Quantum Computing and Software Engineering Superposition:

$\frac{1}{\sqrt{2}}(|QC\rangle + |SE\rangle)$

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Laboratório de Inovação, Pesquisa e Engenharia de Software

Outline I

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Outline II

1. Who Am I?

Who Am I?

FILIPE FERNANDES

- Professor at IF Sudeste MG [since 2016]
- Head of LIPES
- Doctoral degree COPPE/UFRJ [2023]
- Master's degree COPPE/UFRJ [2017]
- Software Engineering (SE) Areas:
  - Software Visualization
  - SE Education
  - Metaverse Engineering
  - Immersive Learning
  - Quantum SE (*on going*)
  - Software-powered Innovation (*on going*)

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Professor and Researcher

- IF Sudeste MG - Campus Manhuaçu
- Software Engineering and Human-Computer Interaction disciplines
- Current projects:
  - Development of a Metaverse Platform as an Innovative Technological Strategy for Basic Education (FAPEMIG)
  - Identification of solutions, problems and challenges in methods, techniques and tools that support the development of applications for the Metaverse (FAPEMIG)
  - Transforming Manhuaçu into a Smart City (IF Sudeste MG)
- NITTEC coordinator

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Master's dissertation

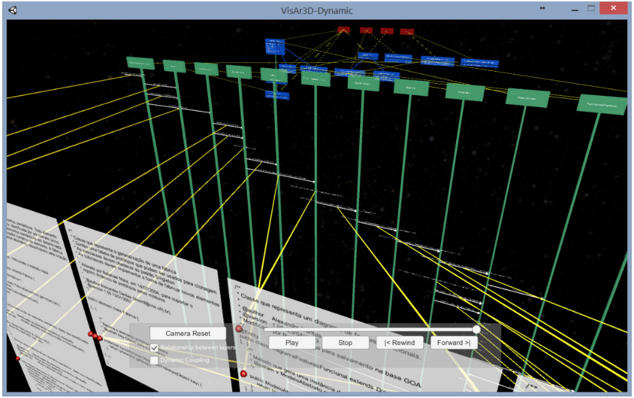

Figure: Perspectives visualization of VisAr3D-Dynamic (FERNANDES, 2017)

Thesis

Metaverse-based Software Engineering Education (MetaSEE)

- *How to support SEE through Immersive Learning?*

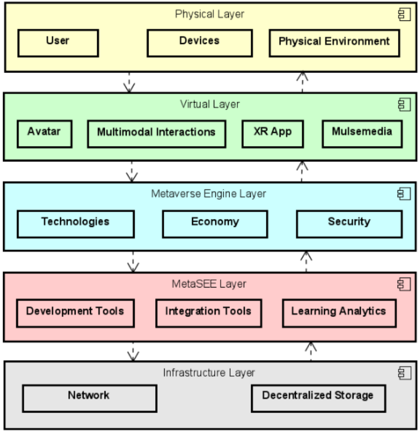

Figure: (FERNANDES, 2023)

Thesis

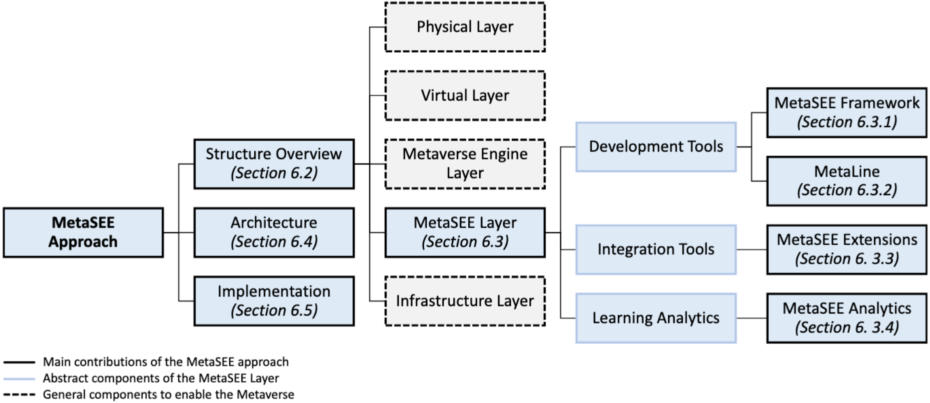

Figure: MetaSEE approach contributions (FERNANDES, 2023)

