

# Quantum Autumn School 2024

Recent developments in quantum technology are bringing the world closer to a new technological revolution – the advent of usable quantum computers able to provide enormous acceleration to important computational tasks. In coming years, quantum computing is expected to have a significant impact on many areas of research that can utilise computational modelling. Indeed, significant efforts and investments are currently underway in Europe to [bolster skills and capacity within quantum computing](#).

ENCCS joins forces again this year with [NordIQuEst](#), to deliver a three-day quantum autumn school in early December 2024! The school will also be visited by and contributed to by several companies who are developing in-house expertise in various application domains of quantum computing.

NordIQuEst brings together a consortium of seven partners from five Nordic and Baltic countries to connect world leading traditional HPC resources and quantum computers across national borders with the aim to establish a quantum computing platform customised to the needs of the region.

The quantum autumn school will be held in Stockholm in hybrid form, in-person and online.

## Prerequisites

For the hands-on tutorials, basic familiarity with Python and some experience working in a Unix environment are desirable. Some previous experience with quantum computing is expected.

## Setup

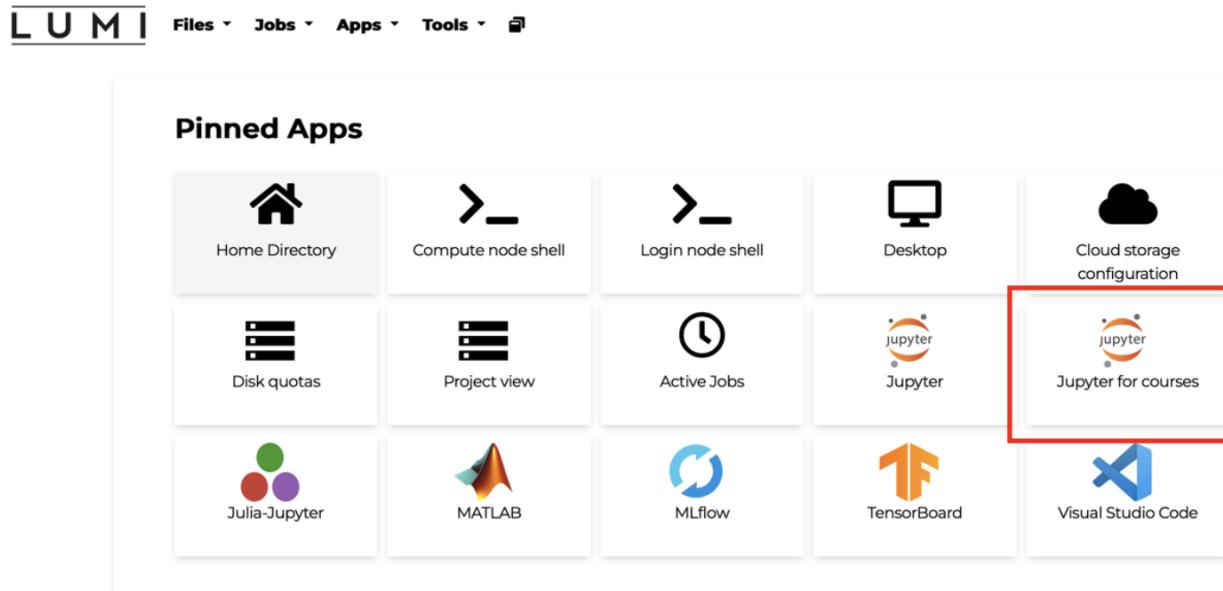
Participants can run the course notebooks either on the Helmi quantum computer through the LUMI Open OnDemand platform, or locally on their laptops. Please refer to step by step instructions below to get started!

## Using Helmi via the Custom Quantum Course Environment on LUMI Open OnDemand

A course environment has been made with preloaded modules ([qiskit-iqm](#)) and resource settings for connecting to Helmi. This section offers guidance on accessing this environment.

See also these  up-to-date instructions.

1. Log in to [LUMI Open OnDemand / web interface](#) with your MyCSC / Haka account
2. Click on [Jupyter for Courses](#)



The screenshot shows the LUMI Open OnDemand interface. At the top, there is a navigation bar with links for Files, Jobs, Apps, Tools, and Help. Below this is a section titled "Pinned Apps" containing a 3x5 grid of icons. The icons represent various services: Home Directory, Compute node shell, Login node shell, Desktop, Cloud storage configuration, Disk quotas, Project view, Active Jobs, Jupyter (which is highlighted with a red box), Julia-Jupyter, MATLAB, MLflow, TensorFlow, and Visual Studio Code.

3. You should get a prefilled page shown below, you can change a few variables such as your [working directory](#).

- Please note what you selected as your working directory when launching your Jupyter Notebook as this will determine where your file is saved.
- You can find more information about storage on LUMI here: [https://docs.lumi-supercomputer.eu/storage/#\\_tabbed\\_1\\_1](https://docs.lumi-supercomputer.eu/storage/#_tabbed_1_1)

**Apps**

Editors

- Visual Studio
- Code

Graphical applications

- Desktop

Servers

- MLflow

Julia-Jupyter

MATLAB

TensorBoard

Jupyter

Tools

- Compute node shell

Course environments

- Jupyter for courses

## Jupyter for courses

Interactive Jupyter session specifically for courses

Documentation

Reservation

quantum\_autumn\_school (active from 2024-12-02)

Project

project\_465001468 (LUST Training / 2024-12-2-4 Q1)

Course module

quantum-autumn-school

Working directory

/scratch/project\_465001468

Show custom resource settings

**Launch**

**Reset to default settings**

\* The Jupyter for courses session data for this session can be accessed under the [data root directory](#).

4. You also have the flexibility to adjust some resource settings. By clicking [show custom resource settings](#) (Please note that memory should be kept under 3GB).

Jupyter

Tools

> Compute node shell

Course environments

Jupyter for courses

Show custom resource settings

Partition  
q\_fiqci

## Resources

Number of CPU cores  
1

SMT is enabled for the selected partition. 2 threads per core will be allocated.

Memory (GB)  
2

Number of GPUs  
0

Time  
01:00:00  
d-hh:mm:ss, or hh:mm:ss

Launch

Reset to default settings

5. Once you are ready, click on Lunch.

Apps

Editors

Visual Studio Code

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Working directory

/scratch/project\_465001468

Show custom resource settings

**Launch**

**Reset to default settings**

\* The Jupyter for courses session data for this session can be accessed under the [data root directory](#).

6. Depending on the queue, it might take a few minutes before you can access your session.  
Once your session is ready, you should see a page like this:

Session was successfully deleted.



Home / My Interactive Sessions

**Apps**

- Editors
  - Visual Studio Code
- Graphical applications
- Desktop
- Servers
- MLflow
- Julia-Jupyter
- MATLAB
- TensorBoard
- Jupyter
- Tools

**Jupyter for courses (8310225)**    **1 node | 2 cores | Running**

**Host:** >\_nid002343    **Cancel**

**Created at:** 2024-10-31 15:02:55 UTC

**Time Remaining:** 59 minutes

**Session ID:** 23bec8a6-e750-4a35-b131-1e933ca2b72e

If you run into issues, please include the following log file in the support ticket:  
[output.log](#)

**Project:** project\_465001468  
**Partition:** q\_fiqci  
**Cores:** 2  
**Memory:** 2048M

**Connect to Jupyter**

7. Click on the big blue **Connect to Jupyter** button and it will launch a Jupyter notebook on a separate tab. Navigate to the new tab.

8. Now you can create and run codes on a jupyter notebook. A sample is shown in the image below.

The screenshot shows a Jupyter Notebook interface with a sidebar on the left containing a file browser and a list of files. The main area displays a code cell with Python code related to quantum computing using Qiskit and IQMProvider. The code includes imports for os, iqm.qiskit\_iqm, and qiskit, along with definitions for shots, qreg, circuit, and provider. It also shows the execution of the circuit, job submission, and printing of the result counts.

```
import os
from iqm.qiskit_iqm import IQMProvider
from qiskit import QuantumCircuit, QuantumRegister, transpile

shots = 1000 # Number of repetitions of the Quantum Circuit

qreg = QuantumRegister(2, "qb")
circuit = QuantumCircuit(qreg, name='Bell pair circuit')

circuit.h(qreg[0])
circuit.cx(qreg[1], qreg[0])
circuit.measure_all()

HELMI_CORTEX_URL = os.getenv('HELMI_CORTEX_URL')

provider = IQMProvider(HELMI_CORTEX_URL)
backend = provider.get_backend()

circuit_decomposed = transpile(circuit, backend=backend) ***

job = backend.run(circuit_decomposed, shots=shots)

job.status()

<JobStatus.DONE: 'job has successfully run'>

counts = job.result().get_counts()
print(counts)

{'00': 604, '01': 383, '10': 10, '11': 3}
```

9. You can save your notebooks like this:

- go to the top left corner, click on file
- click on `Save notebook` to save a specific file or `Save all` to save all file & changes

10. This environment gives each user 2 hours and 2GB per session. It is configured to load the `helmi_qiskit` (qiskit-iqm) module and connect to Helmi.

11. To add extra python packages use `pip install --user <package-name>`

## Useful Links

- [https://fiqci.fi/\\_posts/2024-08-23-Lumi\\_web\\_introduction](https://fiqci.fi/_posts/2024-08-23-Lumi_web_introduction)
- <https://docs.csc.fi/computing/quantum-computing/helmi/running-on-helmi/>

## Locally with your laptop

All of the course contents can be followed along locally on your laptop. Each tutorial will provide installation instructions.

If you already have a preferred way to manage Python versions and libraries, you can stick to that. If not, we recommend that you install Python3 and all libraries using `miniconda` a free minimal installer for the package, dependency and environment manager for `conda`.

Please follow the installation instructions on <https://docs.conda.io/en/latest/miniconda.html> to install Miniconda3.

Make sure that both Python and conda are correctly installed:

```
$ python --version
$ # should give something like Python 3.11.7
$ conda --version
$ # should give something like conda 24.9.2
```

A `requirements.txt` file is provided which contains all of the python packages to install a local software environment on your computer. Using this a `conda` environment can be created using the command:

```
$ conda create --name qas2024 -y python=3.11.7 pip
```

Which creates a new conda environment with Python 3.10 and `pip`. You can then activate it and install the python packages:

```
$ conda activate qas2024  
$ pip install -r requirements.txt
```

You can download the [requirements.txt](#) [here](#).

To get access to the notebooks covered during the school, you can clone the Git repository behind this lesson page:

```
$ git clone https://github.com/ENCCS/qas2024.git  
$ cd content/notebooks
```

Alternatively, you can navigate to <https://github.com/ENCCS/qas2024>, click the green “Code” button, and select “Download ZIP”.

## (Backup approach) [Notebooks.csc.fi](#)

CSC’s notebooks platform provides a preconfigured python environment and jupyter-lab server for running all of the jupyter notebooks shown in this course. **No setup is required** to run the notebooks.

Please find [instructions here](#).

## Welcome and introduction

### Agenda

Time	Topic
10:00-11:00	Arrival and registration
11:00-11:15	Welcome and introduction to NordIQuEst, ENCCS and SQS
11:15-12:00	HPC/QC integration and the NordIQuEst application library
12:00-13:00	Lunch
13:00-14:00	Introduction to the Helmi quantum computer
14:00-17:00	Intro to variational quantum algorithms: QAOA theory and hands-on
17:30-18:30	Study visit to quantum optics labs at Albanova University Center
18:30-21:00	Self-organised dinner in Stockholm

Time	Topic
09:00-12:00	Error correction – theory and hands-on
12:00-13:00	Lunch

Time	Topic
13:00-14:00	Quantum computing hardware
14:00-15:00	Quantum Monte Carlo and quantum finance
15:00-16:30	QMC and quantum finance tutorial
16:30-17:00	Overview of the Quantum Sweden Innovation Platform – QSIP
17:00-17:30	Post-quantum cryptography
18:00-21:00	QAS dinner, drinks and Pecha Kucha social event

Time	Topic
09:00-10:00	Solving Flight Scheduling Optimization using QAOA – Theory
10:00-11:00	Solving Flight Scheduling Optimization using QAOA – Hands-on
11:00-12:00	Quantum walk – seminar and demo
12:00-13:00	Lunch
13:00-14:00	Quantum chemistry and materials science seminar
14:00-15:00	Quantum chemistry and materials science hands-on
15:00-15:30	Quantum extreme learning machine: presentation and case study
15:30-16:15	Overview of the Tergite framework

## About ENCCS

GET  
MORE  
COMPUTING  
POWER

We help you gain access  
And use Europe's most  
powerful supercomputers  
for your projects **for free**

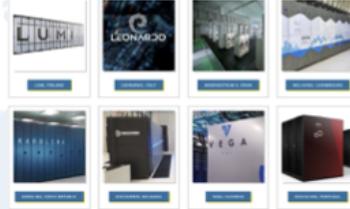
**SUPPORT**

- ✓ Software support
- ✓ HPC usage
- ✓ System access

**TRAINING**

- ✓ GPU/CPU coding
- ✓ HPC & HPDA
- ✓ AI/Deep Learning

**INDUSTRY**  
**PUBLIC ADMINISTRATION**  
**ACADEMIA**

[enccs.se](http://enccs.se) [info@enccs.se](mailto:info@enccs.se)









LINKÖPING UNIVERSITY



EuroHPC  
Joint Undertaking

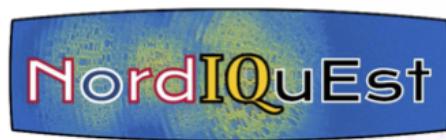


Swedish  
Research  
Council



VINNOVA  
Sweden's Innovation Agency

# About NordIQuEst



## The Nordic-Estonian Quantum Computing e-Infrastructure Quest

Quantum Autumn School 2024

2024-12-02



### NordIQuEst

**Partners:** Chalmers (SE), CSC (FI) , DTU (DK) , SINTEF (NO), SRL (NO), University of Tartu (EE), VTT (FI)

**Started:** 1.4.2022

#### Main goals and motivations

- Combine Nordic efforts for establishing and spreading know-how of quantum computing
- Provide a sustainable quantum computing platform **customised to the needs of the Nordic region**, free from outside commercial interests
- Collaboration within the Nordics crucial for reaching **critical mass**: Success requires collaboration across national borders – the QC know-how is dispersed across Europe

#### Combine several HPC resources and quantum computers

into a unified Nordic **HPC+QC** platform:

- QAL 9000 / Sweden (Chalmers)
- Helmi / Finland (VTT)
- LUMI / EuroHPC (hosted at CSC)
- eX3 / Norway (SRL)

1) Library of example algorithms

2) Unified access/project handling



## Integration of High Performance Computing and Quantum Computing

Slides

## Introduction to Helmi

Slides

# Tutorial - Introduction to Helmi

## Estimating the GHZ fidelity

### Preparing the GHZ circuit

```
# Importing the required modules
import os
import networkx as nx
import numpy as np
import itertools
from iqm.qiskit_iqm import IQMProvider
from iqm.qiskit_iqm.fake_backends import fake_adonis
from iqm.qiskit_iqm.iqm_transpilation import optimize_single_qubit_gates
from qiskit.compiler import transpile
from qiskit import QuantumCircuit, QuantumRegister, ClassicalRegister
from qiskit.visualization import plot_histogram
from qiskit.result import marginal_counts
from functools import reduce
import matplotlib.pyplot as plt
from scipy.optimize import minimize
```

```
# Set up the Helmi backend
HELMI_CORTEX_URL = os.getenv('HELMI_CORTEX_URL')
if not HELMI_CORTEX_URL:
    raise ValueError("Environment variable HELMI_CORTEX_URL is not set")

provider = IQMProvider(HELMI_CORTEX_URL)
backend = provider.get_backend() # fake_adonis.IQMFakeAdonis()
shots = 1024
n_qubits = 5
```

```
print(f"Native operations: {backend.operation_names}")
print(f"Number of qubits: {backend.num_qubits}")
print(f"Coupling map: {backend.coupling_map}")
```

```
G = nx.Graph()
G.add_edges_from(backend.coupling_map)
node_labels = {node: f"QB{node + 1}" for node in G.nodes}
nx.draw(G, labels=node_labels, node_color="skyblue", node_size=500, font_size=10)
```

Let us first prepare the GHZ circuit.

```

# Simple GHZ circuit
qubits: dict[str, QuantumRegister] = {i: QuantumRegister(1, "QB" + str(i)) for i in
range(1, 6)}
qc = QuantumCircuit(*qubits.values())
qc.h(qubits[3])
qc.cx(qubits[3], qubits[2])
qc.cx(qubits[3], qubits[4])
qc.cx(qubits[3], qubits[1])
qc.barrier()
qc.cx(qubits[3], qubits[5])
qc.measure_all() #expected equal majority counts of '00000' and '11111'
qc.draw(output="mpl")

```

Here is how the circuit will look like if we convert to Helmi's native gateset.

```

# Optimising for Helmi ->
initial_layout: list[int] = [backend.qubit_name_to_index(qubit) for qubit in
qubits.values()]
transpiled_circuit = transpile(qc, backend, initial_layout= initial_layout,
optimization_level=0)
transpiled_circuit.draw(output="mpl")

```

As the RZ gates commute with the CZ gates, and the measurement is not affected by the final RZ gate, we can optimise those away to decrease the number of gates we perform.

```

transpiled_circuit = optimize_single_qubit_gates(transpiled_circuit)
transpiled_circuit = transpile(transpiled_circuit, backend, optimization_level=0)
transpiled_circuit.draw(output="mpl")

```

```

job = backend.run(transpiled_circuit, shots=shots)
result = job.result()
counts = result.get_counts()

```

```
plot_histogram(counts)
```

```
print("Unmitigated GHZ fidelity =", (counts["00000"] + counts["11111"])/shots)
```

## Applying readout mitigation

The code used here was modified from [this tutorial](#) from NVIDIA.

To perform readout mitigation with the minimum number of jobs, we will prepare the  $\mid 00000 \rangle$  and  $\mid 11111 \rangle$  and see which states we actually measure.

First, we observe how the  $\mid 00000 \rangle$  state is not strongly affected by state preparation and measurement (SPAM) errors.

```
qubits: dict[str, QuantumRegister] = {i: QuantumRegister(1, "QB" + str(i)) for i in range(1, 6)}
qc_0s = QuantumCircuit(*qubits.values())
qc_0s.measure_all()

initial_layout: list[int] = [backend.qubit_name_to_index(qubit) for qubit in qubits.values()]
qc_0s = transpile(qc_0s, backend, initial_layout = initial_layout,
optimization_level=0)
```

```
job_0s = backend.run(qc_0s, shots=shots)
result_0s = job_0s.result()
counts_0s = result_0s.get_counts()
plot_histogram(counts_0s)
```

Next, we can observe how the  $\mid 11111 \rangle$  is much more strongly affected by SPAM error. Part of this comes from the  $\mid 1 \rangle$  state relaxing to  $\mid 0 \rangle$ , however, the exact ways in which Helmi is calibrated also plays an important role here.

```
qubits: dict[str, QuantumRegister] = {i: QuantumRegister(1, "QB" + str(i)) for i in range(1, 6)}
qc_1s = QuantumCircuit(*qubits.values())
for qubit in range(1,6):
    qc_1s.x(qubits[qubit])
qc_1s.measure_all()

initial_layout: list[int] = [backend.qubit_name_to_index(qubit) for qubit in qubits.values()]
qc_1s = transpile(qc_1s, backend, initial_layout = initial_layout,
optimization_level=0)
```

```
job_1s = backend.run(qc_1s, shots=shots)
result_1s = job_1s.result()
counts_1s = result_1s.get_counts()
plot_histogram(counts_1s)
```

```

local_states = ["0" * n_qubits, "1" * n_qubits]
results = {"00000": result_0s, "11111": result_1s}
for state in local_states:
    res = dict(list(results[state].get_counts().items()))
    print(f"{state} becomes {res}")

```

```

possible_counts = [
    dict(list(results[state].get_counts().items())) for state in local_states
]
matrices = []

for k in range(n_qubits):
    matrix = np.zeros([2, 2], dtype=float)
    marginalized_counts = []
    total_shots = []
    for i in local_states:
        marginal_cts = marginalized_counts(results[i], indices = [k]).get_counts()
        marginalized_counts.append(marginal_cts)
        total_shots.append(sum(marginal_cts.values()))

    # matrix[i][j] is the probability of counting i for expected j
    for i in range(2):
        for j in range(2):
            matrix[i][j] = marginalized_counts[j].get(str(i),
                0) / total_shots[j]
    matrices.append(matrix)

```

We have just prepared the confusion matrices for each of the  $\backslash(5\backslash)$  qubits using just  $\backslash(2\backslash)$  jobs, which can be used to calculate the confusion matrix for the whole system. This does assume that measurement or doing gates on one qubit does not affect other gates. We could create these confusion matrices using  $\backslash(2n_{\text{qubits}}\backslash)$ , or even more properly using  $\backslash(2^{n_{\text{qubits}}}\backslash)$  jobs, however, just these  $\backslash(2\backslash)$  jobs should suffice.

```

for i, matrix in enumerate(matrices):
    print(f"Confusion matrix for QB{i+1}:")
    print(matrix, "\n")

```

```

labels = list(map(list, itertools.product([0, 1], repeat=n_qubits)))
states = list(map(lambda label: "".join(map(str, label)), labels))

```

Let us have another look at the counts from the GHZ circuit. We will perform readout error mitigation on it, and hopefully, improve the GHZ state fidelity.

```
new_counts = dict(counts.items())
noisy_counts = np.array(
    [new_counts.get(state, 0) for i, state in enumerate(states)])
noisy_counts
```

```
def find_closest_distribution(empirical_dist):
    """
    Find the closest distribution to an empirical distribution by minimizing the L1
    norm.

    Args:
        empirical_dist: Empirical distribution that you want to find the closest
        distribution to.

    Returns:
        Closest distribution to `empirical_dist`
    """

    def objective(x):
        return np.linalg.norm(empirical_dist - x, ord=1)

    # Constraint: all elements of p must be positive, and the distribution must sum to
    1
    cons = (
        {
            "type": "ineq",
            "fun": lambda p: p
        },
        {
            "type": "eq",
            "fun": lambda p: np.sum(p) - 1
        },
    )
    bnds = [(0, 1) for _ in range(len(empirical_dist))]
    initial_value = np.random.uniform(size=len(empirical_dist))

    res = minimize(
        objective,
        initial_value,
        method="SLSQP",
        options={"maxiter": 1000},
        bounds=bnds,
        constraints=cons,
    )

    return res.x
```

```

def get_counts_from_distribution(n_qubits, size, dist):
    """
    Generates samples based on a given distribution and returns the counts of each
    sample value.

    Args:
        n_qubits: The number of qubits in the quantum circuit.
        dist: The probability distribution from which samples are drawn.

    Returns:
        An array of counts for each possible value in the distribution. The array has a
        length of  $2^{n_qubits}$ .
    """
    samples = np.random.choice(np.arange(2**n_qubits), size=size, p=dist)
    values, counts = np.unique(samples, return_counts=True)
    res = np.zeros(2**n_qubits, dtype=int)
    res[values] = counts
    return res

```

```

# Function to draw the confusion matrix
def plot_cmat(mat):
    fig, ax = plt.subplots()
    n = len(mat)
    im2 = ax.matshow(mat, cmap=plt.cm.Reds, vmin=0, vmax=1.0)
    ax.set_yticks(np.arange(n))
    ax.set_xticks(np.arange(n))
    ax.set_yticklabels(n * [""])
    ax.set_xticklabels(n * [""])
    ax.set_title(r"Confusion Matrix", fontsize=16)
    ax.set_xlabel("Prepared State")
    ax.xaxis.set_label_position("top")
    ax.set_ylabel("Measured State")
    fig.colorbar(im2, ax=ax)
    plt.show()

```

First, we invert the confusion matrix for each individual qubit. Next, we approximate the inverse confusion matrix for Helmi using the tensor product. Now, we can simply apply this to our “noisy” results and we should have mitigated the effects of the readout errors.

As this is a mathematical operation, we can end up with negative counts, which lack any physical meaning. We can find another distribution with all positive values that is similar to our mitigated distribution. We sample this distribution probabilistically to obtain our corrected counts.

```

pinv_confusion_matrices = [np.linalg.pinv(m) for m in matrices]
A_pinv = reduce(np.kron, pinv_confusion_matrices)
mitigated = np.array(np.dot(A_pinv, noisy_counts), dtype=int)
print(f"Mitigated counts:\n{mitigated}")

if not np.all(mitigated >= 0):
    positive_dist = find_closest_distribution(mitigated / shots)
    mitigated = get_counts_from_distribution(n_qubits, shots, positive_dist)
    print(f"\nCorrected for negative counts:\n{mitigated}")

A_joint = reduce(np.kron, matrices)
plot_cmat(A_joint)

```

As we can see, the mitigated fidelity is higher than the unmitigated fidelity, at the cost of two more jobs run.

```
plot_histogram([counts, dict({bin(i)[2:]: x for i, x in enumerate(mitigated)})), legend=["Unmitigated", "Mitigated"])
```

```
print("Unmitigated GHZ fidelity =", (counts["00000"] + counts["11111"])/shots)
print("Corrected GHZ fidelity =", (mitigated[0] + mitigated[-1])/shots)
```

## Multiple Quantum Coherences

### Theory

[Multiple Quantum Coherences](#) (MQC) offers an alternative way to estimate the GHZ fidelity. It allows us to calculate a lower and upper bound on the GHZ fidelity, as well as calculating the exact GHZ fidelity if run alongside a GHZ circuit.

MQC works by utilising phase kickback, a highly versatile tool used in many algorithms to “kick” a phase from a target qubit “back” to a control qubit. First, we prepare a  $(N)$ -qubit GHZ state, and then we apply a phase  $\phi$  to all  $N$  qubits. Then, we “undo” the GHZ state, and this “kicksback” the phase to the control qubit, applying a phase shift of  $\phi$  to the control qubit.

To help explain this more easily, I will quote the paper directly here.

- Starting from the  $|N\rangle$ -qubit ground state:  $|\text{GS}\rangle = |000..00\rangle$ , apply a Hadamard gate on qubit  $|0\rangle$  followed by a sequence of CX gates. Ideally this brings the system into the GHZ state:  $|\text{GHZ}\rangle = \frac{1}{\sqrt{2}}(|000..00\rangle + e^{i\phi}|111..11\rangle)$
- Apply a collective rotation given by the unitary  $U_{\{\phi\}}$  on all qubits. This amounts to adding a phase  $e^{iN\phi}$  to the GHZ state:  $|\text{GHZ}\rangle = \frac{1}{\sqrt{2}}(|000..00\rangle + e^{-iN\phi}|111..11\rangle)$
- Disentangle the GHZ state by performing the CX gate sequence in reverse order. The amplified phase is mapped onto qubit  $|0\rangle$ :  $\frac{1}{\sqrt{2}}(|000..00\rangle + e^{-iN\phi}|111..11\rangle) \otimes |00..00\rangle$
- Read out the amplified phase by measuring the probability of the system returning to its initial state:  $|\text{GS}\rangle$ . The measured signal of this protocol is given by  $S_{\{\phi\}} = |\langle 000..00 | U^{\dagger} | \text{GHZ} \rangle|$  where  $U_{\{\text{GHZ}\}} = U_{\{\text{CZ}\}} H_0$ , and  $\rho_{\{\phi\}} = U_{\{\phi\}} \rho U_{\{\phi\}}^{\dagger}$ .

