
structure: # gates, depth,
non-local gates, # parameters

Operators

mutation: add / delete / move / alter / swap gate change qubits, ...

crossover: one-point, two-point, ...

selection: tournament, ...

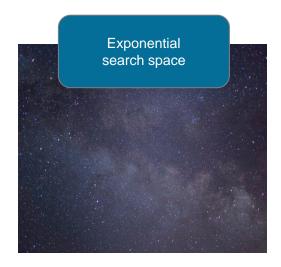
Algorithms

use of classical meta-heuristic algorithms: GA, NSGA-II, NSGA-III, ...

Is this all we need?



Dealing with several challenges

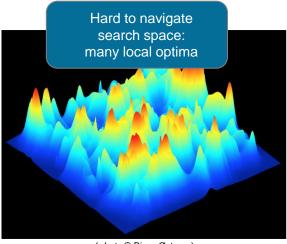


→ Shrink search space



(photo © Florian Hirzinger)

→ Speed up or avoid simulation



(photo © Bjørn Østman)

→ Make search more efficient



Challenge: Hard to navigate search space Hybrid Quantum State Synthesis

Problem

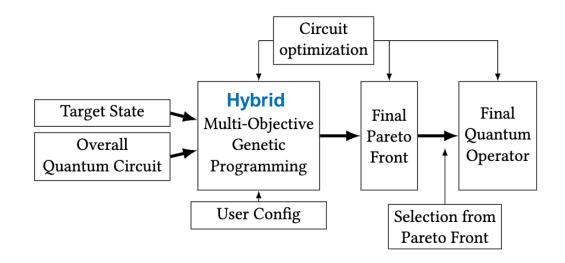
• Some gates (e.g., RX θ , RY θ , RZ θ) require parameters $\theta \in (0, 2\pi)$

Core Idea

 Embed parameter optimization (Nelder-Mead) within evolutionary search

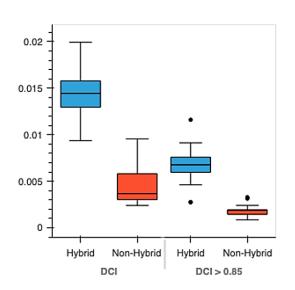
Results

- Higher diversity
- Faster convergence

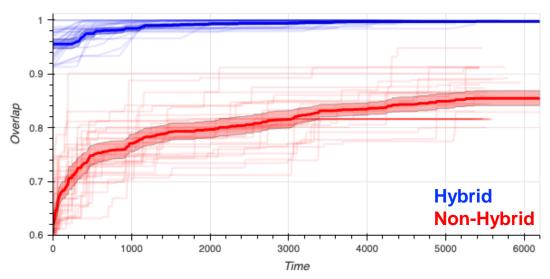




Challenge: Hard to navigate search space Hybrid Quantum State Synthesis



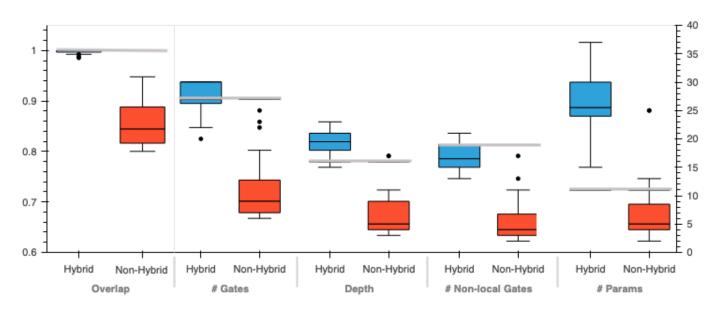
RQ1: better diversity



RQ2: Hybrid has higher overlap + faster convergence



Challenge: Hard to navigate search space Hybrid Quantum State Synthesis



RQ3: higher overlap, but more costly circuits

Hybrid Non-Hybrid



Challenge: Hard to navigate search space Hybrid Quantum Debugging and Optimization