2. Introduction

Introduction

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Computing Types

Classical Computing

- Governed by the laws of classical mechanics
- Deterministic theory
- Uses digital computers to perform computation

Quantum Computing (QC)

- Governed by the laws of quantum mechanics
- Probabilistic theory
- Uses quantum computers to perform computation
  - Quantum circuits and
  - Adiabatic computing

Information Unit

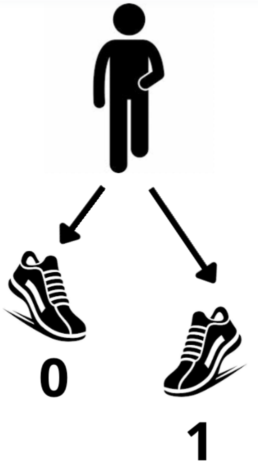
Classical Computing

- Bit = Binary Digity
- Values = 0 or 1

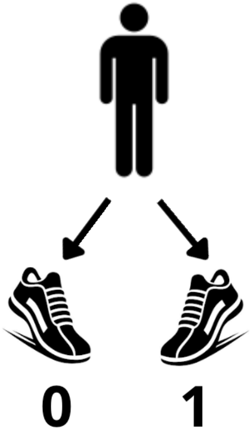
Quantum Computing

- Qubit = Quantum Bit
- Values = 0, 1, 0 and 1 at the same time

Classical Bit



Quantum Bit (Qubit)



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Applications

- **Simulations for complex quantum experiments**: complex chemistry, physics, and biology problems (SCHAETZ; MONROE; ESSLINGER, 2013)
- **Weather prediction**: forecast of natural disasters and allied complex tasks (FROLOV, 2017)
- **Post-quantum cryptography**: classic computer systems are safe with quantic computers attacks (BERNSTEIN *et al.*, 2017)
- **Quantum Finance**: optimize portfolios, model risks, and accelerate complex calculations (CANABARRO *et al.*, 2022)
- **Quantum Internet**: instant transmission of quantum information with lower latency and greater resistance to interference (CACCIAPUOTI *et al.*, 2020; UFF, 2024)
- **Quantum AI**: efficient processing of large amounts of data and the optimization of complex models exponentially faster (PERDOMO-ORTIZ *et al.*, 2018)
- Among others

QC Goal

- QC offers different solutions to computational problems and enables more efficient problem-solving than what is possible with classical computations (GYONGYOSI; IMRE, 2019)
  - Example: *while a problem with 30 variables would take around 17 minutes to solve, the same problem with 50 variables would take more than 35 years* (CANABARRO *et al.*, 2022)
- Quantum Mechanics Concepts
  - Estates superposition
  - Quantum entanglement

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3. Quantum Mechanics Concepts

Young or Elderly?

Answer the questionnaire

Observation

States superposition

$$|Person\rangle = \frac{1}{\sqrt{2}}(|Young\rangle + |Elderly\rangle)$$

P(Y) = 50% e P(E) = 50%

Coin superposition

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$$|Coin\rangle = \frac{1}{\sqrt{2}}|Heads\rangle + \frac{1}{\sqrt{2}}|Tails\rangle$$