If we run this on a noiseless quantum computer, we expect  $S_{\{\phi\}} = \frac{1}{2}(1 + \cos(N\phi))$ . We can then measure  $S_{\{\phi\}}$  for multiple angles  $\{\phi\}$ , and then perform a Fourier transform to find which frequency our  $S_{\{\phi\}}$  actually corresponds to.

$$[I_q=\mathcal{N}^{-1}|\sum_\phi e^{i q \phi} S_\phi|]$$

Ideally, it should be completely dependent on  $N$ , and have no reliance on any of the other frequencies - however, due to noise, we shall get a spread of frequencies with varying amplitudes. We can then use these to estimate the lower and upper bounds of the GHZ fidelity.

$$[2 \sqrt{I_N} \leq F \leq \sqrt{I_0 / 2} + \sqrt{I_N}]$$

## Preparing the MQC circuits

First, let us define a parametrised circuit for the MQC experiment. Developed based on the original paper.

```

def mqc_circuit(angle: float):
    qubits: dict[str, QuantumRegister] = {i: QuantumRegister(1, "QB" + str(i)) for i in range(1, 6)}
    mqc = QuantumCircuit(*qubits.values())
    mqc.h(qubits[3])
    mqc.cx(qubits[3], qubits[2])
    mqc.cx(qubits[3], qubits[4])
    mqc.cx(qubits[3], qubits[1])
    mqc.cx(qubits[3], qubits[5])
    for qubit in qubits.values():
        mqc.x(qubit) # We will comment out this line later
        mqc.rz(angle, qubit)
    mqc.cx(qubits[3], qubits[5])
    mqc.cx(qubits[3], qubits[2])
    mqc.cx(qubits[3], qubits[4])
    mqc.cx(qubits[3], qubits[1])
    mqc.h(qubits[3])
    mqc.measure_all()
    return mqc

```

Next, we define which  $\phi$  to sweep over, and how many shots to execute for each circuit. We need a minimum of 12 experiments here, so that our Fourier transform can detect frequencies upto 6.

```

n_exp = 2 * n_qubits + 2
angles = [2 * np.pi * j / n_exp for j in range(n_exp)]
shots = 16_384

```

The parameterized circuits are collected in a list `mqc_circuits`.

```

mqc_circuits = []

for angle in angles:
    mqc = mqc_circuit(angle)
    mqc_circuits.append(mqc)

```

Let us observe how the untranspiled circuit looks.

```
mqc_circuits[1].draw(output='mpl')
```

Before running, we transpile each circuit to the native gate set and map the logical qubits to the physical qubits.

```

initial_layout: list[int] = [backend.qubit_name_to_index(qubit) for qubit in ["QB1",
"QB2", "QB3", "QB4", "QB5"]]

fidelity_circuits = transpile(mqc_circuits, backend, initial_layout=initial_layout,
optimization_level=2)
fidelity_circuits = optimize_single_qubit_gates(fidelity_circuits)
fidelity_circuits = transpile(fidelity_circuits, backend, initial_layout=
initial_layout, optimization_level=0)

```

Let's have a look at the transpiled circuit.

```
fidelity_circuits[1].draw(output='mpl')
```

## With Ideal Backend

```
fake_backend = fake_adonis.IQMFakeAdonis()
```

```
fake_jobs = fake_backend.run(fidelity_circuits, shots=shots)
```

```
fake_results = fake_jobs.result()
fake_counts = fake_results.get_counts()
```

```
plot_histogram(fake_counts[1])
```

After running the circuit, we should only have the states  $\lvert 00000 \rangle$  and  $\lvert 00100 \rangle$ .

```
fake_outcomes = [fake_count['00000'] / (fake_count['00000'] + fake_count['00100']) for
fake_count in fake_counts] # (fake_count['00000'] + fake_count['00100'])
```

```

fig, ax = plt.subplots(1, 1, figsize=(10, 6))
all_angles = np.linspace(0, 2 * np.pi, 10_000)
expected_fidelity = [(1 + np.cos(n_qubits * j)) / 2 for j in all_angles]
ax.plot(all_angles, expected_fidelity, '-', label='Expected', color='black')
ax.plot(all_angles, fake_outcomes, 'o', label='Fake', color='red')
ax.set_xlabel('Angle  $\phi$ ')
ax.set_ylabel('$S_\phi$')
ax.legend(loc='lower right')
plt.show()

```

```

I_0 = 0
I_n = 0
for i, angle in enumerate(angles):
    I_0 += fake_outcomes[i]
    I_n += np.exp(1j * n_qubits * angle) * fake_outcomes[i]
I_0 = np.abs(I_0 / n_exp)
I_n = np.abs(I_n / n_exp)
print("Lower bound for MQC fidelity = " + str(2 * np.sqrt(I_n)))
print("Upper bound for MQC fidelity = " + str(np.sqrt(I_0 / 2) + np.sqrt(I_n)))

```

## Simulations vs Actual Hardware

Let us now rerun this, but comment out the `mqc.x(qubit)` line at the very start of the circuit. Similarly, try changing the `n_exp` to a higher value. What changes do you observe?

► Spoiler warning

### With Helmi Backend

```
jobs = backend.run(fidelity_circuits, shots=shots)
```

```
jobs.status()
```

```
mqc_results = jobs.result()
mqc_counts = mqc_results.get_counts()
```

```
mqc_results.timestamps
```

```
plot_histogram(mqc_counts[1])
```

```
outcomes = [mqc_count['00000'] / (mqc_count['00000'] + mqc_count['00100']) for
mqc_count in mqc_counts] # (mqc_count['00000'] + mqc_count['00100'])
```

```

fig, ax = plt.subplots(1, 1, figsize=(10, 6))
all_angles = np.linspace(0, 2 * np.pi, 10_000)
expected_fidelity = [(1 + np.cos(n_qubits * i)) / 2 for i in all_angles]
ax.plot(angles, fake_outcomes, 'o', label='Simulated', color='red')
ax.plot(angles, outcomes, 'o', label='Experimental', color='blue')
ax.plot(all_angles, expected_fidelity, '-', label='Expected', color='black')
ax.set_xlabel('Angle $(\phi)$')
ax.set_ylabel('$S_{\phi}$')
ax.legend(loc='lower right')
plt.show()

```

```

I_0 = 0
I_n = 0
for i, angle in enumerate(angles):
    I_0 += outcomes[i]
    I_n += np.exp(1j * n_qubits * angle) * outcomes[i]
I_0 = np.abs(I_0 / n_exp)
I_n = np.abs(I_n / n_exp)
print("Lower bound for MQC fidelity = " + str(2 * np.sqrt(I_n)))
print("Upper bound for MQC fidelity = " + str(np.sqrt(I_0 / 2) + np.sqrt(I_n)))

```

What we observe is that removing the  $\langle X \rangle$  gates results in a noticeable phase shift in the results, even though it should technically not matter. The presenter's hypothesis is that this phenomenon is related to qubit relaxation, which causes the state  $|\text{mid } !00000\rangle$  to dominate over  $|\text{mid } !11111\rangle$ , even though they should be even. Consequently, applying the  $\langle X \rangle$  gates inverts this distribution, and further relaxation should lead to a more balanced ratio of these states. An analogy can be drawn to the Hahn-Echo experiment, where a  $\langle Z \rangle$  gate can help cancel out some of the dephasing effects.

Furthermore, running more experiments provides a higher fidelity. The presenter hypothesises that this can be attributed to the noise after the Fourier transform being spread out over more frequencies, leading to improved results. We are not changing the experiment - just collecting additional data to help average out errors.

## Introduction to variational quantum algorithms: VQE and QAOA

 [Slides](#)

# Tutorial - Variational Quantum Algorithms

## Exercise 1: Max 4-Cut

### 1. Problem Definition

The Max 4-Cut problem is defined on a graph  $G = (V, E)$ , with a corresponding problem Hamiltonian given by:

$$H_P = \sum_{e \in E} w_e H_e, ]$$

where  $w_e$  represents the weight of edge  $e \in E$ , and  $H_e$  is the Hamiltonian associated with that edge.

## 2. Generic Graph Problem

In this exercise, the class `GraphProblem` from the `qaoa.problems` module is used to define the problem. The class requires two inputs:

1. A networkx graph  $(G)$ ,
2. The number of qubits per vertex/node.

The `GraphProblem` class includes a method to create a quantum circuit for implementing the phase separating Hamiltonian  $(e^{-i\theta} H_P)$ .

## 3. Specific problem implementation

However, `GraphProblem` relies on an abstract method, `create_edge_circuit`, which must be implemented to define the phase separating Hamiltonian  $(H_e)$  for an edge.

```

import networkx as nx
import numpy as np

from qaoa.problems import GraphProblem

from qiskit import QuantumCircuit
from qiskit.circuit.library import PhaseGate

class Max4Cut(GraphProblem):
    def __init__(self, G: nx.Graph) -> None:

        N_qubits_per_node = 2
        super().__init__(G, N_qubits_per_node)

        # each color is associated with a bitstring combination
        self.colors = {
            "color1": ["00"],
            "color2": ["01"],
            "color3": ["10"],
            "color4": ["11"],
        }

        # Create a dictionary to map each index to its corresponding set
        self.bitstring_to_color = {}
        for key, indices in self.colors.items():
            for index in indices:
                self.bitstring_to_color[index] = key

    def create_edge_circuit(self, theta):
        qc = QuantumCircuit(2 * self.N_qubits_per_node)

        """
        -----#
        # implement the circuit#
        -----#"

        return qc
    def create_edge_circuit_fixed_node(self, theta):
        pass

```

Show the circuit for one edge

```

test = Max4Cut(nx.Graph([(0, 1, {"weight": 1.0})]))
test.create_edge_circuit(0.2).draw("mpl")

```

Graph contains nodes with one or zero edges. These can be removed to reduce the size of the problem.

#### 4. Graph instance

Let's start by defining a Graph with 10 nodes

```

import matplotlib.pyplot as plt
# Create a graph with 8 nodes
G = nx.Graph()
# Add nodes
G.add_nodes_from(range(8))
# Add edges (example connections)
edges = [
    (0, 1), (0, 2), (1, 3), (1, 4), (2, 4), (2, 5),
    (3, 6), (4, 7), (5, 6), (6, 7), (7, 3), (3, 5)
]
G.add_edges_from(edges)

# Draw the graph
plt.figure(figsize=(3,3))
nx.draw(G, with_labels=True, pos = nx.circular_layout(G))

```

## 5. Problem instance

Now we can instantiate a Max4Cut problem with the graph and create and draw the resulting circuit for the phase separating Hamiltonian. Observe that there is one circuit per edge in the graph.

```

max4cut = Max4Cut(G)
max4cut.create_circuit()
max4cut.circuit.draw("mpl")

```

## 5. QAOA instance

We create a QAOA instance using

- as initial state we use the  $\langle + \rangle$  state,
- as mixing operator the  $X$ -mixer, and
- as phase separation operator our newly created max4cut instance.

```

from qaoa import QAOA
from qaoa.initialstates import Plus
from qaoa.mixers import X
from qiskit_algorithms.optimizers import COBYLA

settings = {"maxiter": 100, "tol": 1e-3, "rhobeg": 0.1}
optimizer = [COBYLA, settings.copy()]

qaoa_k4 = QAOA(initialstate=Plus(), problem=max4cut, mixer=X(), optimizer=optimizer)

```

## 5. Run QAOA

- Sample the cost landscape and plot it.

```

from mpl_toolkits.axes_grid1 import make_axes_locatable
def plot_E(qaoa_instance, fig=None):
    angles = qaoa_instance.landscape_p1_angles
    dgamma = (qaoa_instance.gamma_grid[1]-qaoa_instance.gamma_grid[0])/2
    dbeta = (qaoa_instance.gamma_grid[1]-qaoa_instance.gamma_grid[0])/2
    extent = [
        angles["gamma"][0]-dgamma,
        angles["gamma"][1]+dgamma,
        angles["beta"][0]-dbeta,
        angles["beta"][1]+dbeta,
    ]
    return __plot_landscape(qaoa_instance.exp_landscape(), extent, fig=fig)

def __plot_landscape(A, extent, fig):
    if not fig:
        fig = plt.figure(figsize=(6, 6), dpi=80, facecolor="w", edgecolor="k")
    _ = plt.xlabel(r"$\gamma$")
    _ = plt.ylabel(r"$\beta$")
    ax = fig.gca()
    _ = plt.title("Expectation value")
    im = ax.imshow(A, interpolation="nearest", origin="lower", extent=extent)
    divider = make_axes_locatable(ax)
    cax = divider.append_axes("right", size="5%", pad=0.05)
    _ = plt.colorbar(im, cax=cax)

qaoa_k4.sample_cost_landscape( angles={"gamma": [0, np.pi, 20], "beta": [0, np.pi, 20]} )
plot_E(qaoa_k4)

```

```

2024-12-02 13:36:14 [info      ] Calculating energy landscape for depth p=1...
file=qaoa.qaoa func=sample_cost_landscape
2024-12-02 13:36:15 [info      ] Executing sample_cost_landscape file=qaoa.qaoa
func=sample_cost_landscape
2024-12-02 13:36:15 [info      ] parameters: 2                      file=qaoa.qaoa
func=sample_cost_landscape
2024-12-02 13:36:15 [info      ] Done execute                         file=qaoa.qaoa
func=sample_cost_landscape
2024-12-02 13:36:22 [info      ] Done measurement                     file=qaoa.qaoa
func=sample_cost_landscape
2024-12-02 13:36:22 [info      ] Calculating Energy landscape done file=qaoa.qaoa
func=sample_cost_landscape

```

- Use a local optimizer to find the optimum for  $\langle p=1 \rangle$ . We converge quickly to the local optimum.

```

qaoa_k4.optimize(depth=1)

fig = plt.figure(figsize=(6, 6))
gamma = []
beta = []
angles = qaoa_k4.optimization_results[1].angles
for i in range(len(angles)):
    gamma.append(angles[i][0])
    beta.append(angles[i][1])
plt.plot(gamma, beta, "x-k")
plt.plot(gamma[0], beta[0], "wo")
plt.plot(gamma[-1], beta[-1], "or")
plot_E(qaoa_k4, fig=fig)

```

```

2024-12-02 13:36:23 [info      ] cost(depth 1 = -10.727539062500002 file=qaoa.qaoa
func=optimize

```

- Run QAOA up to depth  $\backslash(p=5\backslash)$ . We can see how the approximation ratio increases with  $\backslash(p\backslash)$ .

```

maxdepth = 5
qaoa_k4.optimize(depth=maxdepth)

p = np.arange(1, len(np.array(qaoa_k4.get_Exp())) + 1)
maxval=12
plt.plot(p, -np.array(qaoa_k4.get_Exp()) / maxval, marker="x")
plt.xlabel("depth")
plt.ylabel("Approx. ratio")
plt.title("QAOA Max 4-Cut")
plt.ylim([0, 1])
plt.show()

```

```

2024-12-02 13:36:25 [info      ] cost(depth 2 = -11.204101562499991 file=qaoa.qaoa
func=optimize
2024-12-02 13:36:29 [info      ] cost(depth 3 = -11.468749999999988 file=qaoa.qaoa
func=optimize
2024-12-02 13:36:34 [info      ] cost(depth 4 = -11.54296875      file=qaoa.qaoa
func=optimize
2024-12-02 13:36:39 [info      ] cost(depth 5 = -11.604492187500007 file=qaoa.qaoa
func=optimize

```

## Exercise 2: Max 3-Cut using the full Hilbert space

- Find the circuit with pen and paper

Given  $\backslash(\operatorname{operatorname}{clr}^3_{< 3}\backslash)$  we now want to devide the states into the following sets (containing power of two states),

- set one consist of  $\backslash(\ket{1011}, \ket{1110}\backslash)$ , and
- set two consists of  $\backslash(\ket{0000}, \ket{0101}, \ket{1010}, \ket{1111}, \backslash)$ .

Apply Theorem 1 from [1] and work out what the circuit for an edge should look like, using pen and paper.

Are there any gates that cancel?

## 2. Specific problem implementation

```
class Max3CutFullH(GraphProblem):
    def __init__(self, G: nx.Graph) -> None:
        N_qubits_per_node = 2
        super().__init__(G, N_qubits_per_node)

        self.colors = {
            "color1": ["00"],
            "color2": ["01"],
            "color3": ["10", "11"]
        }
        # Create a dictionary to map each index to its corresponding set
        self.bitstring_to_color = {}
        for key, indices in self.colors.items():
            for index in indices:
                self.bitstring_to_color[index] = key

    def create_edge_circuit(self, theta):
        qc = QuantumCircuit(2 * self.N_qubits_per_node)

        """
        implement the circuit
        """

        return qc

    def create_edge_circuit_fixed_node(self, theta):
        pass
```

```
test = Max3CutFullH(nx.Graph([(0, 1, {"weight": 1.0})]))
test.create_edge_circuit(0.2).draw("mpl")
```

Graph contains nodes with one or zero edges. These can be removed to reduce the size of the problem.

## 3. Run QAOA

```
qaoa_k3_fullH = QAOA(initialstate=Plus(), problem=Max3CutFullH(G), mixer=X(),
optimizer=optimizer)
```

```
qaoa_k3.fullH.optimize(depth=1, angles={"gamma": [0, np.pi, 20], "beta": [0, np.pi, 20]}).
```

```
fig = plt.figure(figsize=(6, 6))
gamma = []
beta = []
angles = qaoa_k3.fullH.optimization_results[1].angles
for i in range(len(angles)):
    gamma.append(angles[i][0])
    beta.append(angles[i][1])
plt.plot(gamma, beta, "x-k")
plt.plot(gamma[0], beta[0], "wo")
plt.plot(gamma[-1], beta[-1], "or")
plot_E(qaoa_k3.fullH, fig=fig)
```

```
2024-12-02 13:36:39 [info] Calculating energy landscape for depth p=1...
file=qaoa.qaoa func=sample cost landscape
```

```
IndexError                                     Traceback (most recent call last)
Cell In[18], line 1
----> 1 qaoa_k3.fullH.optimize(depth=1, angles={"gamma": [0, np.pi, 20], "beta": [0, np.pi/2, 10]}).
      3 fig = plt.figure(figsize=(6, 6))
      4 gamma = []
```

```
File c:\Users\rubenb\OneDrive - SINTEF\Desktop\test_qas\.venv\Lib\site-packages\qaoa\qaoa.py:451, in QAOA.optimize(self, depth, angles)
    449 if self.current_depth == 0:
    450     if self.Exp_sampled_p1 is None:
--> 451         self.sample_cost_landscape(angles=angles)
    452     ind_Emin = np.unravel_index(
    453         np.argmin(self.Exp_sampled_p1, axis=None), self.Exp_sampled_p1.shape
    454     )
    455     angles0 = np.array(
    456         (self.gamma_grid[ind_Emin[1]], self.beta_grid[ind_Emin[0]]),
    457     ).
```

```
File c:\Users\rubenb\OneDrive - SINTEF\Desktop\test_qas\.venv\Lib\site-packages\qaoa\qaoa.py:352, in QAOA.sample_cost_landscape(self, angles)
    350     logger.info("Done measurement").
    351 else:
--> 352     self.createParameterizedCircuit(depth)
    353     gamma = [None] * angles["beta"][2] * angles["gamma"][2].
    354     beta = [None] * angles["beta"][2] * angles["gamma"][2].
```

```
File c:\Users\rubenb\OneDrive - SINTEF\Desktop\test_qas\.venv\Lib\site-packages\qaoa\qaoa.py:248, in QAOA.createParameterizedCircuit(self, depth)
    245 for d in range(depth):
    246     self.gamma_params[d] = Parameter("gamma_" + str(d)).
    247     tmp_circuit = self.problem.circuit.assign_parameters(
--> 248         {self.problem.circuit.parameters[0]: self.gamma_params[d]},.
    249         inplace=False,
    250     )
    251     self.parameterized_circuit.compose(tmp_circuit, inplace=True).
    253 if self.usebarrier:
```

```
File c:\Users\rubenb\OneDrive - SINTEF\Desktop\test_qas\.venv\Lib\site-packages\qiskit\circuit\parametertable.py:241, in ParameterView.__getitem__(self, index)
    239 def __getitem__(self, index):
    240     """Get items."""
--> 241     return self.data[index].
```

```
IndexError: list index out of range
```

```
maxdepth = 5
qaoa_k3.fullH.optimize(depth=maxdepth)

p = np.arange(1, len(np.array(qaoa_k3.fullH.get_Exp().))+1)
maxval=12
plt.plot(p, -np.array(qaoa_k3.fullH.get_Exp()) / maxval, marker="x")
plt.xlabel("depth")
plt.ylabel("Approx. ratio")
plt.title("QAOA Max 3-Cut using the full Hilber space")
plt.ylim([0, 1])
plt.show()
```

## Exercise 3: Max 3-Cut using subspaces

1. Show that the Grover mixer is valid using pen and paper

$$\begin{aligned} U_m(\beta) &= e^{-i\beta} |E\rangle\langle E|, \quad \text{where } U_S |0\rangle = |E\rangle := \\ &\quad \frac{1}{\sqrt{|B|}} \sum_{x \in B} |x\rangle \end{aligned}$$

2. Create circuit for Grover mixer

Using the package `qaoa` create a Grover mixer for  $(|000\rangle + |011\rangle + |111\rangle)/\sqrt{3})$ . For this we import the following:

```
from qaoa.initialstates import LessThanK
ltk3 = LessThanK(3)
ltk3.create_circuit()
ltk3.circuit.draw("mpl")
```

Create a circuit for  $(|000\rangle + |011\rangle + |111\rangle)^{\otimes 3}$ . For this we can use the Tensor class.

```
from qaoa.initialstates import Tensor
numNodes = 3
phi0 = Tensor(ltk3, numNodes)
phi0.create_circuit()
phi0.circuit.draw("mpl")
```

create the Grover mixer for  $(|000\rangle + |011\rangle + |111\rangle)^{\otimes 3}$ .

```
from qaoa.mixers import Grover
grover =
" -----"
" define the Grover mixer"
" -----"
```

3. Numerically test that the Grover mixer is valid

Show that we have a valid mixer by plotting the overlap  $\langle z_1 | U_M(\beta) | z_2 \rangle$ , depending on  $(\beta)$ :

- Pick two feasible computational basis states  $(|z_1\rangle \neq |z_2\rangle)$  and see that the overlap is nonzero for some values of  $(\beta)$ .
- Pick a feasible and an infeasible state, and show that the overlap is always zero

Let's start by importing the necessary things, before we can do some plots.

```

import numpy as np
import matplotlib.pyplot as pl
from tqdm import tqdm
from qiskit.aer import Aer
from qiskit import (
    QuantumCircuit,
    QuantumRegister,
    ClassicalRegister,
    transpile,
)
backend=Aer.get_backend("qasm_simulator")

```

```

overlap = []
betavalues = np.linspace(0,2*np.pi,50)
shots=10**5
for beta in tqdm(betavalues):
    q = QuantumRegister(numNodes*2)
    c = ClassicalRegister(numNodes*2)
    circuit = QuantumCircuit(q,c)
    " -----"
    " implement a circuit for <z_1|"
    " -----"
    circuit.barrier()
    circuit.append(grover.circuit,q)
    circuit.measure(q,c)
    circuit = transpile(circuit, backend)

    # Assign float values to the parameters
    parameters = list(circuit.parameters)
    parameter_values = [beta]
    bound_circuit = circuit.assign_parameters(dict(zip(parameters, parameter_values))).

    # Run the job
    job = backend.run(bound_circuit, shots=shots)
    counts = job.result().get_counts()
    overlap.append(counts.get(
        " -----"
        " choose string for |z_2>"
        " -----",
        0.)/shots))

# bound_circuit.draw('mpl')
pl.plot(betavalues, overlap)

```

#### 4. Problem class

```

class Max3Cut(GraphProblem):
    def __init__(self, G: nx.Graph) -> None:
        N_qubits_per_node = 2
        super().__init__(G, N_qubits_per_node)

        # each color is associated with a bitstring combination
        self.colors = {
            "color1": ["00"],
            "color2": ["01"],
            "color3": ["10"]
        }
        # Create a dictionary to map each index to its corresponding set
        self.bitstring_to_color = {}
        for key, indices in self.colors.items():
            for index in indices:
                self.bitstring_to_color[index] = key

    def create_edge_circuit(self, theta):
        qc = QuantumCircuit(2 * self.N_qubits_per_node)

        qc.cx(0, 2)
        qc.cx(1, 3)
        qc.x([2, 3])
        phase_gate = PhaseGate(-theta).control(1)
        qc.append(phase_gate, [2, 3])
        qc.x([2, 3])
        qc.cx(1, 3)
        qc.cx(0, 2)

    return qc

    def create_edge_circuit_fixed_node(self, theta):
        # we will not use this function, so we can skip it
        pass

```

## 5. Initial state class

To run QAOA we need to implement the `InitialState` class that creates a Tensor of  $\langle \text{tk3} |$  state, which can be done just as above

```

from qaoa.initialstates import InitialState
class Max3CutInitialState(InitialState):

    def create_circuit(self) -> None:

        numQubitsPerNode = 2
        self.num_V = int(self.N_qubits/numQubitsPerNode)

        tg =
        """
        " -----"
        " define the initial state"
        " -----"

        tg.create_circuit()
        self.circuit = tg.circuit

```

## 6. Mixer class

We also need to implement the `Mixer` class that creates a Tensor of Grover mixer, which can be done just as above

```

from qaoa.mixers import Mixer
class Max3CutGrover(Mixer):

    def create_circuit(self) -> None:

        numQubitsPerNode = 2
        self.num_V = int(self.N_qubits/numQubitsPerNode)

        gm =
        """
        " -----"
        " define the Box Grover mixer"
        " -----"

        gm.create_circuit()
        self.circuit = gm.circuit

```

## 7. Run QAOA

create an instance of QAOA and plot the resulting landscape

```

qaoa_k3_subH = QAOA(
    initialstate=Max3CutInitialState(),
    problem=Max4Cut(G),
    mixer=Max3CutGrover(),
    optimizer=optimizer)

qaoa_k3_subH.optimize(depth=1, angles={"gamma": [0, 2*np.pi, 20], "beta": [0, 2*np.pi, 20]}).

fig = plt.figure(figsize=(6, 6))
gamma = []
beta = []
angles = qaoa_k3_subH.optimization_results[1].angles
for i in range(len(angles)):
    gamma.append(angles[i][0])
    beta.append(angles[i][1])
plt.plot(gamma, beta, "x-k")
plt.plot(gamma[0], beta[0], "wo")
plt.plot(gamma[-1], beta[-1], "or")
plot_E(qaoa_k3_subH, fig=fig)

```

## 8. Comparison for MAX 3-CUT

Compare the convergence for the method using the full Hilbert space and the subspace encoding up to d

```

maxdepth = 5
qaoa_k3_subH.optimize(depth=maxdepth)

p = np.arange(1, len(np.array(qaoa_k3_subH.get_Exp())) + 1)
maxval=12
plt.plot(p, -np.array(qaoa_k3_fullH.get_Exp()) / maxval, marker="x", label="full H")
plt.plot(p, -np.array(qaoa_k3_subH.get_Exp()) / maxval, marker="x", label="sub H")
plt.xlabel("depth")
plt.ylabel("Approx. ratio")
plt.legend()
plt.title("QAOA Max 3-Cut comparison")
plt.ylim([0, 1])
plt.show()

```

For more info you can look into the following reference.