Problem

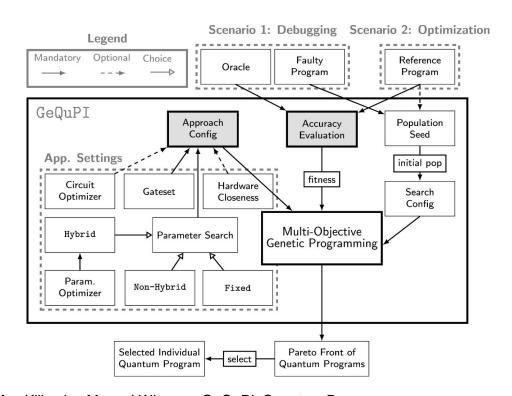
 Sometimes we already have a scaffold or almost correct quantum circuit

Core Idea

 Use existing information as "seed" for searching for better versions

Results

 Can fix buggy and optimize inefficient quantum circuits





Debugging capabilities?

- Hybrid can optimize
 - for specific input states
 - with Non-Hybrid & Fixed sometimes only equally good solutions are found

- Hybrid can repair arbitrary inputstate programs
 - Non-Hybrid & Fixed have problems

Debugging capabilities: number of runs per category and use case. (Hybrid / Non-Hybrid / Fixed).

(a) RQ1.1 (Perfect Accuracy)

Input state	Problem	Optimized	Pareto Equal	Worse	Faulty
Specific	QG_8 (2 qubits)	30/30/30	0/0/0	0/0/0	0/0/0
	QSO_6 (2 qubits)	26/0/0	4/30/30	0/0/0	0/0/0
	QSO_5 (3 qubits)	30/30/30	0/0/0	0/0/0	0/0/0
	QSE_15 (4 qubits)	30/30/30	0/0/0	0/0/0	0/0/0
	QSE_3 (5 qubits)	30/30/30	0/0/0	0/0/0	0/0/0
Arbitrary	QSE2_2 (2 qubits)	30/0/0	0/0/30	0/16/0	0/14/0
	QSE2_3 (3 qubits)	0/0/0	17/0/0	8/0/8	5/30/22
	QSE2_4 (4 qubits)	0/0/0	0/0/0	7/0/0	23/30/30
	QSE2_5 (5 qubits)	0/0/0	0/0/0	6/0/0	24/30/30



Optimization capabilities?

- All approaches can optimize
- Hybrid performs (almost) consistently better
- Hybrid improves by 35%
- Hybrid compared to "standard approach" (Qiskit built-in optimizer):
 - optimize in significantly more cases
 - and higher on average

Optimization capabilities (Hybrid / Non-Hybrid / Fixed).

(a) RQ2.1 (Perfect Accuracy)

	Optimized	Pareto Equal	Worse	Faulty
Total	541/135/105	143/84/64	50/10/14	406/911/957
Specific	274/63/45	89/84/64	23/10/14	124/353/387
Arbitrary	267/72/60	54/0/0	27/0/0	282/558/570
2 qubits	135/101/90	40/30/30	19/0/0	16/79/90
3 qubits	248/17/11	37/20/2	9/7/14	66/316/333
4 qubits	120/6/2	55/32/30	14/3/0	141/289/298
5 qubits	38/11/2	11/2/2	8/0/0	183/227/236

Lesson Learned:

Simulation of the candidate circuits consumes majority of the execution time of the discussed approaches!



Ongoing work: Simulation with Caching

Problem

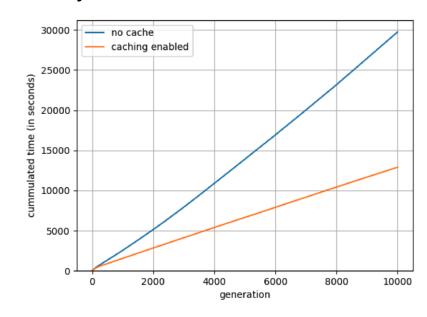
- QCS (often) operates on **circuit populations** (e.g., when using GAs)
- Populations (often and on purpose) contain redundancy

Core Idea

 Identify recurring gate patterns and aim for reuse of the results → reduce computations

Results

- Clear reduction in simulation time (depending on redundancy and qubits)
 - > 50% time savings in GAs