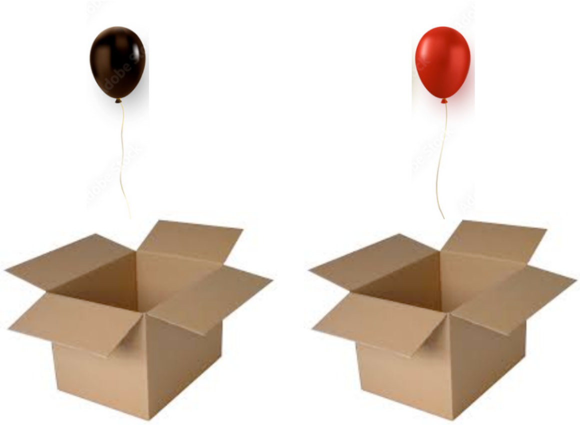
or simply

$$|Coin\rangle = \frac{1}{\sqrt{2}}(|Heads\rangle + |Tails\rangle)$$

Entanglement

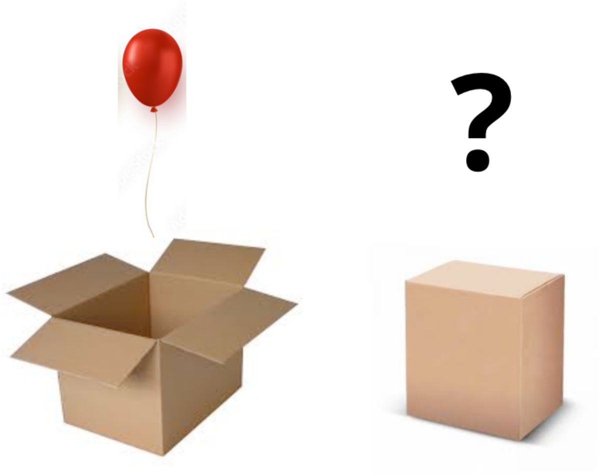
- In an entangled state, the properties of qubits are linked to each other, in spite of physical separation between them (GILL *et al.*, 2022)

Entanglement example



Entanglement example

Entanglement example



4. Quantum Computing

Quantum Computing

(GILL *et al.*, 2022)

QC is an emerging paradigm with the potential to **offer significant computational advantage** over conventional classical computing by **exploiting quantum-mechanical principles** such as superposition and entanglement

Algebraic Representation

$$|Coin\rangle = \frac{1}{\sqrt{2}}|Heads\rangle + \frac{1}{\sqrt{2}}|Tails\rangle$$

Algebraic representation

$$|\Psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle \qquad \alpha, \beta \in \mathbb{C}$$

- α and β are **probabilities amplitudes**
- $|\alpha|^2 + |\beta|^2 = 1$
- Computational base:

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Geometrical Representation

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{-i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle$$

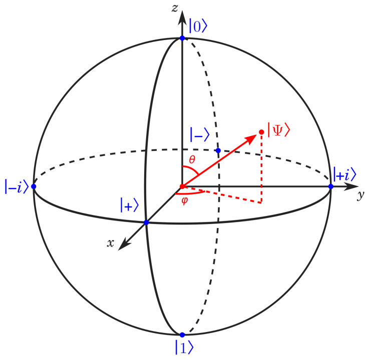


Figure: Bloch sphere

Access simulation

Bloch Sphere Example

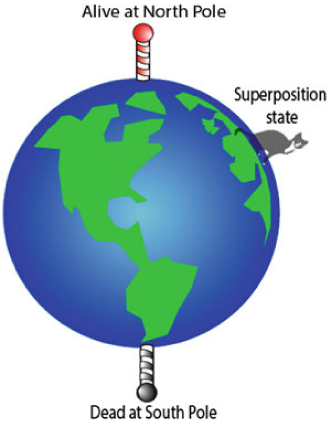


Figure: A cartoon of the Bloch sphere (HUGHES *et al.*, 2021)

Qubit States

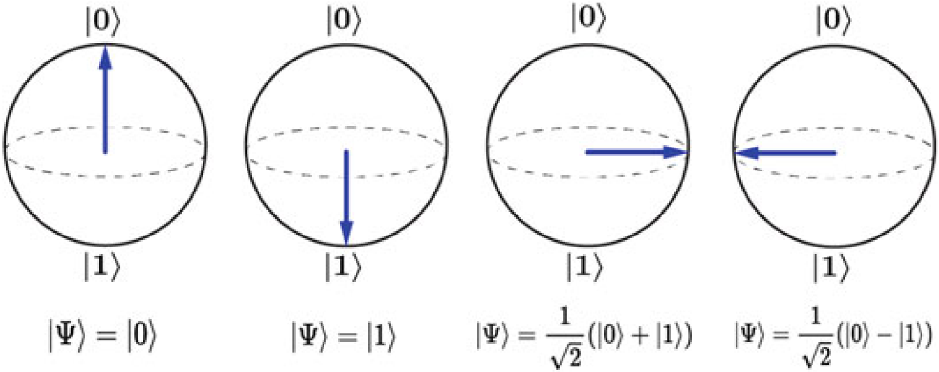
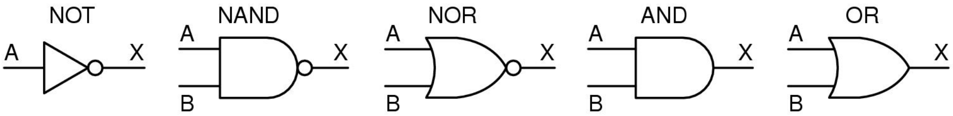