## References

[1] Fuchs, Franz G., Ruben P. Bassa, and Frida Lien. “Encodings of the weighted MAX k-CUT on qubit systems.” Preprint arXiv 2024. [arXiv:2411.08594](https://arxiv.org/abs/2411.08594)

[2] Fuchs, Franz G., Ruben P. Bassa. “LX-mixers for QAOA: Optimal mixers restricted to subspaces and the stabilizer formalism.” Quantum 8 (2024): 1535. [10.22331/q-2024-11-25-1535](https://doi.org/10.22331/q-2024-11-25-1535)

[3] Bärtschi, Andreas, and Stephan Eidenbenz. "Grover mixers for QAOA: Shifting complexity from mixer design to state preparation." In 2020 IEEE International Conference on Quantum Computing and Engineering (QCE), pp. 72-82. IEEE, 2020. [10.1109/QCE49297.2020.00020](https://doi.org/10.1109/QCE49297.2020.00020)

## Introduction to Quantum Error Correction

 Slides

## Tutorial - MAP Decoding Exercise

The goal of MAP decoding is to find the most probable error vector  $e$  given the syndrome  $s$ . We optimize:

```
max P(e | s)
```

Given the constraints from the parity-check matrix  $H$ :

```
H @ e = s (mod 2)
```

Throughout the exercise we will assume that errors are iid with  $p < 1/2$ .

### 1. MAP Decoding for [7,4] Hamming code

```
import numpy as np
from itertools import product

# Function to compute the syndrome for a given error vector
def compute_syndrome(H, e):
    return np.mod(H @ e, 2)

# Example of a parity-check matrix for a [7,4] Hamming code
H = np.array([
    [1, 1, 0, 1, 1, 0, 0],
    [1, 0, 1, 1, 0, 1, 0],
    [0, 1, 1, 1, 0, 0, 1],
])
e = np.array([1, 0, 0, 0, 0, 0, 0])

s = np.mod(H@e, 2)
print("\nReceived syndrome, s= ", s)
```

Received syndrome, s= [1 1 0].

## 2. Exhaustive MAP Decoding

Now let's assume we only received the syndrome  $s$  and want to find the most likely error vector  $e$ .

Let's simulate the decoding process by searching through all possible error vectors.

- Generate all possible error vectors  $e$ .
- Check which satisfy  $H @ e = s \pmod{2}$ .
- Among valid solutions, select the one with the smallest Hamming weight.

```
# Generate all possible error vectors for n = 7
n = H.shape[1]
error_vectors = [np.array(e) for e in product([0, 1], repeat=n)].

# Find all error vectors that satisfy H @ e = s (mod 2)

print("Valid error vectors, with weight:")
valid_errors = []
for e in error_vectors:
    if np.array_equal(compute_syndrome(H, e), s):
        valid_errors.append(e)
        print(e, np.sum(e))

# Select the error vector with the smallest Hamming weight
best_error = min(valid_errors, key=lambda e: np.sum(e))

print("\nBest error vector (minimum weight):", best_error, np.sum(best_error))
print("We needed to search", len(error_vectors), "error vectors.")
```

Valid error vectors, with weight:

```
[0 0 0 0 1 1 0] 2
[0 0 0 1 0 0 1] 2
[0 0 1 0 1 0 1] 3
[0 0 1 1 0 1 0] 3
[0 1 0 0 0 1 1] 3
[0 1 0 1 1 0 0] 3
[0 1 1 0 0 0 0] 2
[0 1 1 1 1 1 1] 6
[1 0 0 0 0 0 0] 1
[1 0 0 1 1 1 1] 5
[1 0 1 0 0 1 1] 4
[1 0 1 1 1 0 0] 4
[1 1 0 0 1 0 1] 4
[1 1 0 1 0 1 0] 4
[1 1 1 0 1 1 0] 5
[1 1 1 1 0 0 1] 5
```

Best error vector (minimum weight): [1 0 0 0 0 0 0] 1  
We needed to search 128 error vectors.

### 3. Heuristic Approach: Greedy Decoding

Instead of checking all error vectors, we can approximate the solution using a greedy algorithm:

- Start with an initial guess (e.g., all zeros).
- Iteratively flip bits to reduce the syndrome error.

This is not guaranteed to find the optimal solution but can be faster in practice.

Observe that the number of steps varies with each run, and it can give solutions that do not minimize the weight.

```
# Greedy decoding algorithm
def greedy_decoder(H, s, max_iter=10):
    steps = 0
    n = H.shape[1]
    e = np.zeros(n, dtype=int) # Start with no errors
    for _ in range(max_iter):
        steps+=1
        syndrome = compute_syndrome(H, e)
        if np.array_equal(syndrome, s):
            break # Decoded successfully
        # Find a bit to flip (choose one randomly for simplicity)
        flip_index = np.random.choice(np.where(syndrome != s)[0])
        e[flip_index] ^= 1 # Flip the bit
    return e, steps

# Run the greedy decoder
decoded_error, steps = greedy_decoder(H, s)
print("\nDecoded error vector using heuristic:", decoded_error)
print("Number of steps required:", steps)
```

```
Decoded error vector using heuristic: [1 0 0 0 0 0 0].
Number of steps required: 2
```

## Tutorial - Fault-Tolerant Quantum Computing with CSS codes

In this notebook we'll explore how fault-tolerant quantum computing looks like at the circuit-level.

For our exploration we'll introduce the Steane Code, proposed by Andrew Steane in 1996. It is a quantum code from the class of Calderbank-Shor-Steane (CSS) codes which was introduced in the lecture.

Our goal is to understand:

- How is a logical qubit prepared at the circuit-level?
- How can we implement logical gates between those logical qubits?
- How does the quantum error correction procedure looks like at the circuit-level?

Let's explore the Steane code! 

## Steane Code

The Steane code is a  $\mathcal{[[7,1,3]]}$  stabilizer code, which means that it encodes 7 physical qubits into 1 logical qubits. Its code distance is  $d=3$ , meaning that it will correct up to  $t = \lfloor 3 - 1/2 \rfloor = 1$  errors.

## Code Construction

### CSS codes:

The class of Calderbank-Shor-Steane (CSS) codes provides a simple recipe of constructing quantum error correcting codes from classical linear codes. In a linear  $\mathcal{([n,k])}$ -code  $\mathcal{C}$ , the code space is defined by the kernel of a parity check matrix  $H \in \mathbb{Z}_{2^{n-k}}$ .

Meaning that for a code word  $x \in \mathbb{Z}_{2^n}$ , we must have:

$$\exists [Hx = 0]$$

Since we have to protect our quantum state from Pauli- $(X)$  and Pauli- $(Z)$  errors, CSS codes combine two classical linear codes  $\mathcal{C}_1$  and  $\mathcal{C}_2$ . The respective parity check matrices  $H_1$  and  $H_2$  define the  $(X)$  and  $(Z)$  stabilizers. To emphasize this fact, we'll denote the matrices as  $(H_X)$  and  $(H_Z)$ .

The rows of the parity check matrices define the stabilizer.

Example: If the  $i$ -th row of  $(H_X)$  is given as  $(1001)$  then the corresponding stabilizer is  $(X_1 X_4 = X_1 \otimes I_2 \otimes I_3 \otimes X_4)$ .

Since all stabilizers from the same parity check matrix necessarily commute, we need to make sure that rows from  $(H_X)$  and  $(H_Z)$  commute. This is ensured if the number of qubits targeted by both stabilizer types is even for each possible pair of stabilizers.

Example:  $(X_1 X_2 X_5 X_6)$  and  $(Z_1 Z_2 Z_3 Z_4)$  commute as they both target qubits 1 and 2 which is an even number of qubits.

### Parity Check Matrix:

For the Steane code, we have  $(H_X = H_Z = H)$  with

$\begin{aligned} H = \begin{bmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 & 1 & 1 & 1 & 0 \end{bmatrix} \end{aligned}$

### Stabilizers:

We can now define the generators of the stabilizer group corresponding to the Steane code based on  $\langle H \rangle$ :

$\begin{aligned} S_X = \langle X_1X_2X_3X_4, X_2X_3X_5X_6, X_3X_4X_6X_7 \rangle \\ S_Z = \langle Z_1Z_2Z_3Z_4, Z_2Z_3Z_5Z_6, Z_3Z_4Z_6Z_7 \rangle \end{aligned}$

### Exercise 1

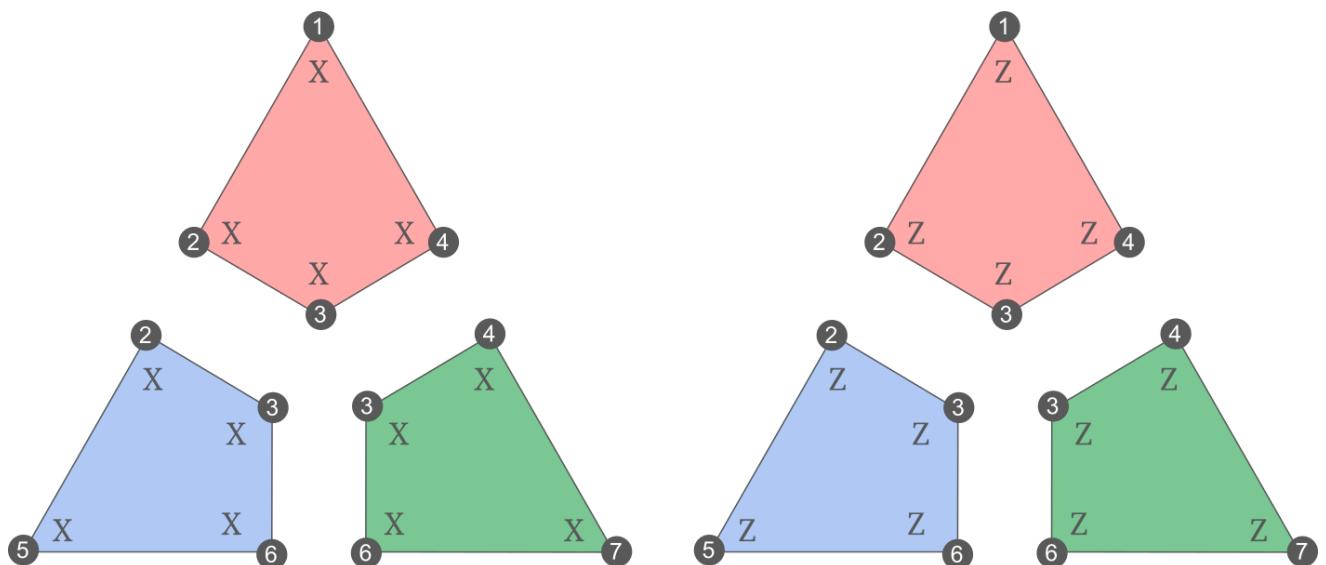
Given the stabilizers, write down a valid code state  $(|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle \otimes |\psi_3\rangle \otimes |\psi_4\rangle \otimes |\psi_5\rangle \otimes |\psi_6\rangle \otimes |\psi_7\rangle)$  of the Steane code.

As a reminder, a valid code state is the simultaneous Eigenstate of all stabilizers such that:  $\langle S|\psi\rangle = |\psi\rangle ; \forall S \in S_X \cup S_Z$

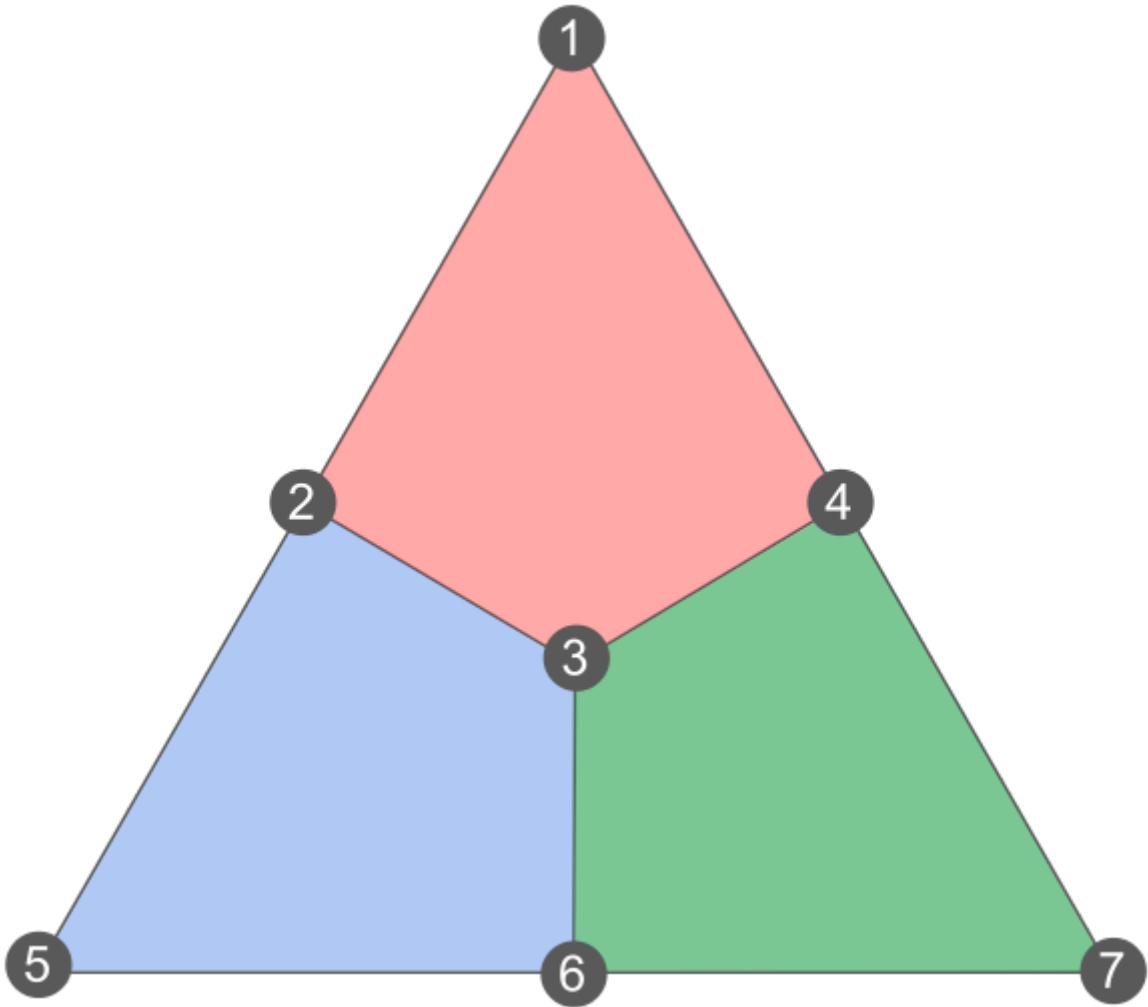
**Tip:** Any stabilizer can be decomposed into a product of generators. This means that only generators have to be considered when checking the stabilizing property.

### Visualizing the Steane Code

To think about the properties of quantum error correcting codes it is often beneficial to visualize them. In the picture below, the vertices represent the physical qubits. Each coloured face defines an  $\langle X \rangle$ - and  $\langle Z \rangle$ -type stabilizer.



Putting the stabilizers together we get triangle with three faces also called *plaquettes* in the literature.



Source: [Arthur Pesah's blog post on the stabilizer formalism](#).

### **Excursion: Stim and Stabilizer formalism**

To implement the Steane Code, we'll use **Stim**, a stabilizer simulator developed by Google, which is used for quantum error correction research.

We'll introduce the 3 most important objects, which are:

- **PauliString** : Representation of a Pauli string such as  $\langle X_1 X_4 \rangle$ .
- **Tableau** : A table holding the current stabilizers of a circuit.
- **circuit** : Representation of quantum circuit similar to Qiskit.

### **Pauli Strings**

A Pauli string is an  $\langle n \rangle$ -qubit operator formed by taking the tensor product of single-qubit Pauli operators:

$\langle P = P_1 \otimes P_2 \otimes \dots \otimes P_n, \text{ where } P_i \in \{I, X, Z, Y\} \rangle$   
For example, a two-qubit Pauli string might be  $\langle P = X \otimes Y \rangle$ , often written as  $\langle XY \rangle$ .

**Note:** We usually omit the identity gates, by adding indices. For example, for  $\langle P = X \otimes I \otimes Y \rangle$  is written as  $\langle X_1 Y_3 \rangle$ .

## Efficient Encoding of Pauli Strings in Software:

Stim is designed to allow the simulation of very large stabilizer codes, so an efficient representation on a computer is crucial. There are 4 different single-qubit Pauli operators, so 2 bits are required to represent them. Stim uses the following encoding:

$$\begin{aligned} \text{enc(I)} &= 00 \\ \text{enc(X)} &= 10 \\ \text{enc(Z)} &= 01 \\ \text{enc(Y)} &= 11 \end{aligned}$$

This encoding is chosen to reflect the algebraic properties of Pauli operators, also called a **group homomorphism**:  $(\text{enc} : (G_1, \cdot) \rightarrow (\mathbb{Z}_2^2, \oplus))$ .

The first bit indicates the presence of an  $\langle X \rangle$  operation, while the second bit indicates a  $\langle Z \rangle$  operation. The  $\langle Y \rangle$  operator, can be decomposed into  $\langle X \cdot Z \rangle$  and has therefore both bits set to 1.

This enables multiplication of Pauli operators through simple bitwise operations. For two Pauli operators  $\langle A \rangle$  and  $\langle B \rangle$ , their product (up to a global phase) is computed by:

$$\text{enc}(A \cdot B) = \text{enc}(A) \oplus \text{enc}(B)$$

where  $\oplus$  represents bitwise XOR. For example:

$$\begin{aligned} \text{enc}(X \cdot Y) &= \text{enc}(X) \oplus \text{enc}(Y) \\ &= 10 \oplus 11 \\ &= 01 \end{aligned}$$

This matches the algebraic relation  $\langle XY = iZ \rangle$  (ignoring the phase factor  $i$ ).

Let's explore Stim's `PauliString` API:

```
import stim

xx = stim.PauliString("+XX")
zz = stim.PauliString("+ZZ")

# Pauli strings can be multiplied
mul_res = xx * zz
print("Multiplication: XX * ZZ = ", mul_res)

# Pauli strings can be concatenated
add_res = xx + zz
print("Addition: XX + ZZ = ", add_res)

# We can check if 2 Pauli strings commute
print("XX and ZZ commute: ", xx.commutes(zz))
```

## Tableau

A tableau is the foundation of efficient simulation of stabilizer circuits. That is circuits, only composed of Clifford gates, mapping Pauli operators to other Pauli operators.

Reminder: a Clifford operator  $\langle C \rangle$ , applied to a product of Pauli's  $\langle P \rangle$ , maps it to  $\langle CPC^{\dagger} \rangle$  which is again a Pauli product.

During execution of a quantum circuit consisting only of Clifford gates, we only need to update the stabilizer generator Pauli strings by applying the update rule above. With our efficient encoding, this can be done very fast.

```
# Define a Tableau simulator
simulator = stim.TableauSimulator()
```

```
# Prepare GHZ state
simulator.h(0)
simulator.cx(0,1)
simulator.cx(0,2)
simulator.measure_many(0,1,2).
```

While it is important to understand how the Tableau works, Stim's Tableau is heavily optimized which increases its complexity. A nice introduction on Tableau simulation is given by Aaronson and Gottesman in "[Improved Simulation of Stabilizer Circuits](#)".

For now, we are happy that we can apply gates to the Tableau and obtain correct measurements.

## Circuit

Stim allows us to also define quantum circuits with a API like Qiskit or Cirq. Below we create the same 3 qubit circuit preparing a GHZ state.

```
c = stim.Circuit()

c.append("H", 0)
c.append("CNOT", [0,1,0,2])
c.append("M", [0,1,2])
```

We can print the circuit using the `diagram` method of `stim.Circuit`.

There are different options to print the circuit:

- `timeline-text` : ASCII diagram
- `timeline-svg` : SVG image
- `timeline-svg-html` : Resizable SVG image
- `timeline-3d-html` : A 3d model, in GLTF format embedded in HTML
- `timeslice-svg` : Prints circuit between "TICK" operations (more on that later)

```
c.diagram('timeline-text').
```

We can sample from the circuit by compiling a sampler

```
sampler = c.compile_sampler()
samples = sampler.sample(shots=10).
```

As expected roughly half of our measurements are  $|00\rangle$  and the other half is  $|11\rangle$ .

```
samples
```

We can also execute the circuit with a Tableau simulator:

```
# Reset all qubits
simulator.reset(0,1,2)
simulator.do(c).
```

```
# All measurements are stored in the measurement record of the Tableau simulator
simulator.current_measurement_record()[-3::].
```

## Logical Operators of the Steane Code

The Steane code has exactly 6 stabilizer generators, imposing independent constraints on the logical qubit state:  $\langle S|\psi\rangle = \langle\psi|S\rangle; \forall S \in S_X \cup S_Z$

Intuitively, this means that for 7 qubits we have 1 degree of freedom left, meaning that the Steane code encodes a single logical qubit.

It can be shown, that for  $m$  stabilizers and  $n$  qubits, the number of logical qubits is  $k = n - m$ .

Assuming, that we have found a logical operator  $O_L$ , then applying it to the logical qubit should result in another valid code state. We can express this condition as:

$$\langle O_L |\psi\rangle = O_L S |\psi\rangle = |\psi\rangle$$

Therefore  $O_L$  must be a stabilizer and the following must hold

$$\langle O_L S |\psi\rangle = \hat{S} |\psi\rangle$$

As a reminder, the stabilizer generators for the Steane code are  $\langle S \rangle = \langle X_1X_2X_3X_4, X_2X_3X_5X_6, X_3X_4X_6X_7 \rangle$ ,  $\langle Z \rangle = \langle Z_1Z_2Z_3Z_4, Z_2Z_3Z_5Z_6, Z_3Z_4Z_6Z_7 \rangle$

We can see that the operators

$$\langle X_L = X_5X_6X_7 \rangle; \langle Z_L = Z_5Z_6Z_7 \rangle$$

satisfy the conditions above. We have found logical  $\langle X_L \rangle$  and  $\langle Z_L \rangle$  operators!

Note: Although it is custom to denote the Pauli string containing Pauli- $\langle Z \rangle$  as  $\langle Z_L \rangle$ , the naming is completely arbitrary. We only care about the algebraic properties of the operators.

## Exercise 2

(a) Verify in Stim, that the logical operators map the set of generators to itself and that  $\langle X_L \rangle$  and  $\langle Z_L \rangle$  anti-commute.

```
from stim import PauliString

steane_stabilizer = [
    PauliString("XXXXIII"),
    PauliString("IXXIXXI"),
    PauliString("IIIXXXX"),
    PauliString("ZZZZIII"),
    PauliString("IZZIZZI"),
    PauliString("IIIZZZZ"),
]

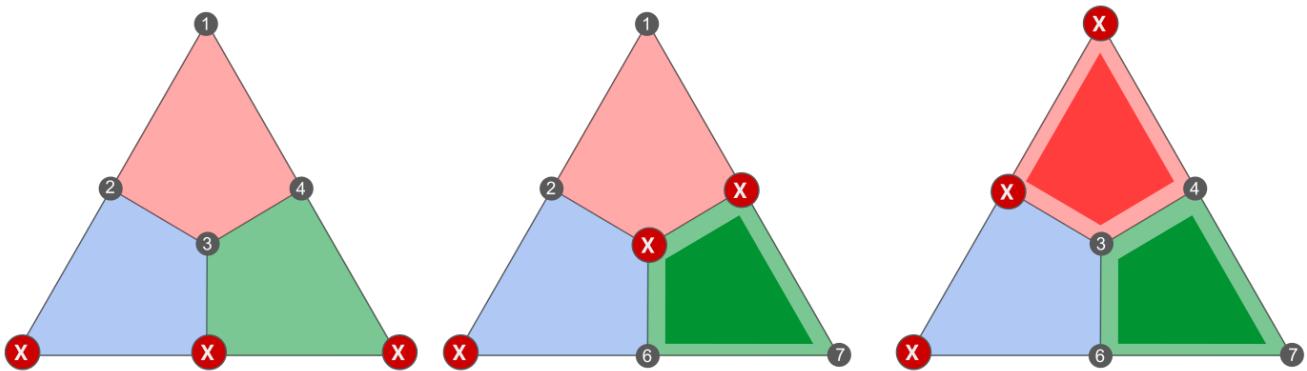
log_x = None # TODO
log_z = None # TODO

# Conjugate the stabilizers one by one with the logical observables and compare the lists
conj_log_x = []
conj_log_z = []

display(conj_log_x)
display(conj_log_z)

# Logical operators anti-commute
# TODO
```

(b) Applying a stabilizer to a logical qubit does not change its state. This means that logical observables form equivalence classes modulus the stabilizers. Use Stim to find equivalent logical observables



Source: [Arthur Pesah's blog post on the stabilizer formalism](#).

**(c) - Pen & Paper** The Steane code is a CSS code, meaning that logical Clifford gates can be performed transversally. Verify that  $(H_L = H^{\otimes 7})$  is a logical operator. Then show that it corresponds to a logical Hadamard based on how it acts on  $(X_L)$  and  $(Z_L)$ .

Note: In the same manner it can be shown that  $(S_L = S^{\otimes 7})$  implements the logical  $(S_L)$  operator.

## Quantum Computing with Logical Qubits

### State Initialization

Quantum circuits usually expect their qubits to be initialized in state  $(|0\rangle)$ . Unfortunately,  $(|0000000\rangle)$  is not a valid code state.

**Question:** Which stabilizers do not stabilize this state?

Therefore, an important, but usually costly, part of QEC is the logical qubit initialization. A naive approach is to prepare the physical qubits in state  $(|0\rangle)$  and measure all stabilizers.

**Question:** How many entangling gates are needed to measure all stabilizers of the Steane code naively in sequence?

To allow for fault-tolerant preparation of the logical qubit, avoiding spreading of errors due to entangling gates, various efficient schemes have been developed.

In the following we provide code for a scheme proposed by [Goto](#).