Ongoing work: Divide & Conquer Simulation

Problem

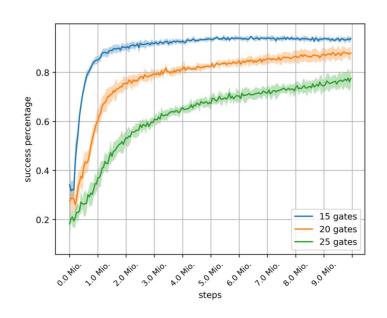
 Cost of simulation grows exponentially in number of qubits

Core Idea

Use Reinforcement Learning to split synthesis problem and solve subproblems independently

Results

- Agent was able to divide in > 75% of all cases
- Much fewer gates needed for separation than for synthesis of the circuits





Summary – Lessons Learned

Technological Spaces

- Integrating QC into "your" technologies (we did this for the EMF ecosystem)
- Allows to reuse existing tooling (which is often defined on the meta-level)
- Model transformations, code generation, validation, ...

Adaptation of Methodologies

- Possible, but requires completely novel treatments for particular subproblems
- Requires interdisciplinary exchange and new skills for researchers



Quantum Europe Strategy

https://digital-strategy.ec.europa.eu/en/policies/quantum

Area 5 - Quantum Skills: Building a diverse, world-class workforce through coordinated education, training, and talent mobility across the EU

"However, this is still insufficient to meet the projected demand from EU's startups and industry, which faces **major shortages of professionals** with relevant applied skills."

"Shortages are **most critical** in applied fields, including **quantum software engineering**, system integration, and quantum cybersecurity, slowing the commercialisation path for EU-based startups and scaleups."

Taken from:

https://digital-strategy.ec.europa.eu/en/library/quantum-europe-strategy







Academic Study Programmes

100+ Programmes Worldwide



Characteristics

- Heterogeneous landscape of programmes
- Focus on MSc degree (typically building on CS or physics)
- Industry Partners: IBM, Microsoft, Google, AWS, ...
- Include Q-Programming, more advanced software engineering topics rarely embedded within broader QC curricula

Notable Examples

- Quantum Master Barcelona (incl. Quantum Software track)
- Aalto: BSc → MSc → PhD in Quantum Technology
- Gdansk: International MSc in QIT

What is Missing

- Dedicated Programme for Quantum <u>Software</u>
 (Software Specialisation only at KAIST, SDU, UTS)
- Shared understanding on "how to design such a programme"



QSE Community Building

SE Field



- Includes a symposium (especially for industry), workshop
- International Workshop on Quantum Software Engineering (Q-SE) @ ICSE
- + many more workshops

Quantum Field

- IEEE Quantum Week Flagship Conference on Quantum Technologies
 - Quantum System Software Track
 - Quantum Science and Engineering Education Conference (QSEEC)

Journals

- SE: ACM TOSEM (Continuous Special Section on Quantum SE)
- Quantum: ACM TQC, IEEE TQE
- 0 ...





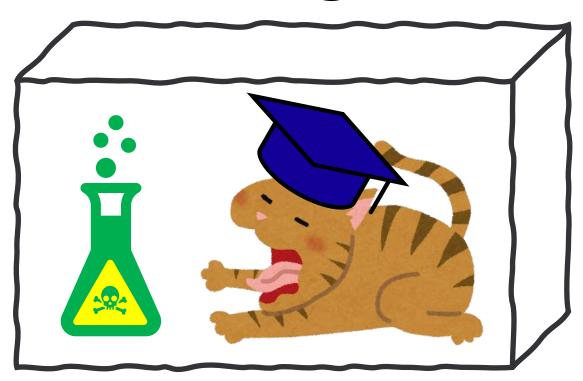


Wrap-Up

- Quantum computers made a huge progress in the last decade, roadmaps look ambitious
 - Quantum Utility still to be shown!
- Innovations of quantum computing will be driven by quantum software
 - What role will Computer Science play here?
- Current practices of developing quantum software are improving, but are still limited
 - What can be reused from classical SE?
 - How are quantum components integrated in larger software systems?
 - How can we scale up current practices supporting 10-100 qubit systems to 1k qubit systems and beyond?
- What type of organizational change is required here?
 - Dedicated quantum groups + software, software groups + quantum, software groups + quantum groups, ...



We're hiring!









From qubits to qudits ©





Thank you!

Comments? Questions? Feedback?

Looking forward to discussions and collaborations!





Many THANKS to my Quantum Software Co-Authors:

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