Figure: The state of a qubit is represented by an arrow on the Bloch sphere (HUGHES *et al.*, 2021)

Classic Logic Gates



A	X
0	1
1	0

(a)

A	B	X
0	0	1
0	1	1
1	0	1
1	1	0

(b)

A	B	X
0	0	1
0	1	0
1	0	0
1	1	0

(c)

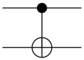
A	B	X
0	0	0
0	1	0
1	0	0
1	1	1

(d)

A	B	X
0	0	0
0	1	1
1	0	1
1	1	1

(e)

Quantum Logic Gates

Operator	Gate(s)		Matrix
Pauli-X (X)	X	⊕	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)	Y		$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)	Z		$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard (H)	H		$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Controlled Not (CNOT, CX)			$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$

Pauli Gates

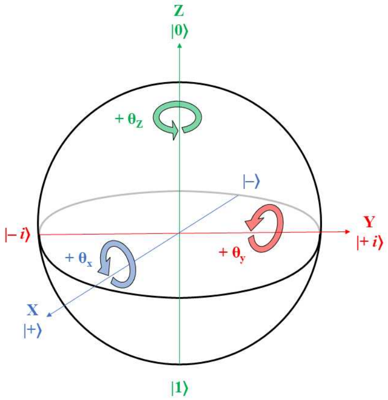


Figure: Access simulation

- **Pauli-X**: bit-flip

$$\sigma_x |0\rangle = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} = |1\rangle$$

- **Pauli-Z**: phase-flip

$$\sigma_z |1\rangle = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \cdot \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ -1 \end{bmatrix} = - \begin{bmatrix} 0 \\ 1 \end{bmatrix} = - |1\rangle$$

- **Pauli-Y**: bit-phase-flip

$$\sigma_y |0\rangle = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ i \end{bmatrix} = i |1\rangle$$

Hadamard Gate

- Creating the quantum superposition:

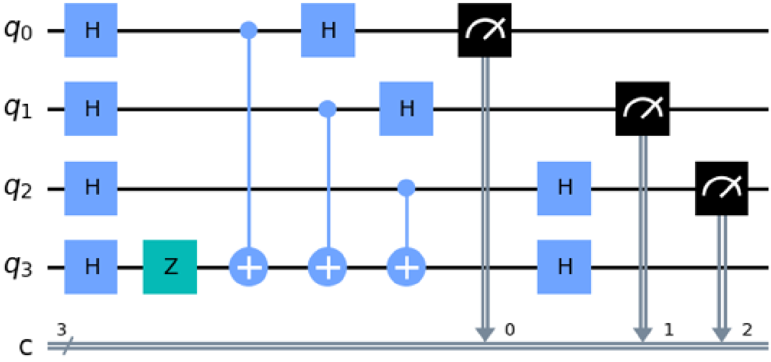
$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

- Example:

$$H\left|1\right\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \cdot \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix} =$$

$$\boxed{\frac{1}{\sqrt{2}}(\left|0\right\rangle - \left|1\right\rangle) \text{ ou } \frac{(\left|0\right\rangle - \left|1\right\rangle)}{\sqrt{2}} \text{ ou } \left|-\right\rangle}$$

Quantum Circuits



Example (equation)

$$|\psi\rangle = CX \cdot (I\,|0\rangle \otimes H\,|0\rangle)$$

$$|\psi\rangle = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \left[\left(\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \right) \otimes \left(\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \right) \right] = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix} \text{ ou } \frac{1}{\sqrt{2}}(|00\rangle + |01\rangle)$$

Example (circuit)

$$|\psi\rangle = CX \cdot (I\,|0\rangle \otimes H\,|0\rangle)$$

Example (qiskit code)

```
from qiskit import QuantumRegister, QuantumCircuit
from numpy import pi

qreg_q = QuantumRegister(2, 'q')
circuit = QuantumCircuit(qreg_q)

circuit.h(qreg_q[0])
circuit.cx(qreg_q[0], qreg_q[1])
```

Question 1

How to convert real problems into quantum algorithms?