The scheme requires 8 CNOT gates to prepare the state, followed by a measurement of  $(Z_L)$  via 3 CNOT gates using an ancilla qubit. If the measured ancilla is in the state  $(|0\rangle)$  then we successfully prepared the state  $(|0\rangle_L)$ , otherwise we reset all qubits and repeat the procedure.

```

def encoding_circuit(log_qb_idx: int = 0) -> stim.Circuit:
    """Encoding scheme proposed by Goto 2015: https://www.nature.com/articles/srep19578
    To prepare the logical Steane qubit in state  $|0\rangle_L$ .
    The qubit index allows shifting the indices so that we can prepare multiple logical
    qubits
    """
    c = stim.Circuit()
    # shift registers to target logical qubit with given index
    s = log_qb_idx * 8

    c.append("H", [s, 4+s, 6+s])
    c.append("CNOT", [s, 1+s])
    c.append("CNOT", [4+s, 5+s])
    c.append("CNOT", [6+s, 3+s])
    c.append("CNOT", [6+s, 5+s])
    c.append("CNOT", [4+s, 2+s])
    c.append("CNOT", [0+s, 3+s])
    c.append("CNOT", [4+s, 1+s])
    c.append("CNOT", [3+s, 2+s])

    # Entangle with ancilla qubit and measure logical Pauli-Z
    c.append("CNOT", [1+s, 7+s])
    c.append("CNOT", [3+s, 7+s])
    c.append("CNOT", [5+s, 7+s])
    c.append("M", [7+s])

return c

```

The encoding circuit can be visualized in Stim by printing the [diagram](#)

```

c = stim.Circuit()
c += encoding_circuit()
c.diagram('timeline-svg')

```

Given the encoding scheme, we should verify if it actually prepares a state with the correct stabilizers.

```

t = c.to_tableau(ignore_measurement=True)
print("Stabilizers")
t.to_stabilizers()

```

We can see that the state prepared by the circuit is stabilized by  $\langle X_1 X_2 X_3 X_4 \rangle; \langle X_2 X_3 X_5 X_6 \rangle; \langle X_3 X_4 X_6 X_7 \rangle$

What about the Pauli- $\langle Z \rangle$  stabilizers?

The [Goto scheme](#), prepares the  $|0\rangle_L$  state by measuring only the  $\langle Z\rangle$ -stabilizers. Since arbitrary Pauli- $\langle Z\rangle$  errors are in this case equivalent to no errors or single-qubit  $\langle Z\rangle$  errors which can be corrected by the Steane code.

As a final sanity check, we can sample shots from the circuit and measure  $\langle Z_L \rangle$ . In the absence of noise, we should prepare the state  $|0\rangle_L$  with 100% success rate.

To avoid code repetition, let's first define a method that takes a circuit, samples from it, and returns the measurements

```
import numpy as np

def measure_logical_qubits(log_qubit_indices: list[int] = [0]) -> stim.Circuit:
    c = stim.Circuit()

    for log_qubit_index in log_qubit_indices:
        # shift index
        s = log_qubit_index * 8
        # final measurement
        c.append("M", np.array([0,1,2,3,4,5,6]) + s)

    return c

def sample_from_circuit(c: stim.Circuit, shots: int = 10) -> np.array:
    # compile a sampler and sample 10 shots
    s = c.compile_sampler()
    r = s.sample(shots=shots).astype(int)

    return r
```

### Exercise 3

Given the helper function above, complete the circuit above to correctly compute the logical  $\langle Z_L \rangle$  measurement result given the measurements of the physical qubits.

```
c = stim.Circuit()
# prepare |0>_L
c += encoding_circuit()
# append final measurement
c += measure_logical_qubits()
# sample from circuit
r = sample_from_circuit(c, shots=10)
# compute Z_L observable from measurement
logical_measurement_output = None # TODO
```

Note, that the first column of `r` corresponds to the ancilla qubit measurement and not the first qubit!

```
print("Logical measurement outcome: ", logical_measurement_output)
```

As there is no noise, the ancilla should always be measured in state  $|0\rangle$

```
print("Ancilla qubit measurement outcome: ", r[:,0]).
```

## Different Basis State Preparation

We can prepare the state  $|0\rangle$  with the method above. Next, we'll want to prepare the logical qubit in different basis states

$|0\rangle, |1\rangle, |+\rangle, |-\rangle, |i\rangle, |-i\rangle$   
This can easily be done by using the logical gates  $X$ ,  $Z$ ,  $S$ , and  $H$ , that we identified in the previous section.

## Exercise 4

Complete the lines marked with **TODO** in the function below (Always add the index shift **s** to prepare for operations on multiple logical qubits!)

```

def logical_single_qubit_gate(gate: str, log_qb_idx: int = 0) -> stim.Circuit:
    """
    Supported logical gates:
    - "Z": Logical Z gate
    - "X": Logical X gate
    - "H": Logical Hadamard gate
    - "S": Logical S (phase) gate
    """

    Args:
        c (stim.Circuit): The stim Circuit object to append the logical gate to
        gate (str): The name of the logical gate to apply. Must be one of: "Z", "X",
        "H", "S"
        log_qb_idx (int, optional): Index of the logical qubit to operate on. Used to
        offset the
            physical qubit indices when working with multiple logical qubits. Defaults
        to 0.
            Each logical qubit uses 8 physical qubits (7 data + 1 ancilla).

    Returns:
        stim.Circuit: The modified circuit with the logical gate appended
    """
    c = stim.Circuit()
    # shift registers to target logical qubit with given index
    s = log_qb_idx * 8

    match gate:
        case "Z":
            # TODO
            pass
        case "X":
            # TODO
            pass
        case "H":
            # TODO
            pass
        case "S":
            c.append("S", np.array([0,1,2,3,4,5,6]) + s)
        case "S_DAG":
            c.append("S_DAG", np.array([0,1,2,3,4,5,6]) + s)
        case _:
            raise ValueError(f"Logical gate name '{logical_gate}' undefined")

    return c

```

We define a helper function to prepare the logical qubit in the Eigenstate of a given Stabilizer

```

def prepare_stab_eigenstate(stabilizer: str) -> stim.Circuit:
    """Generates a circuit preparing the Eigenstate of a given single-qubit stabilizer"""
    c = stim.Circuit()

    match stabilizer:
        case "+Z": # |0>
            pass
        case "-Z": # |1>
            c += logical_single_qubit_gate(gate="X")
        case "+X": # |+>
            c += logical_single_qubit_gate(gate="H")
        case "-X": # |->
            c += logical_single_qubit_gate(gate="X")
            c += logical_single_qubit_gate(gate="H")
        case "+Y": # |+i>
            c += logical_single_qubit_gate(gate="H")
            c += logical_single_qubit_gate(gate="S")
        case "-Y": # |-i>
            c += logical_single_qubit_gate(gate="X")
            c += logical_single_qubit_gate(gate="H")
            c += logical_single_qubit_gate(gate="S")
        case _:
            raise ValueError(f"Unknown stabilizer {stabilizer}")

    return c

```

Let's test the state preparation for our logical qubit when measuring in the  $\langle Z \mid L \rangle$  basis

```

c = stim.Circuit()
# prepare |0> L
c += encoding_circuit()
# apply a bit-flip
c += logical_single_qubit_gate(gate="X")
# append final measurement
c += measure_logical_qubits()
# sample from circuit
r = sample_from_circuit(c, shots=10)

logical_measurement_output = r[:,5] ^ r[:,6] ^ r[:,7]
print("Logical bit-flip measurement outcome: ", logical_measurement_output)

```

```

c = stim.Circuit()
# prepare |0> L
c += encoding_circuit()
# apply a logical Hadamard gate
c += prepare_stab_eigenstate("-Z")
# append final measurement
c += measure_logical_qubits()
# sample from circuit
r = sample_from_circuit(c, shots=20)

# compute Z L observable from measurement
logical_measurement_output = r[:,5] ^ r[:,6] ^ r[:,7]
print("Logical Hadamard measurement outcome: ", logical_measurement_output)

```

```

c = stim.Circuit()
# prepare |0> L
c += encoding_circuit()
# apply a logical X by using logical HZH construction
c += logical_single_qubit_gate(gate="H")
c += logical_single_qubit_gate(gate="Z")
c += logical_single_qubit_gate(gate="H")
# append final measurement
c += measure_logical_qubits()
# sample from circuit
r = sample_from_circuit(c, shots=20)

# compute Z_L observable from measurement
logical_measurement_output = r[:,5] ^ r[:,6] ^ r[:,7]
print("Logical bit-flip measurement outcome: ", logical_measurement_output)

```

Based on the results above, we can see that logical operators works as expected and that we prepare any state that we interested in.

## **Measuring in different Basis**

To measure a qubit in a different basis we usually apply single-qubit rotations before the measurement in the  $\langle Z \rangle$ -basis.

For example, if we want to measure in the  $\langle X \rangle$ -basis we need to apply a Hadamard gate before the measurement since

$$\langle \psi | H Z H | \psi \rangle = \langle \psi | X | \psi \rangle$$

### **Exercise 5**

Complete the lines marked with `TODO` in the function below.

```

def rotate_to_measurement_basis(meas_basis: str) -> stim.Circuit:
    """Appends single-qubit rotations to a circuit to prepare measurement in specified
    basis"""
    c = stim.Circuit()

    match meas_basis:
        case "Z":
            pass
        case "X":
            # TODO
            pass
        case "Y":
            c += logical_single_qubit_gate(gate="S_DAG")
            c += logical_single_qubit_gate(gate="H")
        case _:
            raise ValueError("Specified target basis not known")

    return c

```

```

c = stim.Circuit()
# prepare |0> L
c += encoding_circuit()
# rotate to X-basis
c += rotate_to_measurement_basis(meas_basis="X")
# append final measurement
c += measure_logical_qubits()
# sample from circuit
r = sample_from_circuit(c, shots=10)

# compute Z_L observable from measurement
logical_measurement_output = r[:,5] ^ r[:,6] ^ r[:,7]
print("Logical bit-flip measurement outcome: ", logical_measurement_output)

```

## Transversal gates

We have now a good understanding of how to manipulate a single logical qubit. To leverage quantum advantage in the future, we will also need to be able to entangle our logical qubits.

In this section we are going to implement a logical CNOT gate. Then, we'll put everything together to prepare a logical GHZ state using 14 + 2 physical qubits:  $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$

In a first step, we prepare the state  $|0\rangle \otimes |0\rangle$

```

# prepare |0> L x |0> L
c = stim.Circuit()
c += encoding_circuit(log_qb_idx=0)
c += encoding_circuit(log_qb_idx=1).

```

```
c.diagram("timeline-svg").
```

## Logical CNOT Implementation

As shown in the lecture, CSS codes allow for transversal implementation of logical entangling gates such as the logical CNOT gate. In the Steane code the logical transversal CNOT gate is simply the pairwise CNOT between physical qubits at the same index of their respective logical qubit.

Let's write a method that implements the logical CNOT:

```

def logical_cnot(ctrl_idx: int, target_idx: int) -> stim.Circuit:
    """Implement a transversal CNOT by applying CNOT between physical qubits of the
    logical qubits
    """
    c = stim.Circuit()
    if ctrl_idx == target_idx:
        raise ValueError("Control index cannot be equal target index").

    offset_ctrl = ctrl_idx * 8
    offset_target = target_idx * 8

    for i in range(7):
        c.append("CNOT", [i + offset_ctrl, i + offset_target]).

    return c

```

Before applying the logical CNOT, we flip the control logical qubit to be able to test our gate

```
c += logical_single_qubit_gate(gate="X")
```

```
c += logical_cnot(ctrl_idx=0, target_idx=1)
```

```
c += measure_logical_qubits(log_qubit_indices=[0,1]).  
c.diagram("timeline-svg")
```

```
r = sample_from_circuit(c, shots=10)
```

```
logical_measurement_output_qb1 = r[:,6] ^ r[:,7] ^ r[:,8].  
logical_measurement_output_qb2 = r[:,6 + 7] ^ r[:,7 + 7] ^ r[:,8 + 7].
```

```
print(logical_measurement_output_qb1).  
print(logical_measurement_output_qb2).
```

## Logical Bell State

Now, we have all tools to implement a logical Bell state!

```

# prepare |0> L x |0> L
c = stim.Circuit()
c += encoding_circuit(log_qb_idx=0)
c += encoding_circuit(log_qb_idx=1)

# Apply Hadamard to first qubit
c += logical_single_qubit_gate(gate="H", log_qb_idx=0)
# Apply logical CNOT
c += logical_cnot(ctrl_idx=0, target_idx=1)

# Add final measurements
c += measure_logical_qubits(log_qubit_indices=[0,1])

```

```

# Optionally display the circuit
c.diagram("timeline-svg")

```

```

# sample and extract states
r = sample_from_circuit(c, shots=20)

logical_measurement_output_qb1 = r[:,6] ^ r[:,7] ^ r[:,8]
logical_measurement_output_qb2 = r[:,6 + 7] ^ r[:,7 + 7] ^ r[:,8 + 7]

print(logical_measurement_output_qb1)
print(logical_measurement_output_qb2)

```

## Optional: Simulating the Steane Code on noisy Hardware: Quantinuum Experiment

The Steane code has been realized in various experiments:

- [Quantum computations on a topologically encoded qubit, 2014, Nigg et al.](#)
- [Realization of Real-Time Fault-Tolerant Quantum Error Correction, 2021](#)
- [Demonstration of logical qubits and repeated error correction with better-than-physical error rates, 2024](#)

In the following, we provide code to simulate parts of the experiment by Quantinuum in 2021, where they implemented a single logical qubit on their ion-trap device and applied multiple rounds of error correction to it.

This will hopefully give you a better understanding of how rounds of quantum error correction are actually implemented and how errors are handled. Please refer to the paper to learn more about the details of the experiment. Happy exploring!

## Introducing Errors

### Quantinuum error parameters

In their experiment, Quantinuum measured various error sources for their ion-trap device.

<u>Operation</u>	<u>Error Channel</u>	<u>Probability</u>
<u>Initialization</u>	<u>Bit flip</u>	$\backslash(1.66 \cdot 10^{-6}\backslash)$
<u>Measurement</u>	<u>Bit flip</u>	$\backslash(2.4 \cdot 10^{-3}\backslash)$
<u>Single-qubit gate</u>	<u>Depolarizing</u>	$\backslash(7 \cdot 10^{-5}\backslash)$
<u>Two-qubit gate</u>	<u>Depolarizing</u>	$\backslash(3.1 \cdot 10^{-3}\backslash)$

Note: We excluded non-Pauli channels, such as leakage, as they cannot be handled by Stim.

Below, we define a helper function that allows us to inject the noise defined in the paper into our circuits:

```
class NoiseModel:  
    """Applies noise to quantum circuits.  
  
    Adds depolarizing noise after 1 and 2-qubit gates, measurement errors,  
    and initialization errors based on typical superconducting qubit parameters.  
    """  
  
    def __init__(self):  
        self.init_error = 1.66 * 1e-6  
        self.meas_error = 2.4 * 1e-3  
        self.depolarize1 = 7 * 1e-5  
        self.depolarize2 = 3.1 * 1e-3  
        self.enabled = True  
  
    def apply(self, c: stim.Circuit) -> stim.Circuit:  
        if not self.enabled:  
            return c  
  
        cn = stim.Circuit()  
        for op in c:  
            if not op.name == "CX":  
                cn.append(op)  
            if op.name in ["H", "X", "Y", "S", "S DAG"]:  
                cn.append("DEPOLARIZE1", op.targets_copy(), self.depolarize1)  
            if op.name == "M":  
                cn.append("X_ERROR", op.targets_copy(), self.meas_error)  
            if op.name == "R":  
                cn.append("X_ERROR", op.targets_copy(), self.init_error)  
  
        else:  
            targets = op.targets_copy()  
            for i in range(0, len(targets), 2):  
                control = targets[i]  
                target = targets[i+1]  
                cn.append("CX", [control, target])  
                cn.append("DEPOLARIZE2", [control, target], self.depolarize2)  
        return cn
```

```
noise = NoiseModel()
```

## Faulty logical state preparation

To test our noise model, we apply it to the Goto scheme. We expect to see some state preparation failures.

```
c = stim.Circuit()
# prepare |0> L
c += noise.apply(encoding_circuit())
# append final measurement
c += measure_logical_qubits()
```

```
c.diagram("timeline-svg")
```

```
num_shots = 100_000
r = sample_from_circuit(c, shots=num_shots)

# compute Z_L observable from measurement
logical_measurement_output = r[:,5] ^ r[:,6] ^ r[:,7].
```

```
# Measure how often the ancilla qubit is measured in state |0>
print("Success rate: ", (1 - (np.sum(r[:,0]) / num_shots)) * 100, "%")
```

## Syndrome extraction

After succesful state preparation, the logical qubit is idling and the physical qubits will accumulate errors. This will cuase the logical qubit to decohere if we don't measure the stabilizers, effectively digitizing the noise, and tracking the changes in stabilizer measurements!

Below we first provide a function to measure all stabilizers of the code in a sequence.

```

def measure_all_syndromes() -> stim.Circuit:
    """Appends a circuit that measures all 6 stabilizers of the [[7,1,3]]-Steane code"""

    # indices for X-/Z-stabilizers
    syndrome_qubits = [
        [0,1,2,3], # 1st plaquette
        [1,2,4,5], # 2nd plaquette
        [2,3,5,6] # 3rd plaquette
    ]
    # indices for ancilla qubits
    ancilla_qubits = [8,9,10]

    c = stim.Circuit()
    # measure X-stabilizers
    for ancilla, data_qubits in zip(ancilla_qubits, syndrome_qubits):
        for data in data_qubits:
            c.append("CNOT", [data, ancilla])
            c.append("M", ancilla)
            c.append("R", ancilla)

    # measure Z-stabilizers
    for ancilla, data_qubits in zip(ancilla_qubits, syndrome_qubits):
        c.append("H", ancilla)
        for data in data_qubits:
            c.append("CNOT", [ancilla, data])
            c.append("H", ancilla)
            c.append("M", ancilla)
            c.append("R", ancilla)

    return c

```

```

c = stim.Circuit()
c += measure_all_syndromes()
c.diagram('timeline-svg')

```

This approach for syndrome extraction is problematic as it is clearly not fault-tolerant. For example, consider a  $\langle Z \rangle$  error on one of the ancilla qubits. A single error can spread to 4 physical qubits during a single stabilizer measurement!

### Can we do better?

A first approach could be to group the entangling gates, so that we measure the stabilizers in parallel. We can measure at most 3 stabilizers in parallel. This also reduces the time the physical qubits spent idling.

Furthermore, we need to consider the spreading of errors from the ancillas, so called **hook errors**. Since the Steane code is a distance  $\langle d=3 \rangle$  code, we can at most correct a single error and detect two errors.

A simple approach to detect hook errors is to add additional “flag” qubits, which measure parity checks on subsets of ancillas. In the following, we define circuits where the ancillas act themselves as flags for hook errors without the need for additional ancillas (Syndrome qubits reciprocally flag each other).

```
def measure_flagged_syndromes_xzz() -> stim.Circuit:
    """Extracts flagged syndrome measurements for stabilizers 1, 5, 6

    1: XXXXII (Z errors on first plaquette)
    5: IZZIZZI (X errors on second plaquette)
    6: IIZZZZZ (X errors on third plaquette)
    """

    c = stim.Circuit()
    c.append("H", 8)
    c.append("CNOT", [8, 3])
    c.append("CNOT", [2, 10])
    c.append("CNOT", [5, 9])

    # correlate
    c.append("CNOT", [8, 9])
    c.append("CNOT", [8, 0])
    c.append("CNOT", [3, 10])
    c.append("CNOT", [4, 9])
    c.append("CNOT", [8, 1])
    c.append("CNOT", [6, 10])
    c.append("CNOT", [2, 9])

    # correlate
    c.append("CNOT", [8, 10])
    c.append("CNOT", [8, 2])
    c.append("CNOT", [5, 10])
    c.append("CNOT", [1, 9])
    c.append("H", 8)

    # measure ancillas and reset them
    c.append("M", [8, 9, 10])
    c.append("R", [8, 9, 10])

    return c
```

```
xzz = measure_flagged_syndromes_xzz()
xzz.diagram('timeline-svg')
```

```

def measure_flagged_syndromes_zxx() -> stim.Circuit:
    """Extracts flagged syndrome measurements for stabilizers 2, 3, 4

    2: ZZZZIII (X errors on first plaquette)
    3: IXXIXXI (Z errors on second plaquette)
    4: IIIXXIXX (Z errors on third plaquette)
    """

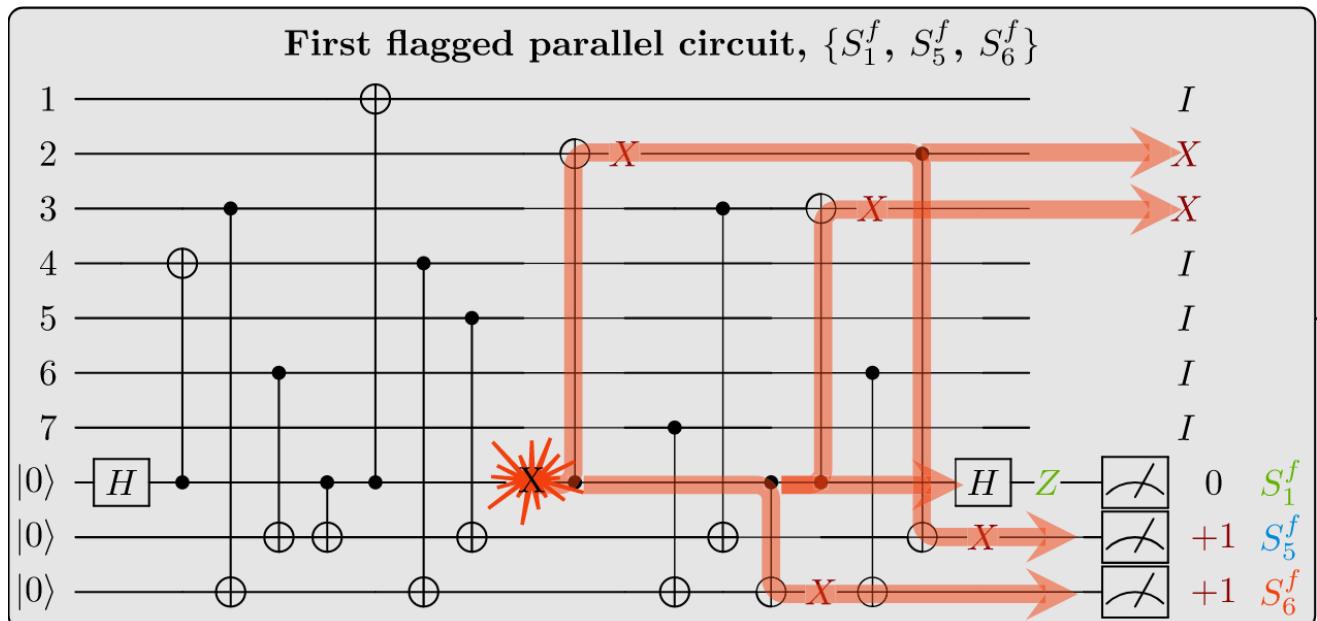
    c = stim.Circuit()

    c.append("H", [9, 10])
    c.append("CNOT", [3, 8])
    c.append("CNOT", [10, 2])
    c.append("CNOT", [9, 5])
    # correlate
    c.append("CNOT", [9, 8])
    c.append("CNOT", [0, 8])
    c.append("CNOT", [10, 3])
    c.append("CNOT", [9, 4])
    c.append("CNOT", [1, 8])
    c.append("CNOT", [10, 6])
    c.append("CNOT", [9, 2])
    # correlate
    c.append("CNOT", [10, 8])
    c.append("CNOT", [2, 8])
    c.append("CNOT", [10, 5])
    c.append("CNOT", [9, 1])
    c.append("H", [9, 10])

    # measure ancillas and reset them
    c.append("M", [8, 9, 10])
    c.append("R", [8, 9, 10])
    return c

```

An example of hook errors with flags is shown in the picture below, taken from the [Quantinuum paper](#):



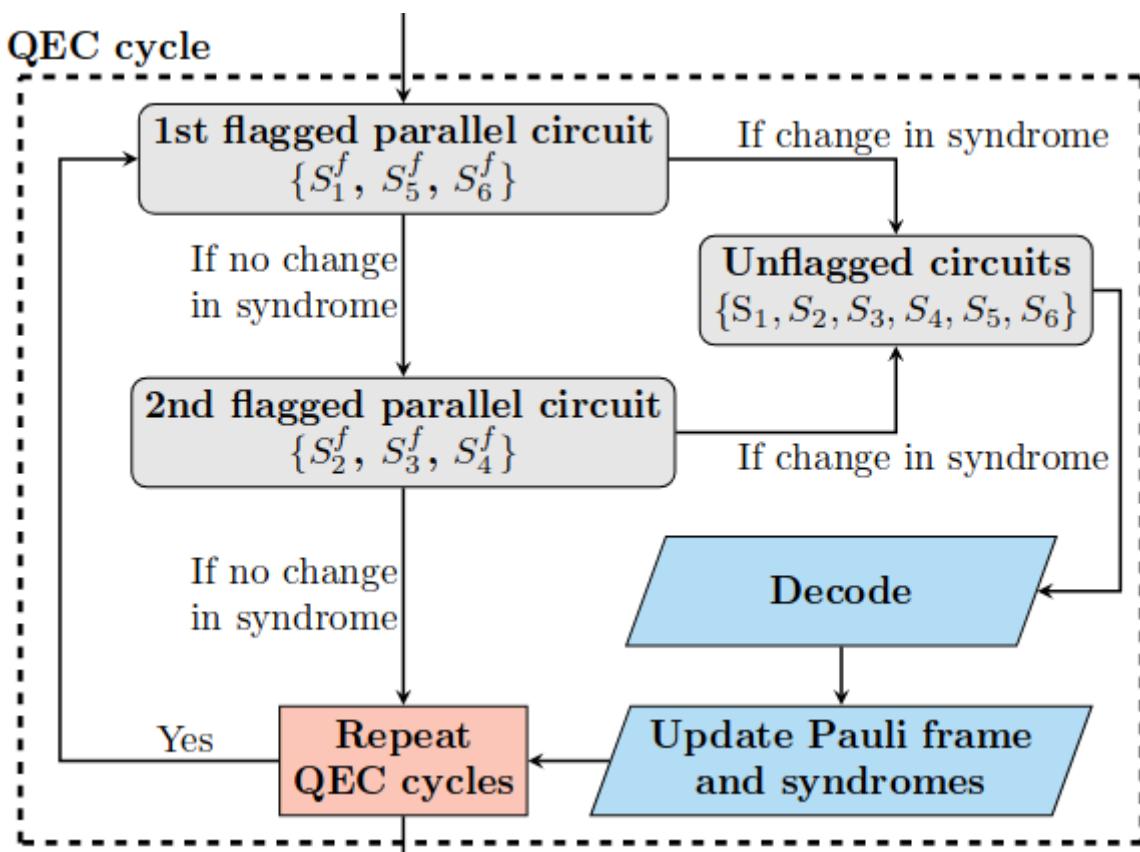
**Full QEC cycle**

We are nearly ready to run our full QEC cycle. We can now come up with a protocol to reliably correct a single physical qubit error. Our flagged syndrome circuits can detect hook errors. To differentiate them from higher weight Pauli errors, we combine flagged and unflagged syndrome extraction.

If the flagged syndrome circuits do not indicate an error, than we are done and the next QEC cycle starts. Otherwise, we know that an error occurred, but we need to measure the complete set of stabilizers to identify whether a hook error occurred.

This combination of conditional syndrome extraction is also known as **adaptive syndrome extraction** and can reduce average QEC cycle time significantly.

The adaptive QEC cycle is depicted in the picture below:



Unfortunately, Stim does not support conditional circuit execution, which means that we need to drive the [TableauSimulator](#) manually.

```
# define a logger allowing us to print the progress of the execution of the QEC experiment
import logging
logging.basicConfig(format='%(message)s')
```

## The Decoder

The decoder is a simple two-stage **Lookup Table Decoder (LUT)**. This means that for each syndrome pattern there is a fixed rule on how to update the **Pauli Frame**, which indicates whether the logical qubit has been flipped or not.

The first stage is used to decode the unflagged syndromes and the second stage decodes the flagged syndromes.

$\Delta(X)\Delta(Z)$ -type errors are handled separately, but since the stabilizers have the same structure we can use the same LUT decoder.

**Note:** We don't provide the syndromes directly to the decoder but only whether the syndromes changed between QEC cycle rounds.

```
def unflagged_decoder(syndromes: np.array) -> int:
    """Given X-/Z-type stabilizer measurements. The syndromes are used to infer whether a logical error has occurred

    This is exactly the case, when there is a change in syndromes for the 2nd/3rd stabilizer
    """
    bad_syndrome_patterns = np.array([[0,0,1], [0,1,0], [0,1,1]]).

    if np.any(np.all(bad_syndrome_patterns == syndromes, axis=1)):
        logging.debug("Unflagged decoder: Logical error detected!")
        return 1
    else:
        return 0

def flagged_decoder(syndromes: np.array, flagged_syndromes: np.array) -> int:
    """
    Handle hook errors.
    """

    if np.all(flagged_syndromes == [1,0,0]) and np.all(syndromes == [0,1,0]):
        return 1
    elif np.all(flagged_syndromes == [1,0,0]) and np.all(syndromes == [0,0,1]):
        return 1
    elif np.all(flagged_syndromes == [0,1,1]) and np.all(syndromes == [0,0,1]):
        return 1
    else:
        return 0

def decoder(syndromes: np.array, flagged_syndromes: np.array) -> list[int, int]:
    """
    pf = unflagged_decoder(syndromes)
    pf_flag = flagged_decoder(syndromes, flagged_syndromes)

    return pf, pf_flag
```

```

def qec_cycle(simulator: stim.TableauSimulator, x_syndromes: np.array, z_syndromes: np.array, pauli_frame: np.array, m_idx: int, noise: NoiseModel) -> int:
    """Run a full QEC cycle for the [[7,1,3]]-Steane code by driving the Tableau simulator manually"""

    # track the delta of previous and current syndrome measurement
    flag_diff_x = np.array([0,0,0]) # track delta of X-stabilizers
    flag_diff_z = np.array([0,0,0]) # track delta of Z-stabilizers

    # first flagged syndrome extraction
    simulator.do(noise.apply(measure_flagged_syndromes_xzz()).)
    # measure first X-stabilizer, and second/third Z-stabilizer
    fx0, fz1, fz2 = simulator.current_measurement_record()[m_idx:m_idx+4]
    # update syndrome delta
    flag_diff_x[0] = fx0 ^ x_syndromes[0]
    flag_diff_z[1] = fz1 ^ z_syndromes[1]
    flag_diff_z[2] = fz2 ^ z_syndromes[2]
    # shift measurement index
    m_idx += 3
    # print delta for debugging
    logging.debug(f"Delta after 1st flagged measurement (XZZ): X {flag_diff_x}, Z {flag_diff_z}")

    # if no syndrome changed continue with second round of flagged syndrome measurements
    if np.all(flag_diff_x == 0) and np.all(flag_diff_z == 0):
        # second flagged syndrome extraction
        simulator.do(noise.apply(measure_flagged_syndromes_zxx()).)
        # measure first Z-stabilizer, and second/third X-stabilizer
        fz0, fx1, fx2 = simulator.current_measurement_record()[m_idx:m_idx+4]
        # update syndrome delta
        flag_diff_z[0] = fz0 ^ z_syndromes[0]
        flag_diff_x[1] = fx1 ^ x_syndromes[1]
        flag_diff_x[2] = fx2 ^ x_syndromes[2]
        # shift measurement index
        m_idx += 3
        # print delta for debugging
        logging.debug(f"Delta after 2nd flagged measurement (ZXX): X {flag_diff_x}, Z {flag_diff_z}")

    # re-measure all syndromes if flagged syndrome extraction indicates changes in syndromes
    if np.any(flag_diff_z == 1) or np.any(flag_diff_x == 1):
        # run full syndrome extraction
        simulator.do(noise.apply(measure_all_syndromes()).)
        s = simulator.current_measurement_record()[m_idx:m_idx+7]
        # update syndromes
        current_z_syndromes = np.array(s[0:3], dtype=int) # First 3 measurements Z-stabilizers
        current_x_syndromes = np.array(s[3:], dtype=int) # Final 3 measurements X-stabilizers
        # compute delta
        diff_x_syndromes = x_syndromes ^ current_x_syndromes
        diff_z_syndromes = z_syndromes ^ current_z_syndromes
        # shift measurement index
        m_idx += 6
        # print new syndrome measurements
        logging.debug(f"Delta after unflagged measurement: X {diff_x_syndromes}, Z {diff_z_syndromes}")

    # call decoder to get updated pauli frame
    pf_x, pf_flag_x = decoder(diff_x_syndromes, flag_diff_x)
    pf_z, pf_flag_z = decoder(diff_z_syndromes, flag_diff_z)

```

```
# update pauli frame
pauli_frame[0] = pauli_frame[0] ^ pf_x ^ pf_flag_x
pauli_frame[1] = pauli_frame[1] ^ pf_z ^ pf_flag_z
logging.debug(f"Pauli frame: Z: {pauli_frame[0]}, X: {pauli_frame[1]}")

# update syndromes
x_syndromes = current_x_syndromes
z_syndromes = current_z_syndromes

return simulator, x_syndromes, z_syndromes, pauli_frame, m_idx
```

For the final round of quantum error correction, we measure all physical qubits simultaneously in the  $\langle Z \rangle$ -basis.

Given the measurement results, we compute the syndrome measurements as well as the logical observable by classically XORing the bits.

Depending on the chosen measurement basis, we need to modify the syndromes.

```

def destructive_logical_measurement(simulator: stim.TableauSimulator, meas basis: str,
x syndromes: np.array, z syndromes: np.array, pauli frame: np.array, m idx: int, noise:
NoiseModel) -> int:
    """Perform final destructive measurement where all physical qubits are measured.

    Returns a single bit, corresponding to the logical qubit measurement in the specified
    measurement basis.
    A final set of syndromes can be computed depending on the measurement basis.
    """

# Measure all seven physical qubits of our logical qubit destructively
simulator.do(noise.apply(measure logical qubits()...))
r = simulator.current measurement record()[m idx:m idx+7]

# Compute the logical observable
log obs = r[4] ^ r[5] ^ r[6]

# Compute syndromes
s1 = r[0] ^ r[1] ^ r[2] ^ r[3] # First plaquette
s2 = r[1] ^ r[2] ^ r[4] ^ r[5] # Second plaquette
s3 = r[2] ^ r[3] ^ r[5] ^ r[6] # Third plaquette
syndromes = np.array([s1, s2, s3], dtype=int)

match meas basis:
    case "X":
        syndrome diff = syndromes ^ x syndromes
    case "Y":
        syndrome diff = syndromes ^ x syndromes
        syndrome diff = syndromes ^ z syndromes
    case "Z":
        syndrome diff = syndromes ^ z syndromes
    case _:
        raise ValueError(f"Unknown measurement basis {meas basis}!")

logging.debug(f"Delta final round: {syndrome diff}")

# Get final corrections from the unflagged decoder
final correction = unflagged decoder(syndrome diff)

# Update the logical obs
log obs = log obs ^ final correction

# Finally, apply correction based on measurement basis
match meas basis:
    case "X":
        log obs = log obs ^ pauli frame[0]
    case "Y":
        log obs = log obs ^ pauli frame[0] ^ pauli frame[1]
        logging.debug("log : %s, pf: %s", log obs, pauli frame)
    case "Z":
        log obs = log obs ^ pauli frame[1]

return log obs

```

```
def expected_result(measure_output: int, stabilizer: str, meas_basis: str) -> int:
        """Evaluate if measurement corresponds to the expected measurement result for a given
    stabilizer and measurement basis."""

        pauli_measurement = stim.PauliString(meas_basis)
        pauli_stabilizer = stim.PauliString(stabilizer)
        commute = pauli_stabilizer.commutes(pauli_measurement)

        if not commute:
            raise ValueError("Anti-commuting stabilizers, measurement is random")

        sign = (pauli_measurement * pauli_stabilizer).sign

        if sign == 1:
            return int(0 == measure_output)
        else:
            return int(1 == measure_output)
```

Finally, we can put everything together and run the whole QEC cycle!

```

def steane_code_exp(initial_state: str = "+Z", meas_basis: str = "Z", num_cycles: int = 1, shots: int = 100, noise = NoiseModel()):
    """Runs an error correction experiment for the Steane [[7,1,3]]-code.

    The quantum state is represented by the state of the stim TableauSimulator.
    """
    results = []

    for _ in range(shots):
        simulator = stim.TableauSimulator()

        m_idx = 0 # shift measurement index

        # state preparation (3 attempts)
        # prepare the logical |0> L state and verify with ancilla
        for _ in range(3):
            simulator.do(noise.apply(encoding_circuit()))
            state_prep_ancilla = simulator.current_measurement_record().m_idx
            logging.debug("State preparation ancilla: %s", int(state_prep_ancilla))
            m_idx += 1
            if not state_prep_ancilla:
                break

        # apply single qubit gate to prepare correct state
        simulator.do(noise.apply(prepare_stab_eigenstate(initial_state)))

        # run QEC cycles
        x_syndromes = np.array([0,0,0])
        z_syndromes = np.array([0,0,0])
        # Pauli frame tracks which logical correction to apply
        # Pauli Frame = [Apply X L?, Apply Z L?]
        pauli_frame = np.array([0,0])

        for i in range(num_cycles):
            logging.debug(f"--- QEC cycle {i}")
            simulator, x_syndromes, z_syndromes, pauli_frame, m_idx = qec_cycle(simulator,
x_syndromes, z_syndromes, pauli_frame, m_idx, noise)

            # Rotate to correct logical measurement basis
            simulator.do(noise.apply(rotate_to_measurement_basis(meas_basis=meas_basis)))

            # Perform final destructive logical measurement
            final_measurement = destructive_logical_measurement(simulator, meas_basis,
x_syndromes, z_syndromes, pauli_frame, m_idx, noise)

            logging.debug(f"Final measurement: {final_measurement}")

            success = expected_result(final_measurement, initial_state, meas_basis)
            logging.debug(f"Success: {success}\n")
            results.append(success)

    return results

```

```

# Uncomment to follow QEC cycle execution
logging.getLogger().setLevel(logging.DEBUG)

noise = NoiseModel()
noise.enabled = False

steane_code_exp(num_cycles=3, shots=1, initial_state=f"+Y", meas_basis=f"Y",
noise=noise).

```

## Simulating Logical Error Rates for Steane Code for each Basis

```

shots = 2048
cycles_sweep = [0,1,2,3,4,5,6]
basis_sweep = ["Z", "X", "Y"]
noise = NoiseModel()
noise.enabled = True

results = []
for basis in basis_sweep:
    cycle_results = []
    for cycles in cycles_sweep:
        exp_results = steane_code_exp(num_cycles=cycles, shots=shots, initial_state=f"+{basis}",
                                       meas_basis=f"{basis}", noise=noise)
        cycle_results.append(np.sum(exp_results)/shots)
    results.append(cycle_results).

```

```

import matplotlib.pyplot as plt

plt.title("Steane Code Logical Error Rate vs. QEC cycles")
plt.xlabel("QEC Cycles")
plt.ylabel("Logical Error Rate")
plt.grid(axis='y')
plt.yscale('log')
for idx, basis in enumerate(basis_sweep):
    plt.scatter(cycles_sweep, 1 - np.array(results[idx]), label=basis)
plt.legend(title="Basis").

```

## Tutorial - Estimating the Surface Code Threshold

In this notebook, we will estimate the threshold of the Surface Code, for a simple phenomenological circuit-noise model.

### Python Dependencies

To run the Jupyter Notebook locally, you'll need the following dependencies:

```

stim~1.14
numpy~1.0 # require for PyMatching
scipy
pymatching
matplotlib

```

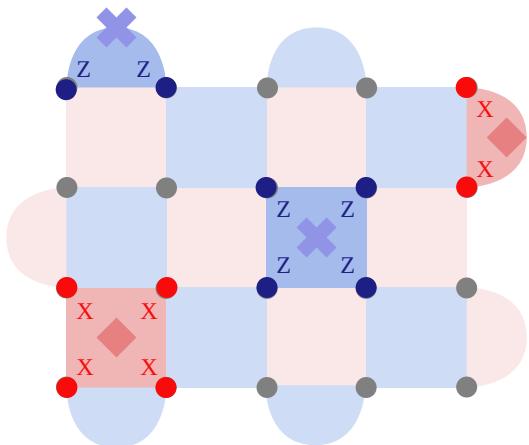
If not already installed in your environment you can install them with

```
pip install stim~=1.14 numpy~=1.0 scipy pymatching matplotlib
```

## The Surface Code

As discussed in the lecture, the Surface Code is a stabilizer code with code distance  $(d)$ ,  $(d^2)$  data qubits, and  $(d^2-1)$  syndrome measurement qubits, embedded in a 2D-plane.

The stabilizers of the code have weight 4 (interior) or 2 (boundary) depending on their location on the surface. In the picture below, a distance  $(d=5)$  Surface Code is shown. The red squares depict the  $(X)$ -type stabilizers, and the blue squares depict the  $(Z)$ -type stabilizers.



Source: [https://errorcorrectionzoo.org/c/rotated\\_surface](https://errorcorrectionzoo.org/c/rotated_surface)

To measure the syndromes, the code requires only local operation between neighboring qubits since each syndrome qubit measures only its neighboring data qubits.

## Surface Code Circuit in Stim

We will use the stabilizer simulator [stim](#) to simulate the circuit code execution and the circuit noise.

Stim allows us to load a set of pre-defined quantum circuits for well-known quantum error correction codes such as the Surface Code.

We'll start by generating a distance  $(d=3)$  Surface Code quantum circuits with 3 rounds of syndrome measurements.

```
import stim

circuit = stim.Circuit.generated(
    "surface_code:rotated_memory_x",
    rounds=2,
    distance=3)
```

```
circuit.diagram('timeline-svg').
```

For  $d=3$ , we expect the circuit to have 9 data qubits and 8 ancilla qubits to measure the stabilizers, so a total of 15 qubits. The circuit generated above contains a few idle wires (corresponding to unused qubits).

A better way to see which qubits are actually utilized is to print a **timeslice diagram** of the circuit. A timeslice diagram depicts the parts of the circuit executed between two **TICK** operations.

**stim** automatically injects **TICK** operations so that we can easily follow the code circuit execution.

```
circuit.diagram('timeslice-svg').
```

We can see that in each round of syndrome measurement, 4 blocks of parallel CNOT gates are applied. In each block, 6 CNOTs are executed - 4 for the stabilizers in the interior of the surface and 2 for the stabilizers at the boundary measuring 2 data qubits.

**Note:** The CNOT gates are executed in a specific order to avoid **hook errors**, which would spread low-weight Pauli errors, to higher weight Pauli errors, making fault-tolerant operations impossible!

After each round, the ancillas are measured, extracting the stabilizer Eigenvalues, followed by a reset operation to re-use them for the next round of error detection.

## Circuit Metadata

In the circuit above, we can see two other annotations, besides the **TICK** operation, which do not correspond to quantum gates operating on the qubits.

The first 16 instructions of the circuit use the **QUBIT\_COORDS(x, y) qubit\_index** annotation to provide Stim information about the qubit's location in space. This information is utilized by various tools to visualize the circuit execution such as the **timeslice** visualizer.

```
circuit[0:17].
```

The second annotation is the `DETECTOR` annotation which is discussed in the next section.

## Detectors

We can see that Stim appended to the end of each QEC cycle a bunch of `DETECTOR` statements.

A detector is a parity check, based on a set of measurements in the **measurement record** denoted as `rec`. Under noiseless execution, the **parity of the detector should never change**.

The latest measurement in the measurement record is accessible through `rec[-1]`.

Each `DETECTOR` can be assigned a location in space-time via a triplet of coordinates  $(x, y, z)$ , which can later be used to display a space-time graph.

If we print the instructions for the first QEC cycle, we see that 4 detectors have been added. Those are used for the  $(Z)$ -type stabilizer parity checks, detecting Pauli- $(X)$  errors.

```
# Instructions for the first QEC cycle
circuit[17:37].
```

What about the  $(X)$ -type stabilizers?

Since at the beginning of the circuit we prepared our qubits in the  $|1\rangle$  state, they are already Eigenvectors of all  $(Z)$ -type stabilizers resulting in a deterministic measurement ( $(Z)$ -type stabilizers have an even amount of Pauli- $(Z)$  operators cancelling out the phase-flip of  $(-1)$  for single physical qubits).

**Example:**  $(ZZZZ|1\rangle\langle 1|) = (-1)^4 |1\rangle\langle 1| = |1\rangle\langle 1|$

For the  $(X)$ -type stabilizers, we require an initial measurement round projecting them randomly onto one of the 2 Eigenspaces  $(+1)/(-1)$ . Subsequent measurements, in the absence of noise, should always yield the same Eigenvalues when measuring the stabilizers.

Therefore, we can add additional `DETECTOR` statements for the  $(X)$ -type stabilizers after the second round of measurements as shown below:

```
circuit[37:60].
```

In the second round, we bitwise XOR the measurement results of the first round, with the measurements of the second round. This way, `DETECTOR` events inform the decoder about changes in the syndromes in the presence of noise.

Note: The `SHIFT_COORDS` instruction can be used to shift the  $\langle z \rangle$ -index (time) by 1, which allows us to reuse the same detector coordinates in every QEC cycle.

## **Final Measurement Round**

At the end of the circuit, all physical data qubits are measured destructively in the  $\langle X \rangle$ -basis, and detectors computing  $\langle Z \rangle$ -type stabilizer parities are defined.

Finally, we define the logical observable measurement as the parity of physical qubits  $\langle 1 \rangle$ ,  $\langle 8 \rangle$ , and  $\langle 15 \rangle$ , corresponding to a logical  $\langle X_L \rangle$  measurement.

```
circuit[60::].
```

## **Detectors in the Absence of Noise**

Without any noise in the circuit, our detectors and the logical observable should always measure the same parities.

We can put this to the test by compiling a `sampler` which will simulate the circuit and collect detector events.

```
# Define a detector sampler
sampler = circuit.compile_detector_sampler().
```

```
# Sample detection events and logical observable
shots = 10

detection_events, observable_flips = sampler.sample(shots, separate_observables=True).
```

Below we can see that the detection events never change parity.

```
print(detection_events).
```

The same applies to the observable

```
print(observable_flips).
```

## Noisy Surface Code Circuits

Now, that we understand how the Surface Code circuit looks like and how detectors behave, we can explore what happens when noise is added to the mix.

Stim doesn't support a noise model, like the ones Qiskit or Cirq support, but we can easily generate the same Surface Code circuit with noisy gates injected.

```
noisy_circuit = stim.Circuit.generated(  
    "surface_code:rotated_memory_x",  
    rounds=2,  
    distance=3,  
    after_clifford_depolarization=0.001,  
    after_reset_flip_probability=0.001,  
    before_measure_flip_probability=0.001,  
    before_round_data_depolarization=0.001).
```

The circuit contains now noise operations, simulating qubit reset, measurement and gate errors.

```
noisy_circuit.diagram('timeline-svg')
```

With the noise, we observe for the first time logical errors after measuring the logical observable

```
import numpy as np  
  
shots = 10_000  
  
sampler = noisy_circuit.compile_detector_sampler()  
detection_events, observable_flips = sampler.sample(shots, separate_observables=True)  
  
print(f"Success rate after 1 QEC cycle: {(1 - (np.sum(observable_flips) / shots)) * 100} %")
```

We also observe detection events in the measured data, indicating the presence of errors:

```
detection_events[0:10]
```

## The Detector Error Model (DEM)

Our goal is to decode the Surface Code. In this section, we introduce a useful abstraction, called the **detector error model (DEM)** which we will use for decoding.

Given a set of measurement parities, defined through detectors and logical observables in the circuit, the detector error model informs the decoder with which probability any of the checks fails due to an error.

For our noisy Surface Code circuit, we can compile a detector model and print the DEM model representation

```
dem = noisy_circuit.detector_error_model()
print(repr(dem))
```

The first instruction

```
error(0.00193118) D0 D2
```

tells us, that there is some error mechanism in our circuit, that occurs with probability \ (0.00193118\) and that will flip the parities of both detectors D0 and D2, defined as

```
detector(2, 0, 0) D0
detector(4, 2, 0) D2
```

in our Surface Code circuit. As a reminder: Detectors are directly associated with stabilizer measurements. This means, that the error probability tells us with which probability a stabilizer measurement will fail given the circuit-level noise model.

## Example: DEM for Repetition Code

Since our noisy Surface Code has many source of errors, retracing the source of error probabilities in the DEM is not a simple task.

Instead, let's continue our analysis for the \(\text{X}\)-flip repetition code:

```
repetition_circuit = stim.Circuit("""
    X_ERROR(0.1) 0 1 2
    CNOT 0 3 1 3 1 4 2 4
    MR 3 4
    DETECTOR(0,0,0) rec[-1]
    DETECTOR(0,0,0) rec[-2]
""").
```

```
repetition_circuit.diagram('timeline-svg')
```

The corresponding DEM has the following form

```
dem = repetition_circuit.detector_error_model()
print(repr(dem))
```

Unsurprisingly, there are three possible errors affecting our detectors. Since both detectors measure the second qubit they will be flipped with probability  $\backslash(0.1\backslash)$ :

```
error(0.1) D0 D1
```

Adding Pauli- $\backslash(Z\backslash)$  errors to our circuit does not affect the DEM as the repetition code cannot detect them:

```
repetition_circuit = stim.Circuit("""
    X_ERROR(0.1) 0 1 2
    Z_ERROR(0.1) 0 1 2
    CNOT 0 3 1 3 1 4 2 4
    MR 3 4
    DETECTOR(0,0,0) rec[-1].
    DETECTOR(0,0,0) rec[-2].
""").
```

```
dem = repetition_circuit.detector_error_model()
print(repr(dem))
```

Replacing the Pauli- $\backslash(X\backslash)$  and Pauli- $\backslash(Z\backslash)$  errors by depolarizing noise, results in the following DEM:

```
repetition_circuit = stim.Circuit("""
    DEPOLARIZE1(0.1) 0 1 2
    CNOT 0 3 1 3 1 4 2 4
    MR 3 4
    DETECTOR(0,0,0) rec[-1].
    DETECTOR(0,0,0) rec[-2].
""").
```

```
dem = repetition_circuit.detector_error_model()
print(repr(dem))
```

For depolarizing noise with probability  $\backslash(p\backslash)$ , Stim applies a given Pauli gate with probability:

- $\backslash(I\backslash): \backslash((1-p)\backslash)$
- $\backslash(X\backslash): \backslash(\frac{p}{3}\backslash)$
- $\backslash(Y\backslash): \backslash(\frac{p}{3}\backslash)$

- $\langle Z \rangle = \frac{1}{3}$

Therefore, we have a probability of  $\frac{2}{3}$  that our detectors are flipped as we only need to take into account Pauli- $X$  and Pauli- $Y$  errors.

## **DEM model and the Tanner Graph**

The detector error model represents a weighted graph, where the nodes are parity checks and the weights represent independent error probabilities affecting the checks.

This representation is very natural for decoders operating on a Tanner graph such as the **Minimum-Weight Perfect Matching** decoder introduced in the lecture.

To further emphasize the relationship, we can visualize the DEM of a larger repetition code using Stim:

```

circuit = stim.Circuit.generated(
    "repetition_code:memory",
    rounds=25,
    distance=9,
    before_round_data_depolarization=0.04,
    before_measure_flip_probability=0.01)

circuit.diagram('timeline-svg').

```

```

dem = circuit.detector_error_model()
dem.diagram('matchgraph-svg').

```

The matching graph is a 2D space-time graph. The  $(x)$ -axis represents space and the  $(y)$ -axis time.

At each time step, we count 8 vertices, representing the 8 detectors. Furthermore, we have two invisible boundary nodes, for matching errors on the outer qubits, which are only measured by a single detector.

For analyzing the Surface Code DEM, it is usually simpler to print the graph in 3D

**Exercise 1:** Test different error mechanisms and see how they affect the connectivity in the DEM graph.

```

noisy_circuit = stim.Circuit.generated(
    "surface_code:rotated_memory_x",
    rounds=25,
    distance=3,
    # before round data depolarization=0.001,
    after_reset_flip_probability=0.001,
    before_measure_flip_probability=0.001)

dem = noisy_circuit.detector_error_model()
dem.diagram('matchgraph-3d')

```

## DEM model for Decoder Research and Reproducibility

Besides being a powerful abstraction, a DEM model is also very useful for sharing noise models.

DEM model errors can be measured on a real device and loaded into Stim, making Stim a powerful tool for evaluating decoders even without access to actual hardware.

DEM models for Google's recent paper: [Quantum Error Correction Below the Surface Code Threshold](#) can be found on [Zenodo](#)

## Decoding Errors: Minimum-Weight Perfect Matching

Given a DEM model, it is straightforward to feed the graph and detector events to a minimum-weight perfect matching decoder.

In this tutorial, we are going to use a MWPM implementation called [PyMatching](#), developed by Oscar Higgots.