Quantum Algorithms

Core computing algorithm	The name of algorithms	Applications	Potential application field
Quantum Fourier Transform (QFT)	Shor's algorithm	RSA decryption	Cryptography
	HHL	Inverse transform of a matrix	Machine learning
Grover's operator	Grover's algorithm	Search problem	Search in unsorted databases
Quantum-classical hybrid methods	Variational Quantum Eigensolver (VQE)	Eigensolver	New material finding
	Quantum Approximate optimization algorithm (QAOA)	Optimization	Financial industry, Satisfiability problems
Quantum adiabatic algorithm	Quantum Annealing algorithm	Optimization	Computing science, Machine learning, Financial industry

Table: Major quantum algorithms and their possible applications (CHO *et al.*, 2021)

Quantum Algorithms Examples

Quantum Finance: portfolio optimization (CANABARRO *et al.*, 2022)

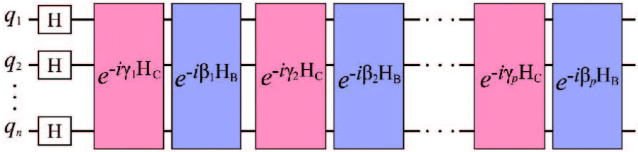


Figure: QAOA circuit implementation (CANABARRO *et al.*, 2022)

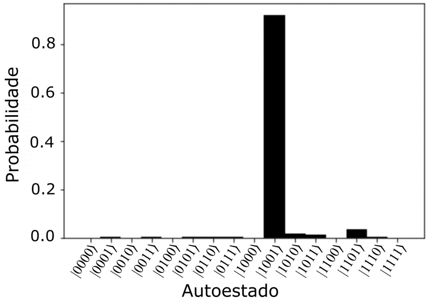


Figure: Histogram of probabilities distribution (CANABARRO *et al.*, 2022)

Quantum Algorithms Examples

Quantum Machine Learning (QML) (GOMES *et al.*, 2024)

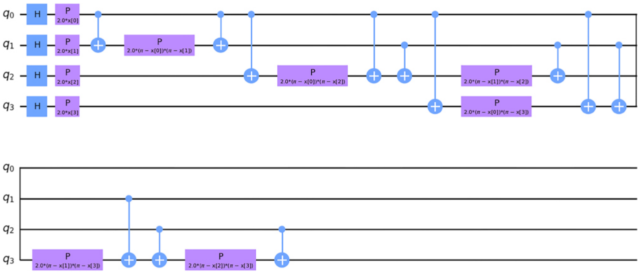


Figure: QML circuit (GOMES *et al.*, 2024)

```python
# Define o ansatz RealAmplitudes
ansatz = RealAmplitudes(num_qubits=n_qubits, reps=2)
ansatz.decompose().draw(output="mpl", style="clifford", fold=20)

# Define o otimizador COBYLA
optimizer = COBYLA(maxiter=50)

# Inicializa o classificador VQC
vqc = VQC(feature_map=feature_map, ansatz=ansatz, optimizer=optimizer)

# Treinamento do modelo VQC e teste
vqc.fit(X_train, y_train)
test_score = vqc.score(X_test, y_test)

# Fazendo previsões no conjunto de teste
y_pred = vqc.predict(X_test)

# Calculando as métricas no conjunto de teste
from sklearn.metrics import accuracy_score, precision_score, recall_score, f1_score

accuracy = accuracy_score(y_test, y_pred)
precision = precision_score(y_test, y_pred, average='weighted')
recall = recall_score(y_test, y_pred, average='weighted')
f1 = f1_score(y_test, y_pred, average='weighted')

# Imprimindo as métricas
print(f"Acurácia: {accuracy:.2f}")
print(f"Precisão: {precision:.2f}")
print(f"Recall: {recall:.2f}")
print(f"F1-Score: {f1:.2f}")
```

Figure: QML code (GOMES *et al.*, 2024)

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Quantum Algorithms Examples

Traveling Salesman Problem with QAOA (RUAN *et al.*, 2020)

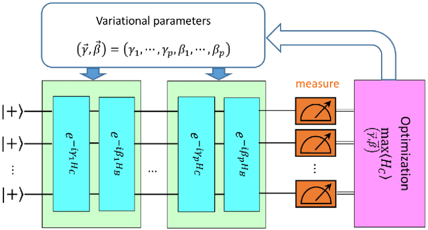

Figure: Schematic diagram of hybrid quantum-classical QAOA (RUAN *et al.*, 2020)

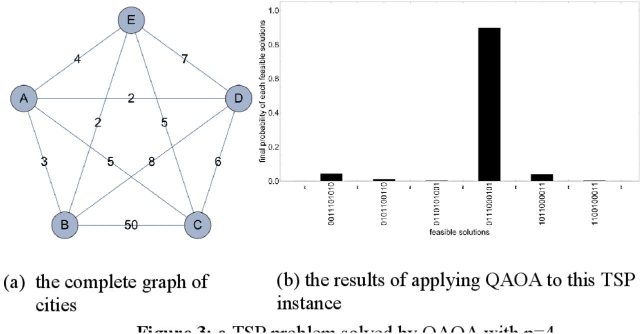

Figure: A TSP problem solved by QAOA with p=4 (RUAN *et al.*, 2020)

Question 2

How to manipulate quantum programs with the same ease and confidence of classic programs?

5. Quantum Software Engineering

Quantum Software Engineering (QSE)

(ZHAO, 2021)

Quantum Software Engineering (QSE) is the use of sound engineering principles for the development, operation, and maintenance of quantum software and the associated document to obtain economically quantum software that is reliable and works efficiently on quantum computers

- "**sound engineering principles**" to Quantum Software (QS) development
- the quantum software should be built **"economically"**
- the quantum software should be **"reliable"** and needs to work **"efficiently"** on quantum computers

QSE needs

- **Methods**
  - To provide the techniques for constructing the quantum software
  - Design of data structures, program architecture, algorithm procedure, coding, testing, and maintenance
- **Tools**
  - To provide automated or semiautomated support for these methods
- **Process**
  - To provide the glue that holds the methods and tools together and enables the rational and timely development of quantum software

Quantum Software Life Cycle

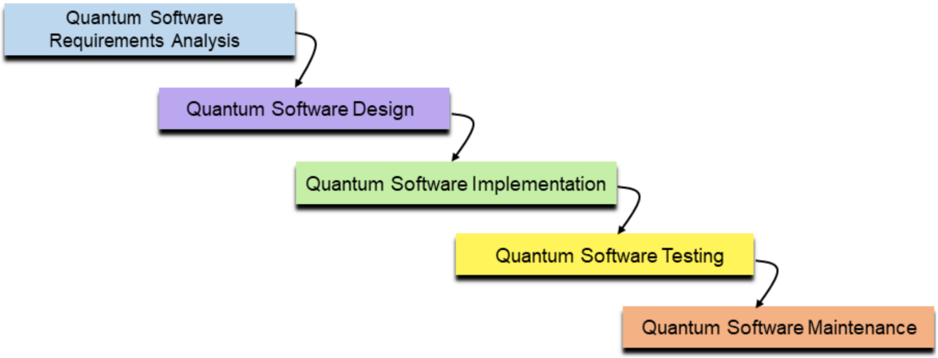

Figure: A quantum software life cycle (ZHAO, 2021)