We'll begin by instantiating a noisy repetition circuit in Stim:

```

# Instantiate noisy repetition code
noisy_repetition_circuit = stim.Circuit.generated(
    "repetition_code:memory",
    rounds=25,
    distance=9,
    before_round_data_depolarization=0.04,
    before_measure_flip_probability=0.01)

# Instantiate a sampler to sample detector events
sampler = circuit.compile_detector_sampler()

# Sample detection events and observable flips
num_shots = 10_000
detection_events, observable_flips = sampler.sample(num_shots,
separate_observables=True)

print(f"Success rate after 25 QEC cycles: {(1 - (np.sum(observable_flips) / num_shots)) * 100} %")

```

Next, we import `PyMatching` and use its bindings to construct a graph from our DEM and return predictions given detection events.

```
import pymatching

# generate DEM for noisy circuit
detector_error_model =
noisy_repetition_circuit.detector_error_model(decompose_errors=True)

# Instantiate MWPM decoder
matcher = pymatching.Matching.from_detector_error_model(detector_error_model)
```

We can print some metadata about the decoder

```
print("Number of detectors:", matcher.num_detectors)
print("Number of nodes:", matcher.num_nodes)
print("Number of edges: ", matcher.num_edges)
```

Now, we are ready to decode our sampled data!

```
predictions = matcher.decode_batch(detection_events)
# print(predictions)
```

Finally, we need to count the decoding mistakes

```
# Count the mistakes.
num_errors = 0
for shot in range(shots):
    actual_for_shot = observable_flips[shot]
    predicted_for_shot = predictions[shot]
    if not np.array_equal(actual_for_shot, predicted_for_shot):
        num_errors += 1

print(f"Number of errors for {num_shots} shots: {num_errors}").
```

## Estimating the Repetition Code Threshold

In order to calculate the threshold of a code for a fixed noise model and decoder, we need to evaluate the decoder at different code distances  $\langle d \rangle$  and noise-levels  $\langle p \rangle$ .

We start by writing a function that automates the steps we performed above:

```

def count_logical_errors(circuit: stim.Circuit, num_shots: int) -> int:
    # Sample the circuit.
    sampler = circuit.compile_detector_sampler()
    detection_events, observable_flips = sampler.sample(num_shots,
    separate_observables=True)

    # Configure a decoder using the circuit.
    detector_error_model = circuit.detector_error_model(decompose_errors=True)
    matcher = pymatching.Matching.from_detector_error_model(detector_error_model)

    # Run the decoder.
    predictions = matcher.decode_batch(detection_events)

    # Count the mistakes.
    num_errors = 0
    for shot in range(num_shots):
        actual_for_shot = observable_flips[shot]
        predicted_for_shot = predictions[shot]
        if not np.array_equal(actual_for_shot, predicted_for_shot):
            num_errors += 1
    return num_errors

```

The function returns the number of logical errors for `num_shots`. From that, we can compute the **logical error rate (LER)** per shot needed for our threshold evaluation.

Next, let's run our threshold estimation for our repetition code:

```

import matplotlib.pyplot as plt

results = []
num_shots = 10_000
for d in [3, 5, 7]:
    print("--- Code distance:", d)
    xs = []
    ys = []
    for noise in [0.1, 0.2, 0.3, 0.4, 0.5]:
        circuit = stim.Circuit.generated(
            "repetition_code:memory",
            rounds=d * 3,
            distance=d,
            before_round_data_depolarization=noise)
        num_errors_sampled = count_logical_errors(circuit, num_shots)
        print(f"Decoding errors at noise level {noise}: {num_errors_sampled}")
        xs.append(noise)
        ys.append(num_errors_sampled / num_shots)
    results.append((d, [xs, ys]))
    plt.plot(xs, ys, label=f"d={d}")
plt.loglog()
plt.xlabel("physical error rate")
plt.ylabel("logical error rate per shot")
plt.legend()
plt.show()

```

The results look very promising. Based on our simulation, the threshold for the repetition code is around  $p=0.4$ !

For physical noise levels  $\leq p$  we observe a significant decrease of the LER, consistent with the threshold theorem.

Unfortunately, the repetition code is not as good as the graph might indicate!

There are several problems with our result:

- The repetition code doesn't consider  $Z$ -type errors
- We didn't introduce any reset or measurement errors
- Our noise model is missing important error processes such as for example leakage, where the qubit escapes its computational subspace and leaks to higher energy states such as  $|\psi_2\rangle, |\psi_3\rangle, \dots$ .

Nevertheless, we were able to estimate the code threshold with a few lines of code, demonstrating the usefulness of Stim :-)

Next, we are going to evaluate the Surface Code under a slightly more realistic noise model to get an idea of the threshold value of a real quantum code.

### **Exercise: Estimating the Threshold of the Surface Code**

Exercise 2: Re-use the code for the repetition code to evaluate the Surface Code threshold. This time introduce reset and measurement errors as well depolarizing errors before the QEC cycles.

Tip 1: The threshold for the Surface Code is significantly lower than the one for the repetition code. Use a noise range between  $[0.002, 0.009]$  to find the threshold.

Tip 2: Observe the number of shots needed to sample a logical error and adjust the number of shots accordingly

Exercise 3: The error suppression factor  $\Lambda = \frac{\epsilon_d}{\epsilon_{d+2}}$  is an important metric to see if our code effectively suppresses the error.

The LER is denoted as  $\epsilon_d$ , at a fixed code distance  $d$  and physical error rate  $p$ .

Calculate  $\Lambda$  at  $p=2 \times 10^{-3}$  and compare it to the theoretical estimate  $(p_{thr}/p)$ .

Tip: You can use the `results` list object for your calculations.

## **References**

To learn more about Stim:

- Read the [Getting Started Tutorial](#) which forms the basis for this notebook.
- Check out the paper [Stim: A fast stabilizer circuit simulator](#) to learn about Stim's internals and how it is leveraging SIMD instructions to squeeze the maximum performance out of our CPUs.

To learn more about the Surface Code:

- [Paper](#) introducing the surface code and logical gates by Fowler et al.
- [Google's Surface Code experiment](#): [Quantum error correction below the surface code threshold](#) contains a lot of details about different noise simulation techniques and other decoder types.

To learn more about QEC codes, visit the QEC Zoo: <https://errorcorrectionzoo.org/> !

## Quantum Monte Carlo and quantum finance

### Option pricing on a quantum computer

 [Slides](#)

### Quantum Amplitude Estimation – Applications to Derivative Pricing

 [Slides](#)

### Pricing a European call option on a quantum computer

This notebook is based on the work of M. Q. Hlatshwayo, [NQCC](#).

A call option is a financial contract in which the holder (buyer) has the right (but not the obligation) to buy a specified quantity of a security at a specified price (strike price) within a fixed period of time (until its expiration).

For the writer (seller) of a call option, it represents an obligation to sell the underlying security at the strike price if the option is exercised. The call option writer is paid a premium for taking on the risk associated with the obligation.

Suppose a European call option with strike price  $\langle K \rangle$  and an underlying asset whose spot price at maturity  $\langle S_T \rangle$  follows a given distribution. The corresponding payoff function is defined as:

$$\langle f(S_T) = \max(S_T - K, 0) \rangle$$

In the following, a quantum algorithm based on amplitude estimation is used to estimate the expected payoff, i.e., the fair price before discounting, for the option:

$\mathbb{E}[f(S_T)] \approx \frac{1}{N} \sum_{i=1}^N f(S_T^{(i)})$   
 The approximation of the objective function and a general introduction to option pricing and risk analysis on quantum computers are given in the following papers:

- [Quantum Risk Analysis. Woerner, Egger. 2018.](#)
- [Option Pricing using Quantum Computers. Stamatopoulos et al. 2019.](#)

## Encoding the probability distribution

We construct a circuit to load a log-normal random distribution into a quantum state. The distribution is truncated to a given interval  $[x_{\min}, x_{\max}]$  and discretized using  $2^n$  grid points, where  $n$  denotes the number of qubits used. The unitary operator corresponding to the circuit implements the following:

$$|\psi\rangle = \sum_{i=0}^{2^n-1} \sqrt{p_i} |i\rangle$$

where  $p_i$  denote the probabilities corresponding to the truncated and discretized distribution and where  $i$  is mapped to the right interval using the affine map:

$$i \in [x_{\min}, x_{\max}] \rightarrow i = \frac{x_{\max} - x_{\min}}{2^n - 1} * i + x_{\min}$$

```

import numpy as np
import matplotlib.pyplot as plt

from qiskit_finance.circuit.library import LogNormalDistribution
from qiskit import QuantumCircuit, QuantumRegister, ClassicalRegister, AncillaRegister
from qiskit_circuit.library import LinearAmplitudeFunction, QFT, GroverOperator
from qiskit_algorithms import EstimationProblem, IterativeAmplitudeEstimation
from qiskit.visualization import plot_distribution
from qiskit_primitives import StatevectorSampler as Sampler

```

```

# number of qubits to represent the stock price
num_uncertainty_qubits = 3

# parameters for considered random distribution
S = 2.0 # initial spot price
vol = 0.4 # volatility of 40%
r = 0.05 # annual interest rate of 4%
T = 40 / 365 # 40 days to maturity

# resulting parameters for log-normal distribution
mu = (r - 0.5 * vol**2) * T + np.log(S)
sigma = vol * np.sqrt(T)
mean = np.exp(mu + sigma**2 / 2)
variance = (np.exp(sigma**2) - 1) * np.exp(2 * mu + sigma**2)
stddev = np.sqrt(variance)

# lowest and highest value considered for the spot price; in between, an equidistant
# discretization is considered.
low = np.maximum(0, mean - 3 * stddev)
high = mean + 3 * stddev

```

```
# construct A operator for QAE for the payoff function by
# composing the uncertainty model and the objective
uncertainty_model = LogNormalDistribution(
    num_uncertainty_qubits, mu=mu, sigma=sigma**2, bounds=(low, high)
).
```

```
# view circuit
uncertainty_model.draw('mpl').
```

```
# view detailed circuit in terms of basis gates
uncertainty_model.decompose().decompose().decompose().draw("mpl").
```

```
%matplotlib inline
# plot probability distribution
x = uncertainty_model.values
y = uncertainty_model.probabilities
plt.figure()
plt.bar(x, y, width=0.2)
plt.xticks(x, size=15, rotation=90)
plt.yticks(size=15)
plt.grid()
plt.xlabel(r"Spot Price at Maturity \$S_T\$ (EUR)", size=15)
plt.ylabel(r"Probability (\$\%\$)", size=15)
plt.show()
```

```
# set the strike price (should be within the low and the high value of the uncertainty)
strike_price = 1.896

# plot exact payoff function (evaluated on the grid of the uncertainty model)
x = uncertainty_model.values
y = np.maximum(0, x - strike_price)
plt.figure()
plt.plot(x, y, "ro-")
plt.grid()
plt.title("Payoff Function", size=15)
plt.xlabel(r"Spot Price at Maturity \$S_T\$ (EUR)", size=15)
plt.ylabel("Payoff Amount (EUR)", size=15)
plt.xticks(x, size=15, rotation=90)
plt.yticks(size=15)
plt.show()
```

The payoff function equals zero as long as the spot price at maturity  $(S_T)$  is less than the strike price  $(K)$  and then increases linearly. The implementation uses a comparator, that flips an ancilla qubit from  $\left|0\right\rangle$  to  $\left|1\right\rangle$  if  $(S_T \geq K)$ , and this ancilla is used to control the linear part of the payoff function.

Eventually, we are interested in the probability of measuring  $\left|1\right\rangle$  in the last qubit. Recall that

$$P(\text{measure } 1) = E[f(X)] = \sum_{i=0}^{2^n-1} f(i)p_i.$$
  
For more details on the implementation, we refer to:

[LinearAmplitudeFunction | IBM Qiskit Documentation](#)

```
# set the approximation scaling for the payoff function
c_approx = 0.25

# setup piecewise linear objective function
breakpoints = [low, strike_price]
slopes = [0, 1]
offsets = [0, 0]
f_min = 0
f_max = high - strike_price
european_call_objective = LinearAmplitudeFunction(
    num_uncertainty_qubits,
    slopes,
    offsets,
    domain=(low, high),
    image=(f_min, f_max),
    breakpoints=breakpoints,
    rescaling_factor=c_approx,
).
```

```
# view payoff function circuit
european_call_objective.draw('mpl').
```

```
# view payoff function circuit
function_circuit =
european_call_objective.decompose().decompose().decompose().decompose().decompose().decompose()
function_circuit.draw("mpl").
```

## Combining the distribution and payoff circuits

We combine the circuits for the underlying distribution and the payoff function, respectively. The  $|q\rangle$  qubit contains the expected value of the payoff. We add a measurement operator for  $|q\rangle$ .

```

# construct A operator for QAE for the payoff function by
# composing the uncertainty model and the objective
num_qubits = european_call_objective.num_qubits
num_clbits = 1
qreg = QuantumRegister(num_uncertainty_qubits, 's')
qreg2 = QuantumRegister(1, 'q')
qreg3 = AncillaRegister(num_qubits - num_uncertainty_qubits - 1, 'a')
creg = ClassicalRegister(num_clbits, 'creg')
european_call = QuantumCircuit(qreg, qreg2, qreg3)
european_call.append(uncertainty_model, range(num_uncertainty_qubits))
european_call.append(european_call_objective, range(num_qubits))
european_call.draw("mpl")

```

We can add a measurement to the objective qubit, in order to run the combined circuit and calculate the average  $\langle \hat{p} \rangle$ . The average is scaled back from the  $[0,1]$  interval to the original  $[x_{\min}, x_{\max}]$  interval.

```

# Add a measurement to the objective qubit
measured_european_call = european_call.copy()
measured_european_call.add_register(creg)
measured_european_call.measure(qreg2, creg)
# draw the circuit
measured_european_call.draw("mpl")

```

```

# Run on local simulator
sampler = Sampler()
n_shots = 10000
result = sampler.run([measured_european_call], shots=n_shots).result()
dist = result[0].data.creg.get_int_counts()

```

```
plot_distribution(dist)
```

```

p_hat = dist[1]/n_shots
p_std = np.sqrt(p_hat*(1-p_hat)/n_shots)

print("raw estimated average:\t%.4f" % p_hat, ", standard deviation:\t%.4f" % p_std)

expectation = european_call_objective.post_processing(p_hat)
upper = european_call_objective.post_processing(p_hat + 2*p_std)
lower = european_call_objective.post_processing(p_hat - 2*p_std)

print("estimation of expected payoff:\t%.4f" % expectation)
print("lower confidence bound:\t%.4f" % lower)
print("upper confidence bound:\t%.4f" % upper)

```

```
raw estimated average: 0.3653 , standard deviation: 0.0048
estimation of expected payoff: 0.1440
lower confidence bound: 0.1215
upper confidence bound: 0.1665
```

```
# evaluate exact expected value (normalized to the [0, 1] interval)
exact_value = np.dot(uncertainty_model.probabilities, y)
print("exact expected value from discretization:\t%.4f" % exact_value)
```

exact expected value from discretization: 0.1623

## Amplitude estimation

### Convergence rate of Classical Monte Carlo

The standard Monte Carlo method for pricing consists in approximating the expected payoff  $\mu = \mathbb{E}[f(S_T)]$  as  $\tilde{\mu} \approx \frac{1}{N} \sum_{i=1}^N f(S_{T^{(i)}})$

where  $(S_{T^{(i)}}, i=1, \dots, N)$  are independent, identically distributed samples from the probability distribution of the underlying asset  $(S)$  at the expiration time  $(T)$ .

A consequence of the central limit theorem is that the estimation error of the Monte Carlo method satisfies  $\sqrt{\frac{1}{N}} \sim \mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$

## Amplitude estimation

Quantum amplitude estimation (QAE) is a quantum algorithm that provides an alternative to classical Monte Carlo in order to compute approximate expectations of random variables.

Suppose we are able to construct a circuit that implements an operator acting on an  $(n+1)$  qubit register as follows  $|U|0\rangle_{n+1} = \sqrt{1-a}|\psi_0\rangle_n|\psi_0\rangle + \sqrt{a}|\psi_1\rangle_n|\psi_1\rangle$  (where  $a \in [0,1]$  is an unknown quantity associated with the value  $\mu$  which we intend to estimate (e.g., an appropriate re-scaling of  $\mu$  to the interval  $[0,1]$ )).

Then, QAE can be used to obtain an estimate of  $a$  through repeated controlled applications of the grover operator  $Q = U S_0 U^\dagger S_{|\Psi_0\rangle}$  and an inverse quantum Fourier transform.

For further details on the algorithm, the reader is referred to [Quantum Amplitude Amplification and Estimation](#). Brassard et. al.

It can be shown that, with high probability ( $(8/\pi^2 \approx 81\%)$ ), the estimate  $\langle \tilde{a} | M \rangle$  provided by QAE satisfies  $\left| \langle \tilde{a} | M - a \rangle \right| \leq \frac{2\pi}{\sqrt{a(1-a)}} \cdot \frac{\sqrt{M}}{M} + \frac{\pi^2}{M^2} \sim \mathcal{O}\left(\frac{1}{M}\right)$ , where  $M=2^m$ , and  $m$  is the number of ancilla qubits used by the algorithm.

That is, QAE provides a quadratic speedup over classical Monte Carlo.

QAE can be applied to the circuit constructed above, which encodes the expected payoff into the amplitude of the objective qubit. To this end, we decompose the circuit into basis gates:

```
european_call =  
european_call.decompose().decompose().decompose().decompose().decompose().decompose().
```

Then, the QAE circuit can be constructed (you can look at the provided code [ae\\_circuit.py](#) to see how this is done).

```

class AECircuit(QuantumCircuit):
    def __init__(self, state preparation circuit, num ancilla qubits, objective qubit):
        self.state preparation circuit = state preparation circuit # The cirtuit
        implementing operator A
        self.num ancilla qubits = num ancilla qubits # Number of ancilla qubits (m in
        IQAE paper)
        self.num state qubits = state preparation circuit.num qubits # Number of qubits
        in circuit A (n+1 in the IQAE paper)
        self.objective qubit = objective qubit # Index of the objective qubit within
        the circuit A (0<=objective qubit<=num state qubits)

        # Initialize circuit
        ancilla register = AncillaRegister(self.num ancilla qubits, name="ancilla")
        state register = QuantumRegister(self.num state qubits, name="state")
        classical register = ClassicalRegister(self.num ancilla qubits, name="creg")
        super().__init__(
            ancilla register,
            state register,
            classical register
        )

        # Hadamard gates on the ancilla qubits
        for j in range(self.num ancilla qubits):
            self.h(ancilla register[j])

        # Circuit A on the state and objective qubits
        A gate = self.state preparation circuit.to_gate(label="$A$")
        self.append(A gate, state register[:])

        self.barrier()

        # Powers of Q
        Q = self.groverOp(self.state preparation circuit, self.objective qubit)
        for j in range(num ancilla qubits):
            Qj = Q_power(2**j).to_gate(label=f"$Q^{{\{2**j\}}}\$").control(1) # Controlled
            version of Q^{2j}
            # Apply the controlled Q^{2j} gate on state and objective qubits,
            controlled by the j-th ancilla qubit
            self.append(Qj, [ancilla register[self.num ancilla qubits-j-1]] +
            state register[:])

        self.barrier()

        # Inverse QFT
        QFT gate = QFT(num qubits=self.num ancilla qubits, inverse=True,
        do swaps=False).to_gate(label="$QFT^\dagger$")
        self.compose(QFT gate, ancilla register, inplace=True)

        self.barrier()

        # Measure the ancilla qubits
        self.measure(ancilla register, classical register)

    def groverOp(self, state preparation circuit, objective qubit):
        # construct the grover operator
        oracle = QuantumCircuit(max(state preparation circuit.num qubits -
        state preparation circuit.num ancillas, 1))
        oracle.h(objective qubit)
        oracle.x(objective qubit)
        oracle.h(objective qubit)
        Q = GroverOperator(oracle, state preparation circuit)
        return Q

```

```
num_ancilla_qubits = 7
gae = AECircuit(state_preparation_circuit=european_call,
    num_ancilla_qubits=num_ancilla_qubits, objective_qubit=num_uncertainty_qubits)
```

```
gae.decompose(reps=5).depth()
```

## Run QAE on local simulator

We can run QAE on our local simulator, and check that the estimator it produces is close to the MC estimator.

```
# Run on local simulator
sampler = Sampler()
n_shots = 100
result = sampler.run([gae], shots=n_shots).result()
counts = result[0].data.creg.get_int_counts()
```

```
# QAE post-processing
M = 2**num_ancilla_qubits # Number of grid points = 2^num_ancilla_qubits
q = np.array(list(counts.keys()))
theta_estimates = q*np.pi/M
estimates = np.round(np.sin(theta_estimates)**2,15)
probabilities = np.array(list(counts.values()), dtype="float64")
probabilities /= np.sum(probabilities)

# Combine duplicates
new_estimates = list(set(estimates))
new_probabilities = [np.sum(probabilities[estimates==e]) for e in new_estimates]
estimates = np.array(new_estimates)
probabilities = np.array(new_probabilities)

p_mode = estimates[np.argmax(probabilities)] # Extract estimate with highest probability
gae_expected_payoff = european_call_objective.post_processing(p_mode) # Re-scale estimate to get expected payoff
gae_expected_payoff
```

We can compute the accuracy of QAE as a function of quantum samples

```

def estimate_ae(num_ancilla_qubits):
    # Construct QAE circuit
    qae = AECircuit(state_preparation_circuit=european_call,
num_ancilla_qubits=num_ancilla_qubits, objective_qubit=num_uncertainty_qubits)

    # Run on local simulator
    sampler = Sampler()
    n_shots = 100
    result = sampler.run([qae], shots=n_shots).result()
    counts = result[0].data.creg.get_int_counts()

    # Post-processing
    M = 2**num_ancilla_qubits # Number of grid points = 2^num_ancilla_qubits
    q = np.array(list(counts.keys()))
    theta_estimates = q*np.pi/M
    estimates = np.round(np.sin(theta_estimates)**2,15)
    probabilities = np.array(list(counts.values()), dtype="float64")
    probabilities /= np.sum(probabilities)

    # Combine duplicates
    new_estimates = list(set(estimates))
    new_probabilities = [np.sum(probabilities[estimates==e]) for e in new_estimates]
    estimates = np.array(new_estimates)
    probabilities = np.array(new_probabilities)

    p_mode = estimates[np.argmax(probabilities)] # Extract estimate with highest
probability
    return p_mode

ancillas_range = np.array(range(1, 8))
qae_estimates = np.array([estimate_ae(num_ancilla_qubits) for num_ancilla_qubits in
ancillas_range])

```

```

# Plot results
M = 2**np.array(ancillas_range)
qae_expected_payoffs = qae_estimates

plt.semilogx(2**np.array(ancillas_range), qae_expected_payoffs, ".-", base=2) # QAE
estimates

# Confidence intervals
M = 2**np.array(ancillas_range)
confidence_intervals = 2*np.pi*np.sqrt(qae_estimates[-1]*(1-qae_estimates[-1]))/M +
np.pi**2/M**2
plt.fill_between(M, qae_estimates - abs(confidence_intervals), qae_estimates +
abs(confidence_intervals), color='gray', alpha=0.2)

plt.grid()
plt.xlabel("$M=2^m$");
plt.ylabel("QAE estimates");

```

## Some thoughts

Look at the depth of the QAE circuit. Is this algorithm NISQ-ready?

There are some more advanced versions of QAE, which attempt to reduce the required circuit depth without compromising accuracy. We refer the interested reader to

- [Amplitude estimation without phase estimation. Suzuki et. al.](#),
- [Faster Amplitude Estimation. Nakaji..](#),
- [Iterative Quantum Amplitude Estimation. Grinko et. al..](#)

## Iterative quantum amplitude estimation

Iterative quantum amplitude estimation (IQAE) uses the same ideas as canonical QAE while reducing the while reducing circuit depth and the required number of ancillas.

The `qiskit.algorithms` module implements the method `IterativeAmplitudeEstimation`, which can be used to estimate the expected payoff as follows:

```
from qiskit_aer.primitives import Sampler

epsilon = 0.01
alpha = 0.05

problem = EstimationProblem(
    state_preparation=european_call,
    objective_qubits=[num_uncertainty_qubits],
    post_processing=european_call_objective.post_processing,
)
iae = IterativeAmplitudeEstimation(
    epsilon_target=epsilon, alpha=alpha, sampler=Sampler(run_options={"shots": 100}),
)

result = iae.estimate(problem)

conf_int = np.array(result.confidence_interval_processed)
print("Exact value:          \t%.4f" % exact_value)
print("Estimated value:     \t%.4f" % (result.estimation_processed))
print("Confidence interval:\t[% .4f, %.4f]" % tuple(conf_int))
```

Exact value:	0.1623
Estimated value:	0.1676
Confidence interval:	[0.1615, 0.1737].

## Tutorial - Pricing a European call option using quantum computing

Welcome!  This tutorial notebook is designed such that you will get to work hands-on with pricing a European call option using quantum computing algorithms. It is structured in the following 4 sections:

0. Reminder - what is a European call option?

1. Asset distributions and payoff function
2. Classical Monte Carlo on a QC
3. Quantum Amplitude Estimation (QAE)

If you have any questions or need assistance, dont hesitate to find either one of us in the room and we'll try and help you! 😊

Authors: Björn Löfdahl, Victorio Úbeda Sosa, Wilhelm Ågren

## **0. Reminder - what is a European call option?**

A call option is a financial contract in which the holder (buyer) has the right (but not the obligation) to buy a specified quantity of a security at a specified price (strike price) within a fixed period of time (until its expiration/maturity). For a European call option the holder can only exercise the option at expiry/maturity.

For the writer (seller) of a call option, it represents an obligation to sell the underlying security at the strike price if the option is exercised. The call option writer is paid a premium for taking on the risk associated with the obligation (this is however omitted here as it only offsets the payoff by the premium price).

Suppose a European call option with strike price  $\backslash(K\backslash)$  and underlying asset whose spot price at maturity  $\backslash(S\_T\backslash)$  follows a given distribution, then the corresponding payoff function for the holder is defined as

$$\backslash[ \backslashphi(S\_T) = \backslashmax(S\_T - K, 0). \backslash]$$

For an investor to profit from a European call option, the spot price at maturity  $\backslash(S\_T\backslash)$  has to be high enough above the strike price to cover the cost of the option premium.

### **Simple example**

Assume that Bob is the writer for a European call option with IonQ (NYSE: IONQ) as the underlying with spot price  $\backslash(S\_0=\text{€}30\backslash)$ . The contract has maturity time  $\backslash(T\backslash)$  of 30 days from today, strike price  $\backslash(K=\text{€}35\backslash)$ , with a premium of  $\backslash(\text{€}5\backslash)$  per contract. In this simple example we disregard all brokerage and assume that Bob does not already own the underlying asset (referred to as a naked call option).

Is this premium too high? Is it too low? Is it perhaps a fair price? 🤔

Alice is interested in buying this call option but is unsure whether Bob has a fair premium on the contract. However, Alice strongly believes that IonQ will be trading for  $\backslash(\text{€}50\backslash)$  in 30 days (i.e. at maturity  $\backslash(T\backslash)$ ). Fast forward 30 days and in this case Alices' beliefs turned out to be true, thus she will make  $\backslash(S\_T - K - \text{premium}\backslash) = 50 - 35 - 5 = \text{€}10\backslash$  per contract.

If IonQ would be worth less than the strike price  $(K)$  at maturity  $(T)$  then the option is not exercised and expires worthless. The holder (Alice) loses the premium and the writer (Bob) profits on the premium.

Why would Bob want to write this specific call option? Based on the strike price  $(K=€35)$  and the premium  $(€5)$  we know that Bob makes money if IonQ is trading for less than  $(€40)$  at maturity ( $\text{premium} - (S_T - K) = 5 - (40 - 35) = 5 - 5 = €0$ ). If  $(S_T=€38)$  then Bob makes  $(5 - (38 - 35) = €2)$  per contract. So Bob would only really want to write this call option because he believes that IonQ will not be worth much more in the future.

In our simple case above Alice accepted the premium (the price of the option) based solely on her strong belief that IonQ would be worth much more in the future. But could she in some way have made a better decision on whether or not the premium of the call option was fair?

Yes, she herself could have estimated a fair price of the call option based on e.g. the current spot price  $(S_t)$ , the desired strike price  $(K)$ , the time to maturity  $(T)$ , the risk-free rate  $(r)$ , the assets implied volatility  $(\sigma)$  by, and a prediction on the value of the underlying at maturity, by estimating the discounted expected payoff

$$v = e^{-rT} \mathbb{E}[\phi(S_T)] = e^{-rT} \mathbb{E}[\max(S_T - K, 0)].$$

So what should be the fair price of the European call option? Let's estimate it using quantum computing! 

## 1. Asset distributions and payoff function

The first step in estimating a fair price for the European call option is to encode/load the distribution of the underlying asset on to a quantum circuit. Assume that the underlying asset can be described by the Geometric Brownian Motion

$$dS_t = rS_t dt + \sigma S_t dW_t$$

and that we follow the Black & Scholes model such that the spot price at time  $(S_t)$  is described by the following log-normal distribution

$$\ln(\frac{S_T}{S_t}) \sim N(r - \frac{1}{2}\sigma^2 T, \sigma \sqrt{T})$$

where  $(\mu)$  is the annual drift rate of  $S$  and we denote  $(\sigma')$  as its scaled volatility, such that

$$\begin{aligned} \mu &= (r - \frac{\sigma^2}{2})T + \log(S_0) \\ \sigma' &= \sigma \sqrt{T} \end{aligned}$$

Because we will be working with quantum circuits in this tutorial, we will have to create an equidistant discretization of the distribution on to  $(2^n)$  grid points, where  $(n)$  is the number of qubits of our quantum circuit. To be able to do this we also have to limit the range of the distribution to some interval, e.g., between 3 standard deviations of its mean

$$x \sim N(\mu, \sigma') \in [\mu - 3\sigma', \mu + 3\sigma']$$

### Exercise

Now we want you to:

1. Classically create the distribution that we just defined, and sample from it on an equidistant interval.
2. Change the variables around and see how the distribution of the spot price at maturity \(\(S\_T\)\) changes.
3. What happens if the asset has a large initial spot price \(S\_0 > 10\) with a relatively high volatility  $(\sigma > 0.2)$ ?
  - Hint: perhaps we have too few qubits to represent such a “wide” distribution?

Some help to get you started:

- To calculate  $(\mu)$  and  $(\sigma)$  refer to the above equations.
- To create an equidistant range with  $(2^n)$  grid points you can use the `np.linspace` method.
- Normalizing the distribution in this context means that the probabilities should sum to 1.

```

import numpy as np
import matplotlib.pyplot as plt
from scipy import stats

n_uncertainty_qubits = 3 # change this also if you want to :)
n_qubit_states = 2 ** n_uncertainty_qubits

S = 2 # initial spot price
volatility = 0.4 # implied volatility
r = 0.05 # risk-free market rate
T = 40 / 365 # time to maturity

mu = ... # this should be the annualized drift rate of S
sigma = ... # this should be the scaled volatility

# Some properties of the log-normal distribution
# https://en.wikipedia.org/wiki/Log-normal_distribution
mean = np.exp(mu + 0.5 * sigma ** 2).
variance = (np.exp(sigma ** 2) - 1) * np.exp(2 * mu + sigma ** 2).
std dev = np.sqrt(variance)

low = np.maximum(mean - 3 * std dev, 0)
high = mean + 3 * std dev

# Scipy log-normal distribution
# https://docs.scipy.org/doc/scipy/reference/generated/scipy.stats.lognorm.html
lognorm scale = S * np.exp(r * T - 0.5 * sigma ** 2).
xx = ... # create an equidistant interval from `low` to `high` with `n qubit states` grid points
yy = stats.lognorm.pdf(xx, sigma, scale=lognorm scale) / sigma
yy = ... # normalize the pdf

plt.figure().
plt.bar(xx, yy, width=0.2, alpha=0.5)
plt.plot(xx, yy, linewidth=2, color="blue")
plt.xticks(np.arange(min(xx) - 0.05, max(xx) + 0.05, (max(xx) - min(xx)) / 10), size=12, rotation=70)
plt.yticks(size=12)
plt.title(r"$\ln \frac{S}{T} \sim N((r - \frac{\sigma^2}{2})T, \sigma\sqrt{T})$",
size=20)
plt.xlabel("Spot price at maturity $S/T (\u20ac)", size=15)
plt.ylabel("Probability (%)", size=15)
plt.grid()
plt.show().

```

## Encode the distribution onto a quantum circuit

Next we need to construct a circuit to load the log-normal distribution into a quantum state. The distribution as defined before is truncated to the given interval  $([\mu - 3\sigma, \mu + 3\sigma])$  and discretized using  $(2^n)$  grid points, where  $(n)$  denotes the number of qubits we are using. The unitary operator  $(\mathcal{A})$  corresponding to the circuit can be represented as

$$\sum_{i=0}^{2^n - 1} p_i |\psi_i\rangle$$
 where  $|\psi_i\rangle$  is the  $(i^{\text{th}})$  state,  $p_i$  represents the probability of measuring the  $(i^{\text{th}})$  discretized grid.

We can use a pre-defined circuit from the `qiskit-finance` library which calculates the same probabilities as we did above and then initializes a circuit with gates that encode the probabilities for the states. It uses the `Initialize` class from the main `qiskit` library to create a circuit with gates that represent the provided probabilities.

## Exercise

No we want you to:

1. Change the number of qubits (defined in the code cell above) and see how the depth of the circuit changes.
  - What happens to the depth? Is this a sustainable behaviour?
2. Look at the types of gates and try and think about what would happen if the hardware we wanted to run on only supported a certain set of (native) basis gates. Do you think the circuit would be deeper? Shallower? What are your thoughts?
  - You will get to explore this practically later in the tutorial, but it is good to start thinking about already.
3. Verify that the quantum circuit has implemented the expected distribution (the one you made in the code cell above).

```
from qiskit_finance.circuit.library import LogNormalDistribution

uncertainty_model = LogNormalDistribution(
    n_uncertainty_qubits, mu=mu, sigma=sigma**2, bounds=(low, high))
.)

decomposed_uncertainty_model = uncertainty_model.decompose(reps=10)

print(f"Depth of the P(X) circuit: {decomposed_uncertainty_model.depth()}")
({n_uncertainty_qubits} qubits"))
display(uncertainty_model.draw("mpl"))
display(decomposed_uncertainty_model.draw("mpl"))

# Verify that the circuit encodes the same probability distribution.
# You should see the exact same distribution as above when we used
`scipy.stats.lognorm.pdf`.

xx = uncertainty_model.values
yy = uncertainty_model.probabilities

plt.figure()
plt.bar(xx, yy, width=0.2, alpha=0.5)
plt.plot(xx, yy, linewidth=2, color="blue")
plt.xticks(np.arange(min(xx) - 0.05, max(xx) + 0.05, (max(xx) - min(xx)) / 10),
size=12, rotation=70)
plt.yticks(size=12)
plt.title(r"\$ln \frac{S_T}{S_0} \sim N((r - \frac{\sigma^2}{2})T, \sigma\sqrt{T})$",
size=20)
plt.xlabel(r"Spot price at maturity \$S_T (\u20ac)", size=15)
plt.ylabel(r"Probability (\u20ac)", size=15)
plt.grid()
plt.show()
```

## Encoding the payoff function

Next step is to encode the payoff function onto a quantum circuit. Remember that the payoff function is defined as

$$\lfloor f(X) = \max(X - K, 0) \rfloor$$

and since we have a equidistant discretized grid for the random variable  $\langle X \rangle$  on  $\langle [0, 1, \dots, 2^n - 1] \rangle$  we can define an operator  $\langle \mathcal{F} \rangle$  as

$\lfloor \langle \mathcal{F} \rangle \ket{i}_n \ket{0} = \sqrt{1 - f(i)} \ket{i}_n \ket{0} + \sqrt{f(i)} \ket{i}_n \ket{1} \rfloor$   
where it is required that the function  $\langle f(x) \mapsto [0, 1] \rangle$ . Applying the operator  $\langle \mathcal{F} \rangle$  to our distribution operator  $\langle \mathcal{A} \rangle \ket{0}_n \ket{0}$  yields

$$\lfloor \langle \mathcal{F} \rangle \mathcal{A} \ket{0}_n \ket{0} = \dots \ket{0} + \sum_{i=0}^{2^n-1} \sqrt{f(i)} \sqrt{p_i} \ket{i}_n \ket{1} \rfloor$$

where we get that the probability of measuring  $\langle \ket{1} \rangle$  in the final qubit is

$$\lfloor \sum_{i=0}^{2^n-1} f(i)p_i = \mathbb{E}[f(X)] \rfloor$$

However, we have a problem, because our payoff function does not currently map to the  $\langle [0, 1] \rangle$  interval. To fix this we can rescale it as

$$\lfloor \hat{f}(X) = \frac{f(\phi(X))}{f(X_{\max})}, \text{ with } \phi(X) = X_{\min} + X^* \frac{X_{\max} - X_{\min}}{2^n - 1}. \rfloor$$

### Exercise

No we want you to:

1. Set a desired strike price  $\langle K \rangle$ .
2. Implement the payoff function  $\langle f(X) \rangle$  classically.

Some help:

- Set the strike price based on your belief on how the underlying assets value will evolve until the time to maturity.
- The `np.maximum` method can be used to get the largest of two values.

```

K = ... # define a strike price

xx = uncertainty_model.values
yy = ... # implement the payoff function

plt.figure()
plt.plot(xx, yy, linewidth=2, color="red", marker=".", ms=8)
plt.title(r"Payoff function $\phi(S_T) = \max(S_T - K, 0)$", size=20)
plt.xlabel(r"Spot price at maturity $S_T$ (€)", size=15)
plt.ylabel(r"Payoff amount (€)", size=15)
plt.xticks(np.arange(min(xx) - 0.05, max(xx) + 0.05, (max(xx) - min(xx)) / 10), size=12, rotation=70)
plt.yticks(size=12)
plt.grid()
plt.show()

```

Now we want to implement this function on a quantum circuit. The [LinearAmplitudeFunction](#) in the qiskit circuit library uses [PiecewiseLinearPauliRotations](#) to implement the piecewise linear function which is our payoff function.

### Exercise

1. Set the slopes of the piecewise payoff function.
2. Set the minimum and maximum value that the payoff function can have.

Some help:

- Look at the above plot of the payoff function and try and figure out which two lines together make up the payoff function.
  - Hint: At the strike price  $(K)$  we start making money, before that, we profit nothing (payoff=0).
- What is the minimum amount of money that we can make? Think logically 😊
- The maximum amount of money we can make depends on the highest value in our equidistant range.

```

from qiskit.circuit.library import LinearAmplitudeFunction

# approximation scaling for the payoff function, determines accuracy in the Taylor
# approximation.
# https://www.nature.com/articles/s41534-019-0130-6
c_approx = 0.25

# piecewise linear with breakpoints on x min and when S T >= K.
breakpoints = (low, K)
slopes = ... # set the slopes of the piecewise linear payoff function
offsets = (0, 0)
f_min = ... # set the minimum value that the payoff function can have
f_max = ... # set the maximum value that the payoff function can have
european_call_objective = LinearAmplitudeFunction(
    num_state_qubits=n uncertainty_qubits,
    slope=slopes,
    offset=offsets,
    domain=(low, high),
    image=(f_min, f_max),
    breakpoints=breakpoints,
    rescaling_factor=c_approx,
)
decomposed_european_call_objective = european_call_objective.decompose(reps=10)

print(f"Depth of the f(x) circuit: {decomposed_european_call_objective.depth()}")
(n uncertainty_qubits) qubits))
display(decomposed_european_call_objective.draw("mpl"))

```

## Wait, now we are working with more qubits than we originally specified for $\langle P(X) \rangle$ .. ?

For each qubit in our  $\langle P(X) \rangle$  circuit we need an equal amount of qubits as ancilla qubits for the payoff function circuit, plus one extra qubit which encodes the value that we are trying to estimate in its  $\langle \ket{1} \rangle$  state.

### Exercise

1. For a circuit with  $n$  qubits for the  $\langle P(X) \rangle$  circuit, how many total qubits would we need to construct the full circuit with both  $\langle P(X) \rangle$  and the payoff function circuit?
  - Hint: change the number of qubits for  $\langle P(X) \rangle$  and see how the number of qubits changes for the payoff function circuit.

**Now we need to add the  $\langle P(X) \rangle$  distribution circuit to before the payoff function**

```

from qiskit import AncillaRegister, ClassicalRegister, QuantumCircuit, QuantumRegister

n_payoff_qubits = european_call_objective.num_qubits
n_cl_bits = 1

qreg_s = QuantumRegister(n_uncertainty_qubits, "s")
qreg_target = QuantumRegister(1, "q")
qreg_a = AncillaRegister(n_payoff_qubits - n_uncertainty_qubits - 1, "a")
creg = ClassicalRegister(n_cl_bits, "creg")

european_call = QuantumCircuit(qreg_s, qreg_target, qreg_a)
european_call.append(uncertainty_model, range(n_uncertainty_qubits))
european_call.append(european_call_objective, range(n_payoff_qubits))

measured_european_call = european_call.copy()
measured_european_call.add_register(creg)
measured_european_call.measure(qreg_target, creg)

decomposed_measured_european_call = measured_european_call.decompose(reps=10)
decomposed_measured_european_call = measured_european_call.decompose(reps=10)

print(f"Depth of the P(X) + f operations circuit:\n{decomposed_measured_european_call.depth()}\n({decomposed_measured_european_call.num_qubits} qubits)")

display(measured_european_call.draw("mpl"))
display(decomposed_measured_european_call.draw("mpl"))

```

## **Do you see any potential issues with the circuit depth?**

What would happen to the depth if we had to apply the payoff function circuit  $\backslash(f(x)\backslash)$  multiple times?

## **2. Classical Monte Carlo on a QC**

If we sample multiple times from the circuit that we have defined above then we can get an estimate of the expected payoff, however, this is just classical monte carlo but performed using quantum circuits.

There is no potential speed-up involved by doing this, but doing this step might be helpful for you to see and understand the gains with doing actual Quantum Monte Carlo (also referred to as Quantum Amplitude Estimation), which you will get to do soon in this tutorial.

### **Estimate the expected payoff for the European call option**

Now you will perform classical monte carlo using the quantum circuit that you created above. We are specifically interested in the probability of measuring the  $\backslash(\ket{1})\backslash$  state in the target qubit

$$\mathbb{P}(\text{measure } 1) = \mathbb{E}[f(X)] = \sum_{i=0}^{2^n-1} f(i)p_i$$

and with probability  $\delta$ , the estimate  $\tilde{\mu}$  satisfies  $|\mu - \tilde{\mu}| \leq \epsilon$  with

$$|\mu - \tilde{\mu}| \leq \phi^{-1} \Big( 1 - \frac{\delta}{2} \Big) \frac{\text{Var}(f(S_T))}{\sqrt{N}} \sim \mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$$

## Exercise

1. Determine how many samples you want to take.

- Try both a small - and a large amount, and see how the estimation and its confidence bound changes.

2. Rescale the estimated value to its original interval  $[x_{\min}, x_{\max}]$ .

- Hint: the circuit used for implementing the objective function has a method called `post_processing` that can be used to map the scaled results to its original domain.

3. Define a confidence bound on the estimated value.

- Hint: assume a confidence bound on  $[\mu - 2\sigma, \mu + 2\sigma]$  and use the same method as above to rescale to the correct interval.

```
from qiskit.primitives import StatevectorSampler as Sampler

sampler = Sampler()
n_shots = ... # how many samples do you want to take for your MC?
result = sampler.run([measured_european_call,], shots=n_shots).result()

quasi_dist_dict = result[0].data.creg.get_int_counts()
quasi_dist = np.array([quasi_dist_dict[0], quasi_dist_dict[1]]).T
dist = quasi_dist / quasi_dist.sum()

plt.figure()
plt.bar(["|0>", "|1>"], dist, width=0.2, alpha=0.8)
plt.yticks(size=12)
plt.xticks(size=12)
plt.title(r"Probability of measuring either $|0>$ or $|1>$", size=20)
plt.ylabel(r"Quasi-probability ($\%$)", size=15)
plt.grid()
plt.show()

p_hat = dist[1]
p_std = np.sqrt(p_hat * (1 - p_hat) / n_shots)

print(f"Raw estimated mu={p_hat:.5f}, std={p_std:.5f}")

mc_expectation = ... # estimated value
mc_lower_conf = ... # lower confidence bound
mc_upper_conf = ... # upper confidence bound

print(f"Estimation of the expected payoff:\t\t{mc_expectation:.5f}")
exact_value = np.dot(uncertainty_model.probabilities,
np.maximum(uncertainty_model.values - K, 0))
print(f"Exact expected value from discretization:\t\t{exact_value:.5f}")
print(f"Confidence bound on estimation:\t\t\t{mc_lower_conf:.5f}, {mc_upper_conf:.5f}")
```

### 3. Quantum Amplitude Estimation (QAE)

Remember that the standard Monte Carlo method for pricing consists in approximating the expected payoff  $\langle \mu = \mathbb{E}[f(S_T)] \rangle$  as

$\langle \mu \approx \tilde{\mu} \rangle_N = \frac{1}{N} \sum_{i=1}^N f(S_T^{(i)})$ , where  $(S_T^{(i)}, i=1, \dots, N)$  are i.i.d samples from the probability distribution of the underlying asset  $(S)$  at the expiration time  $(T)$ . Note that a consequence of the central limit theorem is that the estimation error of the classical Monte Carlo method satisfies

$$|\langle \mu - \tilde{\mu} \rangle| \sim \mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$$

and the posed question is whether or not the estimation error rate can be improved on?

Quantum Amplitude Estimation (QAE) is a quantum algorithm that provides an alternative to the classical Monte Carlo in order to compute approximate expectations of random variables.

Suppose we are able to construct a circuit that implements a state preparation operator  $(\mathcal{U})$  acting on an  $((n+1))$  qubit register as follows

$$\langle \mathcal{U}|0\rangle_{n+1} = \sqrt{1-a}|\psi_0\rangle_n|0\rangle + \sqrt{a}|\psi_1\rangle_n|1\rangle$$

where  $(a \in [0, 1])$  is an unknown quantity associated with the value  $(\mu)$  which we want to estimate (e.g. an appropriate re-scaling of  $(\mu)$  to the interval  $([0, 1])$ ).

Then, QAE can be used to obtain an estimate of  $(a)$  through repeated controlled applications of the [Grover operator](#)

$\langle \mathcal{Q} = \mathcal{U}S_0\mathcal{U}^\dagger S_{|\Psi_0\rangle}$  together with an inverse [Quantum Fourier Transform \(QFT\)](#), where  $(S_0)$  is the zero reflection and  $(S_{|\Psi_0\rangle})$  is the phase oracle in the Grover operator. For further details on the algorithm, please refer to [Quantum Amplitude Amplification and Estimation](#). Brassard et al., 2000.

It can be showed that, with high probability  $((8/\pi^2 \approx 81\%))$ , the estimate  $(\tilde{a}_M)$  provided by the QAE satisfies

$$|a - \tilde{a}_M| \leq \frac{2\pi\sqrt{a(1-a)}}{M} + \frac{\pi^2 M^2}{2} \sim \mathcal{O}\left(\frac{1}{M}\right)$$

where  $(M=2^m)$ , and  $(m)$  is the number of ancilla qubits used by the algorithm (which determines how many repetitions of the operator  $(\mathcal{Q})$  should be applied).

Comparing this to classical Monte Carlo and we can see that QAE provides a (theoretical) quadratic speedup.

Quantum Amplitude Estimation can be applied to our circuit that we performed classical Monte Carlo on, and doing QAE should theoretically improve our estimation on the fair price of the European call option.

So lets apply QAE and see if we get a better result than classical Monte Carlo! 

## **Exercise**

1. Pick  $\langle m \rangle$ , i.e., the number of repetitions of  $\langle \mathcal{Q} \rangle$ .
  - How is the depth of the circuit impacted by the choice of  $\langle m \rangle$ ?

```

# Define QAE circuit
from qiskit import QuantumCircuit, QuantumRegister, AncillaRegister, ClassicalRegister
from qiskit.circuit.library import QFT, GroverOperator
class AECircuit(QuantumCircuit):
    def __init__(self, state_preparation_circuit, num_ancilla_qubits, objective_qubit):
        self.state_preparation_circuit = state_preparation_circuit # The circuit
        implementing operator A
        self.num_ancilla_qubits = num_ancilla_qubits # Number of ancilla qubits (m in
        IQAE paper)
        self.num_state_qubits = state_preparation_circuit.num_qubits # Number of qubits
        in circuit A (n+1 in the IQAE paper)
        self.objective_qubit = objective_qubit # Index of the objective qubit within
        the circuit A (0<=objective_qubit<=num_state_qubits)

    # Initialize circuit
    ancilla_register = AncillaRegister(self.num_ancilla_qubits, name="ancilla")
    state_register = QuantumRegister(self.num_state_qubits, name="state")
    classical_register = ClassicalRegister(self.num_ancilla_qubits, name="creg")
    super().__init__(
        ancilla_register,
        state_register,
        classical_register
    )

    # Hadamard gates on the ancilla qubits
    for j in range(self.num_ancilla_qubits):
        self.h(ancilla_register[j])

    # Circuit A on the state and objective qubits
    A_gate = self.state_preparation_circuit.to_gate(label="$A$")
    self.append(A_gate, state_register[:])

    self.barrier()

    # Powers of Q
    Q = self.groverOp(self.state_preparation_circuit, self.objective_qubit)
    for j in range(num_ancilla_qubits):
        Qj = Q**j.to_gate(label=f"$Q^{2**j}$").control(1) # Controlled
        version of Q^{2j}
        # Apply the controlled Q^{2j} gate on state and objective qubits,
        controlled by the j-th ancilla qubit
        self.append(Qj, [ancilla_register[self.num_ancilla_qubits-j-1]] +
        state_register[:])

    self.barrier()

    # Inverse QFT
    QFT_gate = QFT(num_qubits=self.num_ancilla_qubits, inverse=True,
    do_swaps=False).to_gate(label="$QFT^\dagger$")
    self.compose(QFT_gate, ancilla_register, inplace=True)

    self.barrier()

    # Measure the ancilla qubits
    self.measure(ancilla_register, classical_register)

def groverOp(self, state_preparation_circuit, objective_qubit):
    # construct the grover operator
    oracle = QuantumCircuit(max(state_preparation_circuit.num_qubits -
    state_preparation_circuit.num_ancillas, 1))
    oracle.h(objective_qubit)
    oracle.x(objective_qubit)
    oracle.h(objective_qubit)

```

```

Q = GroverOperator(oracle, state_preparation_circuit)
return Q

```

```

m = ... # The number of Q repetitions (number of ancilla qubits)
M = 2 ** m
n_ancilla_qubits = m
qae = AECircuit(
    state_preparation_circuit=decomposed_european_call,
    num_ancilla_qubits=n_ancilla_qubits,
    objective_qubit=n_uncertainty_qubits,
).
decomposed_qae = qae.decompose(reps=10)

print(f"Depth of the full QAE circuit: {decomposed_qae.depth()}")
({decomposed_qae.num_qubits} qubits) ({m} ancilla qubits)).
display(qae.draw("mpl")).


```

Recall from the lecture that quantum amplitude estimation uses a combination of phase estimation and amplitude amplification in order to get an estimate of  $\tilde{\mu}$ , specifically, because of the inverse QFT, what we are measuring from the quantum circuit is a number  $\tilde{q}$  ( $\tilde{q} \in \{0, 1, \dots, 2^m - 1\}$ ) that we have to map to the actual estimate through

$$\tilde{\mu} = \sin^2 \left( \frac{\pi \tilde{q}}{2^m} \right)$$

Now you should run the QAE circuit that was constructed above. Note that in a world with perfect quantum computers, with no errors, we would only have to run this circuit once.

However, we do not (yet?) live in such a world, and thus we have to sample  $\tilde{q}$  multiple times.

### Exercise

1. Define how many times you want to sample/measure from the QAE circuit.

```

sampler = Sampler()
n_shots = ... # how many samples do you want to take for the estimation?
result = sampler.run([qae], shots=n_shots).result()

```

### Exercise

1. Calculate the angles based on the measured values  $\tilde{q}$ :
  - Hint: the formula for the angle is  $\frac{\pi \tilde{q}}{2^m}$
2. Calculate the estimates based on the angles:
  - Hint: the formula for the estimate is  $\tilde{\mu} = \sin^2 \left( \frac{\pi \tilde{q}}{2^m} \right)$
  - Optional: round it to a suitable number of decimals (e.g. 15)
3. Determine which estimate has the highest probability and then post-process it.
  - Hint: you can use the `np.argmax` method to get the index with the largest value.

```

#
# QAE Post-processing
#

counts = result[0].data.creg.get_int_counts()
qq = np.array(list(counts.keys()))

theta_estimates = ... # Calculate the angles
estimates = ... # Calculate the estimates

probabilities = np.array(list(counts.values()), dtype="float64")
probabilities = probabilities / probabilities.sum()

# Combine any estimate or probability duplicates (because sin is periodic)
unique_estimates = list(set(estimates))
unique_probabilities = [np.sum(probabilities[estimates==e]) for e in unique_estimates]
qae_estimates = np.array(unique_estimates)
qae_probabilities = np.array(unique_probabilities)

qae_p_mode = ... # Extract the estimate with the highest probability
qae_expectation = european_call_objective.post_processing(qae_p_mode)

print("Exact MC QAE")
print("="*70)
print(f"Expectation: {exact_value:.5f} {mc_expectation:.5f} {qae_expectation:.5f}")
print(f"Diff (abs): N/A {np.abs(exact_value - mc_expectation):.5f} {np.abs(exact_value - qae_expectation):.5f}")
print(f"Diff (%): N/A {np.abs(exact_value - mc_expectation)/mc_expectation:.5f} {np.abs(exact_value - qae_expectation)/qae_expectation:.5f}")

```

## What if we wanted to run this QMC circuit on a specific backend?

If you for example wanted to run this circuit on the Helmi QC then you would have to transpile the circuit to be compatible with the native gate set of the target backend.

Qiskit has a method for (attempting) translating ([transpiling](#)) your circuit with your gates to the target gate set, this method is called [transpile](#) and composes 6 different stages (each of which can be read about in detail on the provided link).