QS Requirements Analysis

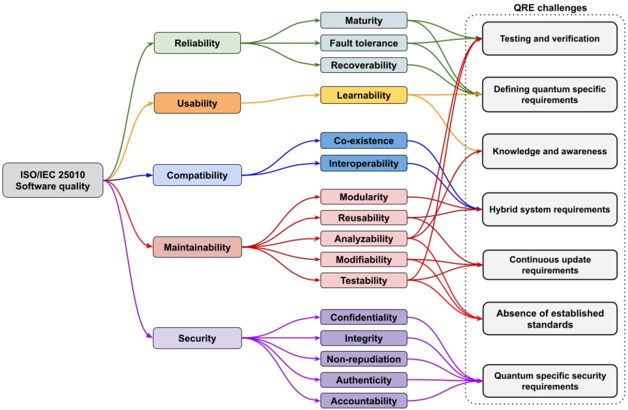

Figure: Quantum Requirements Engineering challenges (SEPúLVEDA *et al.*, 2024)

QS Design

- **Quantum Software Modelling**
  - *UML-Based Modelling language*: an approach to extending the UML to model quantum software systems (PéREZ-DELGADO; PEREZ-GONZALEZ, 2020)
  - *Generic Modelling Languages*: a preliminary conceptual model from the perspective of model-based engineering (ALI; YUE, 2020)
- **Quantum Software Specification**
  - Cartiere (2013) presented some work on defining a formal specification language for quantum algorithms
- **Modular Design of Quantum Systems**
  - Thompson *et al.* (2018) presented a formal framework to specify modularity in quantum systems
  - Sánchez and Alonso (2021) discussed the concept of module (next slide)

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QS Reuse

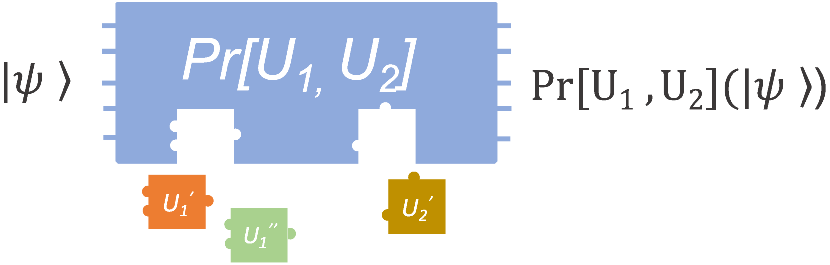

Figure: A modular approximation for quantum computing (SÁNCHEZ; ALONSO, 2021)

QS Implementation

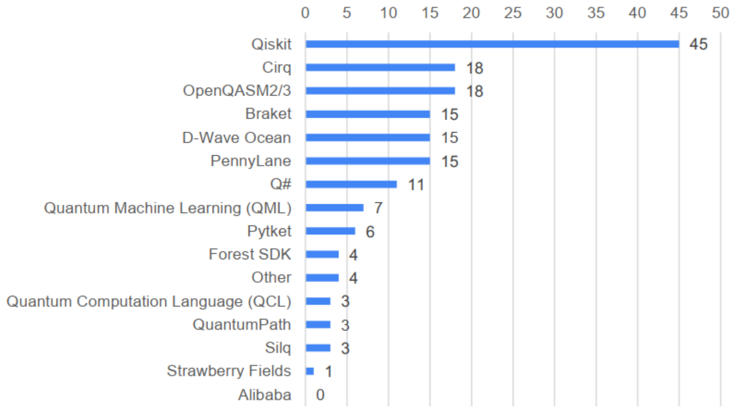

Figure: Quantum programming languages or toolkits used (JIMENEZ-NAVAJAS *et al.*, 2024)

QS Testing

- How to define testing coverage criteria of quantum software?
- How to automatically and efficiently generate test cases for quantum software?
- How to evaluate the test data quality for quantum software?
- How to test quantum software regressively?

(ZHAO, 2021)

QS Maintenance

- How to understand the existing quantum software?
- How to modify the existing quantum software?
- How to re-validate the modified quantum software?

(ZHAO, 2021)

6. Conclusion

Question 3

Is it necessary to adapt all SE to the quantum program paradigm?

- State of the practice
- QSE Education

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Thank You Very Much

Quantum Computing and Software Engineering Superposition: $\frac{1}{\sqrt{2}}(|QC\rangle + |SE\rangle)$

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