The 5th stage in the transpilation process is called [optimization](#) and can be controlled by the user by specifying what optimization level you want to have. The optimization stage is necessary in order to manage increased circuit depths due to the transpilation process potentially adding a lot of gates in order to both: map the source gates to the target gate set, but also to match the target hardware qubit topology. We have discussed circuit depth quite a bit in this tutorial, and one way to (potentially) cope with extremely deep circuits is through [transpilation optimization](#).

The user can specify what optimization level they want to run with:

0. [no optimization](#)
1. [light optimization](#)

2. heavy optimization
3. even heavier optimization

and the default level is 2. The higher the optimization level, the more optimized circuits, at the expense of longer transpilation times. Important to note is that the transpilation process is stochastic and will thus generate circuits with e.g. varying depth and gate layout even for the same source circuit.

### Exercise

1. Decide on a set of native gates that you want to have as target for the transpilation process.
  - If you have the time, you could try and find the specifications of a real QPU and its native gate set and use that. Here is a [link](#) for the IBM QPUs.
2. Set your desired optimization level and see how the depth of the circuit changes as you change the optimization level.
  - How many gates can you remove from the original (extremely deep) QAE circuit by optimizing it?
3. Can you find a gate set that you can't transpile the circuit to? Why do you think that is?

```
from qiskit import transpile
from typing import List

backend_native_gates: List[str] = ... # the native gates of the target backend
optimization_level: int = ... # your desired optimization level [0, 3]

transpiled_circuit = transpile(
    circuits=qae,
    basis_gates=backend_native_gates,
    optimization_level=optimization_level,
).

print(transpiled_circuit.depth())

# You can most likely not display this circuit since the transpilation process
# decomposes any grouped gates, meaning, it will try and draw ~100 000 gates...
# display(transpiled_circuit.draw("mpl"))
```

That's all we had prepared for you today, well done! 🎉🌟

Hopefully you had the time to get a better understanding of how quantum amplitude estimation can be used in finance for pricing options, and also that you had the time to reflect on the suitability of these algorithms in the NISQ era.

---

## Code solutions

If you are stuck on a problem or you want to compare your code to our code, look here. 😎

```

#
# Log-normal distribution (classically)
#



import numpy as np
import matplotlib.pyplot as plt
from scipy import stats

n_uncertainty_qubits = 3
n_qubit_states = 2 ** n_uncertainty_qubits

S = 2 # initial spot price
volatility = 0.4 # implied volatility
r = 0.05 # risk-free market rate
T = 40 / 365 # time to maturity

mu = (r - 0.5 * volatility ** 2) * T + np.log(S)
sigma = volatility * np.sqrt(T).

# Some properties of the log-normal distribution
# https://en.wikipedia.org/wiki/Log-normal_distribution
mean = np.exp(mu + 0.5 * sigma ** 2).
variance = (np.exp(sigma ** 2) - 1) * np.exp(2 * mu + sigma ** 2).
std_dev = np.sqrt(variance).

low = np.maximum(mean - 3 * std_dev, 0)
high = mean + 3 * std_dev

# Scipy log-normal distribution
# https://docs.scipy.org/doc/scipy/reference/generated/scipy.stats.lognorm.html
lognorm_scale = S * np.exp(r * T - 0.5 * sigma ** 2).
xx = np.linspace(low, high, num=n_qubit_states)
yy = stats.lognorm.pdf(xx, sigma, scale=lognorm_scale) / sigma
yy = yy / yy.sum().

plt.figure().
plt.bar(xx, yy, width=0.2, alpha=0.5)
plt.plot(xx, yy, linewidth=2, color="blue")
plt.xticks(np.arange(min(xx) - 0.05, max(xx) + 0.05, (max(xx) - min(xx)) / 10), size=12, rotation=70)
plt.yticks(size=12)
plt.title(r"$\ln \frac{S}{I} \sim N((r - \frac{\sigma^2}{2})T, \sigma\sqrt{T})$",
size=20)
plt.xlabel(r"Spot price at maturity $S/I\$ (\u20ac)", size=15)
plt.ylabel(r"Probability (\u20ac)", size=15)
plt.grid()
plt.show()

```

```

#
# Encoding the payoff function (classically)
#

K = 1.713 # this can be whatever..

xx = uncertainty_model.values
yy = np.maximum(xx - K, 0).

plt.figure()
plt.plot(xx, yy, linewidth=2, color="red", marker=".", ms=8)
plt.title(r"Payoff function $\phi(S_T) = \max(S_T - K, 0)$", size=20)
plt.xlabel(r"Spot price at maturity $S_T$ ($\text{€}$)", size=15)
plt.ylabel(r"Payoff amount ($\text{€}$)", size=15)
plt.xticks(np.arange(min(xx) - 0.05, max(xx) + 0.05, (max(xx) - min(xx)) / 10), size=12, rotation=70)
plt.yticks(size=12)
plt.grid()
plt.show()

```

```

#
# Encoding the payoff function (QC)
#

from qiskit.circuit.library import LinearAmplitudeFunction

# approximation scaling for the payoff function, determines accuracy in the Taylor
# approximation.
# https://www.nature.com/articles/s41534-019-0130-6
c_approx = 0.25

breakpoints = (low, K)
slopes = (0, 1)
offsets = (0, 0)
f_min = 0
f_max = high - K
european_call_objective = LinearAmplitudeFunction(
    num_state_qubits=n_uncertainty_qubits,
    slope=slopes,
    offset=offsets,
    domain=(low, high),
    image=(f_min, f_max),
    breakpoints=breakpoints,
    rescaling_factor=c_approx,
)

decomposed_european_call_objective = european_call_objective.decompose(reps=10)

print(f"Depth of the f(x) circuit: {decomposed_european_call_objective.depth()}")
(f{n_uncertainty_qubits} qubits).
display(decomposed_european_call_objective.draw("mpl"))

```

```

#
# Performing classical MC on a QC
#

from qiskit.primitives import StatevectorSampler as Sampler

sampler = Sampler()
n_shots = 100_000
result = sampler.run([measured_european_call, ], shots=n_shots).result()

quasi_dist_dict = result[0].data.creg.get_int_counts()
quasi_dist = np.array([quasi_dist_dict[0], quasi_dist_dict[1]]).
dist = quasi_dist / quasi_dist.sum()

plt.figure()
plt.bar(["|0>", "|1>"], dist, width=0.2, alpha=0.8)
plt.yticks(size=12)
plt.xticks(size=12)
plt.title(r"Probability of measuring either $|0>$ or $|1>$", size=20)
plt.ylabel(r"Quasi-probability ($\%$)", size=15)
plt.grid()
plt.show()

p_hat = dist[1]
p_std = np.sqrt(p_hat * (1 - p_hat) / n_shots)

print(f"Raw estimated mu={p_hat:.5f}, std={p_std:.5f}")

expectation = european_call_objective.post_processing(p_hat)
lower_conf = european_call_objective.post_processing(p_hat - 2 * p_std)
upper_conf = european_call_objective.post_processing(p_hat + 2 * p_std)

print(f"Estimation of the expected payoff:\t\t{expectation:.5f}")
exact_value = np.dot(uncertainty_model.probabilities,
np.maximum(uncertainty_model.values - K, 0))
print(f"Exact expected value from discretization:\t{exact_value:.5f}")
print(f"Confidence bound on estimation:\t\t\t{lower_conf:.5f}, {upper_conf:.5f}")

```

```

#
# QAE Post-processing
#
counts = result[0].data.creg.get_int_counts()
qq = np.array(list(counts.keys()))

theta_estimates = qq * np.pi / M
estimates = np.round(np.sin(theta_estimates) ** 2, 15)

probabilities = np.array(list(counts.values()), dtype="float64")
probabilities = probabilities / probabilities.sum()

# Combine any estimate or probability duplicates (because sin is periodic)
unique_estimates = list(set(estimates))
unique_probabilities = [np.sum(probabilities[estimates==e]) for e in unique_estimates]
qae_estimates = np.array(unique_estimates)
qae_probabilities = np.array(unique_probabilities)

qae_p_mode = qae_estimates[np.argmax(qae_probabilities)]
qae_expectation = european_call_objective.post_processing(qae_p_mode)

print("Exact MC QAE")
print("="*70)
print(f"Expectation: {exact_value:.5f} {mc_expectation:.5f} {qae_expectation:.5f}")
print(f"Diff (abs): N/A {np.abs(exact_value - mc_expectation):.5f} {np.abs(exact_value - qae_expectation):.5f}")
print(f"Diff (%): N/A {np.abs(exact_value - mc_expectation)/mc_expectation:.5f} {np.abs(exact_value - qae_expectation)/qae_expectation:.5f}")

```

```

#
# Transpiling and optimizing quantum circuits using qiskit
#
from qiskit import transpile
from typing import List

backend_native_gates: List[str] = ["u", "x", "ry", "cx"]
optimization_level: int = 3

transpiled_circuit = transpile(
    circuits=qae,
    basis_gates=backend_native_gates,
    optimization_level=optimization_level,
)

print(transpiled_circuit.depth())

# You can most likely not display this circuit since the transpilation process
# decomposes any grouped gates, meaning, it will try and draw ~100 000 gates...
# display(transpiled_circuit.draw("mpl"))

```

## References

- [Quantum Risk Analysis. Woerner, Egger. 2018.](#)
- [Option Pricing using Quantum Computers. Stamatopoulos et al. 2019.](#)

- [Pricing of a European call option. Pachon, Ricardo. 2014.](#)

# QSIP - Quantum Sweden Innovation Platform

 Slides

## Tutorial - Solving Flight Scheduling Optimization using QAOA

Quantum computing has introduced a new approach for solving complex optimization problems. Notably, the **Quantum Approximate Optimization Algorithm (QAOA)** – a hybrid (quantum-classical) – has emerged as a promising candidate. In this tutorial, we will see how QAOA can be applied to solve a real-world optimization problem, specifically, the tail-assignment problem – with **Qiskit**.

### Requirements

Before starting this tutorial, be sure you have the following installed:

- Qiskit SDK v1.0 or later, with visualization support (`pip install 'qiskit[visualization]'`)
- Qiskit Runtime v0.22 or later (`pip install qiskit-ibm-runtime`)
- Qiskit AER v0.15.0 or later (`pip install qiskit-aer`)

### The Tail-Assignment Problem

The tail-assignment problem is a complex combinatorial optimization challenge arising in the airline industry, specifically in aircraft scheduling tasks. The objective is to assign a specific aircraft (identified by its tail number), also called a *route*, to a sequence of flights while:

1. **Satisfying operational constraints** (e.g., maintenance schedules, turnaround times, crew availability).
2. **Minimizing operational costs** (e.g., fuel usage, delay penalties).

### Why Is It Hard?

The tail-assignment problem is classified as **NP-hard**. This means that as the number of flights and aircraft increases, finding an optimal solution becomes computationally infeasible for traditional algorithms due to exponential growth in complexity. A common classical approach to this problem is **column generation**, which breaks the problem into smaller subproblems to make it manageable.

### Mathematical Formulation

The tail-assignment problem can be formulated as the following integer linear program:

(1)  $\min \sum_{r \in R} c_r x_r$

Such that

(2)  $\sum_{r \in R} A_{fr} x_r = 1, \quad \forall f \in F, \forall r \in R$

Where:

- $\mathcal{R}$ : The set of all possible routes (sequences of flights assigned to an aircraft).
- $c_r$ : The cost associated with route  $r$ .
- $F$ : The set of all activities (e.g., individual flights or sequences of flights).
- $A_{fr}$ : A binary indicator;  $A_{fr} = 1$  if activity  $f$  is part of route  $r$ , and  $0$  otherwise.
- $x_r$ : A binary decision variable;  $x_r = 1$  if route  $r$  is chosen in the solution, and  $0$  otherwise.

## Simplified Problem for This Tutorial

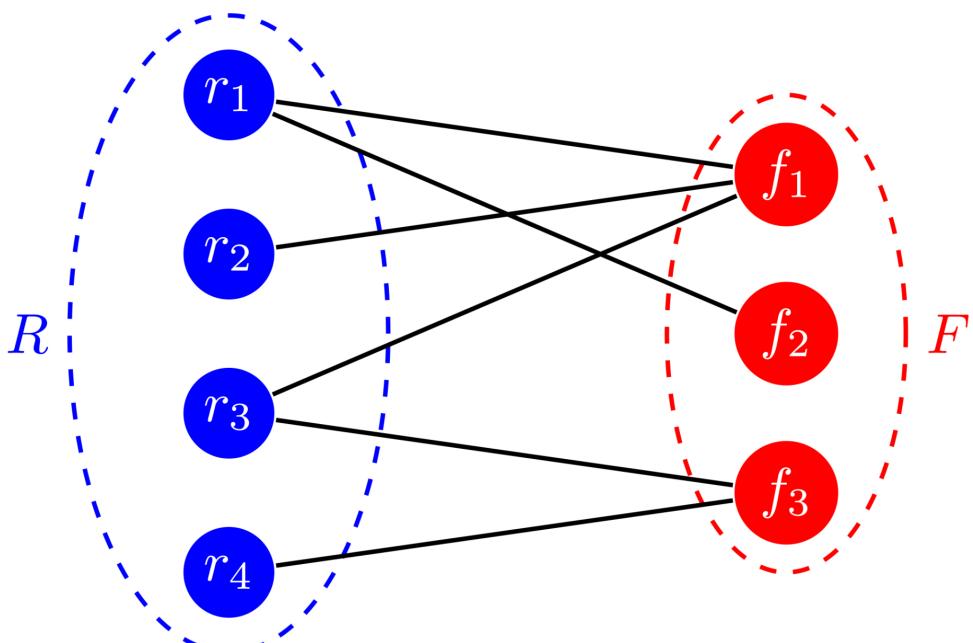
For this tutorial, we focus on a simplified version of the problem where:

- Only one feasible solution exists per instance. This eliminates the need to minimize costs ( $c_r$ ) since it becomes irrelevant when there is a unique solution.
  - The problem reduces to solving the constraints:  $\sum_{r \in R} A_{fr} x_r = 1, \quad \forall f \in F$ , which can be expressed compactly in matrix form as:  $A\vec{x} = \vec{1}$
- $A$ : The constraint matrix.
  - $\vec{x}$ : A vector of binary decision variables.
  - $\vec{1}$ : A vector of ones (length equal to the number of flights).

## Connection to the Exact Cover Problem

This simplified tail-assignment problem is equivalent to the well-known [Exact Cover problem](#). In Exact Cover, the goal is to select a subset of sets such that every element in the universal set is covered exactly once.

## Visual Example:



**Figure Caption:** The Exact Cover problem requires selecting a subset of vertices from  $\{R\}$ , such that exactly one edge connects each vertex in  $\{F\}$ . In the example above, the subset  $\{r_1, r_4\}$  forms an exact cover.

## What You'll Learn in This Tutorial

In this tutorial, we will use the **Quantum Approximate Optimization Algorithm (QAOA)** to solve the simplified tail-assignment problem. We'll explore:

1. How to represent the problem as a quadratic unconstrained binary optimization (QUBO) problem.
2. Mapping the problem to a quantum Hamiltonian.
3. Solving the problem step-by-step using QAOA.

## Loading a problem instance

To begin solving the tail-assignment problem, we need a specific problem instance. In this tutorial, the problem is represented as a constraint matrix  $(A)$ , where:

- Each row corresponds to a flight or activity.
- Each column represents a potential route.
- The entry  $(A_{fr})$  is  $(1)$  if flight  $(f)$  is included in route  $(r)$ , and  $(0)$  otherwise.

By loading the matrix  $(A)$ , we define the structure of the problem and the constraints that must be satisfied. This matrix serves as the foundation for constructing the optimization model.

```
import numpy as np
url = "https://raw.githubusercontent.com/Wikstahl/autumn-school-qas2024/main/data/"
A = np.loadtxt(url + "instance_8.csv", delimiter=',') # load problem data
num_rows, num_cols = A.shape
print(f"Number of flights equals {num_rows}, and number of routes equals {num_cols}.")
```

Number of flights equals 77, and number of routes equals 8.

## Step 1: Map the Optimization Problem to a Hamiltonian

The first step in solving the problem with QAOA is to map the classical optimization problem into quantum circuits and operators. This involves three main steps:

1. **Reformulate the problem using QUBO notation:** Transform the problem into the form of a **Quadratic Unconstrained Binary Optimization (QUBO)**. This step reformulates the problem as a cost function that then makes it easy to map it to a Hamiltonian.

2. **Express the problem as a Hamiltonian:**

Represent the QUBO problem as a Hamiltonian. The goal is to construct a Hamiltonian where the ground state (the lowest energy state) corresponds to the optimal solution of the classical problem.

3. **Design a quantum circuit:** Create a parameterized quantum circuit that creates quantum states representing candidate solutions to the problem. The parameters of this circuit are iteratively adjusted to find states that minimize the Hamiltonian.

By sampling from the quantum states produced by the parametrized quantum circuit (Ansatz), you can evaluate candidate solutions using the cost function encoded in the Hamiltonian.

**Note:** The process combines quantum and classical computation, as the quantum circuit proposes solutions, and a classical optimizer adjusts the circuit's parameters based on feedback from the cost evaluation.

## Map Optimization Problem to QUBO Form

The first step in mapping the tail-assignment problem is to express it in **Quadratic Unconstrained Binary Optimization (QUBO)** form. This involves a notation change, where the optimization problem is represented as:

$$(3) \quad \begin{aligned} f(\vec{x}) = \min_{\vec{x}} \{ & \vec{x} \in \{0, 1\}^n \} \vec{x}^T Q \vec{x}, \\ & \end{aligned}$$

Here:

- $f(x)$  is the **cost function** we aim to minimize.
- $Q$  is an  $(n \times n)$  matrix of real numbers.
- $n$  corresponds to the number of routes.
- $\vec{x}$  is the vector of binary decision variables introduced earlier.
- $\vec{x}^T$  is the transpose of  $\vec{x}$ .

Our next task is to map the tail-assignment problem into QUBO form.

### Step 1.1: Transforming Constraints into a Cost Function

The tail-assignment problem is defined by the constraint  $\langle A \vec{x} \rangle = \langle \vec{1} \rangle$ . To transform this into a QUBO cost function, we subtract  $\langle \vec{1} \rangle$  from the right-hand side and square (via inner product) the expression:

$$(4) \quad \langle A \vec{x} - \vec{1} \rangle^2 = 0$$

This ensures that the cost function evaluates to zero if and only if there exists a binary vector  $\vec{x}$  that satisfy the equation. Thus, the problem can now be expressed as

$$(5) \quad f(\vec{x}) = \min_{\vec{x}} \langle \vec{x} \rangle \in \{0, 1\}^n \langle A \vec{x} - \vec{1} \rangle^2$$

Next we expanding the square of the cost function. Doing this we get:

$$(6) \quad \langle A \vec{x} - \vec{1} \rangle^2 = \langle \vec{x} \rangle^T A^T A \vec{x} - 2 \langle \vec{1} \rangle^T \langle \vec{x} \rangle + \langle \vec{1} \rangle^T \vec{1}$$

Since  $\langle \vec{1} \rangle^T \vec{1}$  is a constant scalar, it does not affect the optimization and can be ignored. This leaves us with two terms:

- $\langle \vec{x} \rangle^T A^T A \vec{x}$ : This term is already in the desired QUBO form.
- $-2 \langle \vec{1} \rangle^T \langle \vec{x} \rangle$ : This is a linear term, which will contribute to the diagonal of the  $(Q)$ -matrix.

To incorporate the linear term into the  $(Q)$ -matrix, we note that:

$$(7) \quad \langle \vec{x} \rangle^T Q \vec{x} = \sum_{i,j} Q_{ij} x_i x_j = \sum_{i=j} Q_{ii} x_i + \sum_{i \neq j} Q_{ij} x_i x_j,$$

where diagonal term is simply  $\langle \sum_i Q_{ii} x_i \rangle$ , since  $\langle x_i x_i \rangle = x_i$ .

Thus, the linear term  $-2 \langle \vec{1} \rangle^T \langle \vec{x} \rangle$  contributes to the diagonal elements of  $(Q)$ . Specifically:

$$(8) \quad -2 \langle \vec{1} \rangle^T \langle \vec{x} \rangle = -2 \sum_{i,j} Q_{ji} x_i$$

This can be written as:

$$(9) \quad -2 \langle \vec{1} \rangle^T \mathbf{diag}(A^T \vec{1}) \vec{x},$$

where  $\mathbf{diag}(A^T \vec{1})$  is a diagonal matrix with diagonal elements:

$$(10) \quad \mathbf{diag}(A^T \vec{1})_j = \sum_i A_{ji}.$$

### Step 1.3: Constructing the $(Q)$ -Matrix

Combining these results, the  $(Q)$ -matrix is given by:

$$(11) \quad Q = A^T A - 2 \mathbf{diag}(A^T \vec{1}).$$

This  $(Q)$ -matrix now fully represents the QUBO form of the tail-assignment problem.

```

def QUBO(A:np.ndarray) -> np.ndarray:
    num_rows = A.shape[0].
    id_vec = np.ones((num_rows,1)) # create column vector with ones
    Q = A.transpose()@A - 2 * np.diag((A.T@id_vec).flatten())
    return Q

Q = QUBO(A)
print(Q).

```

```

[[[-17.,   2.,   0.,   0.,   0.,   3.,   5.,   3.],
 [  2., -18.,   3.,   9.,   4.,   3.,   5.,   2.],
 [  0.,   3., -20.,   0.,   0.,   3.,   5.,   0.],
 [  0.,   9.,   0., -19.,   0.,   6.,   7.,   5.],
 [  0.,   4.,   0.,   0., -21.,   6.,   2.,  12.],
 [  3.,   3.,   3.,   6.,   6., -18.,   3.,   4.],
 [  5.,   5.,   5.,   7.,   2.,   3., -19.,   1.],
 [  3.,   2.,   0.,   5.,  12.,   4.,   1., -20.]]]

```

## Step 2: Reformulate QUBO to Hamiltonian

You can reformulate the QUBO problem as a Hamiltonian (here, a matrix that represents the energy of a system):

$$\langle H \rangle C = \sum_{ij} Q_{ij} Z_i Z_j + \sum_i b_i Z_i.$$

## Reformulation steps from the QAOA problem to the Hamiltonian

To demonstrate how the QAOA problem can be rewritten in this way, first replace the binary variables  $\langle x_i \rangle$  to a new set of variables  $\langle z_i \in \{-1, 1\} \rangle$  via

$$\boxed{x_i = \frac{1-z_i}{2}}$$

Here you can see that if  $\langle x_i \rangle$  is  $\langle 0 \rangle$ , then  $\langle z_i \rangle$  must be  $\langle 1 \rangle$ . When the  $\langle x_i \rangle$ 's are substituted for the  $\langle z_i \rangle$ 's in the optimization problem ( $\langle x^T Q x \rangle$ ), an equivalent formulation can be obtained.

$$\begin{aligned} \langle x^T Q x \rangle &= \sum_{ij} Q_{ij} x_i x_j \\ &= \frac{1}{4} \sum_{ij} Q_{ij} (1-z_i)(1-z_j) \\ &= \frac{1}{4} \sum_{ij} Q_{ij} z_i z_j - \frac{1}{4} \sum_{ij} (Q_{ij} + Q_{ji}) z_i + \frac{1}{4} \sum_{ij} Q_{ij} \end{aligned}$$

Now if we define  $\langle b_i = -\sum_j (Q_{ij} + Q_{ji}) \rangle$ , remove the constant  $\langle 1/4 \sum_{ij} Q_{ij} \rangle$  term, we arrive at the two equivalent formulations of the same optimization problem.

$$\boxed{\min_{x \in \{0,1\}^n} x^T Q x \Longleftrightarrow \min_{z \in \{-1,1\}^n} \frac{1}{4} z^T Q z + \frac{1}{4} b^T z}$$

Here,  $\langle b \rangle$  depends on  $\langle Q \rangle$ .

Now, to obtain a quantum formulation of the problem, promote the  $\langle z_i \rangle$  variables to a Pauli  $\langle Z \rangle$  matrix, such as a  $(2 \times 2)$  matrix of the form

$$\boxed{Z_i = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}$$

When you substitute these matrices in the optimization problem above, you obtain the following Hamiltonian

$$\boxed{H_C = \frac{1}{4} \sum_{ij} Q_{ij} Z_i Z_j + \frac{1}{4} \sum_i b_i Z_i}$$

Also recall that the  $\langle Z \rangle$  matrices are embedded in the quantum computer's computational space, i.e., a Hilbert space of size  $(2^n \times 2^n)$ . Therefore, you should understand terms such as  $\langle Z_i Z_j \rangle$  as the tensor product  $\langle Z_i \rangle \otimes \langle Z_j \rangle$  embedded in the  $(2^n \times 2^n)$  Hilbert space. For example, in a problem with five decision variables the term  $\langle Z_1 Z_3 \rangle$  is understood to mean  $\langle I \otimes Z_3 \otimes I \otimes Z_1 \otimes I \rangle$  where  $\langle I \rangle$  is the  $(2 \times 2)$  identity matrix.

This Hamiltonian is called the **cost function Hamiltonian**. It has the property that its ground state corresponds to the solution that minimizes the cost function  $\langle f(x) \rangle$ . Therefore, to solve your optimization problem you now need to prepare the ground state of  $\langle H_C \rangle$  (or a state with a high overlap with it) on the quantum computer. Then, sampling from this state will, with a high probability, yield the solution to  $\langle \min f(x) \rangle$ .

```

from qiskit.quantum_info import SparsePauliOp

def generate_pauli_terms(Q: np.ndarray, b: np.ndarray) -> list[tuple[str, float]]:
    """Construct the cost Hamiltonian.

    Args:
        Q (ndarray): NxN symmetric matrix of coefficients for Z_i Z_j terms.
        b (ndarray): N-dimensional array coefficients for Z_i terms.

    Returns:
        pauli_list: List of (Pauli string, coefficient) pairs representing the
        Hamiltonian terms.
    """
    N = len(b) # number of qubits

    pauli_list = []

    # Two-qubit terms
    for i in range(N-1):
        for j in range(i + 1, N):
            if Q[i, j] != 0:
                # Create a Pauli string with "Z" at positions i and j
                paulis = ["I"] * N
                paulis[i], paulis[j] = "Z", "Z"
                coeff = 2 * Q[i, j] / 4 # multiply by a factor 2 since we are only
                summing the upper triangular of Q
                pauli_list.append(("".join(paulis)[::-1], coeff))

    # Single-qubit terms
    for i in range(N):
        if b[i] != 0:
            # Create a Pauli string with "Z" at position i
            paulis = ["I"] * N
            paulis[i] = "Z"
            coeff = b[i] / 4
            pauli_list.append(("".join(paulis)[::-1], coeff))

    return pauli_list

b = - sum(Q[:, i] + Q[:, i].T for i in range(Q.shape[0]))
pauli_terms = generate_pauli_terms(Q, b)
cost hamiltonian = SparsePauliOp.from_list(pauli_terms)

print("Cost Function Hamiltonian:", cost hamiltonian)

```

```

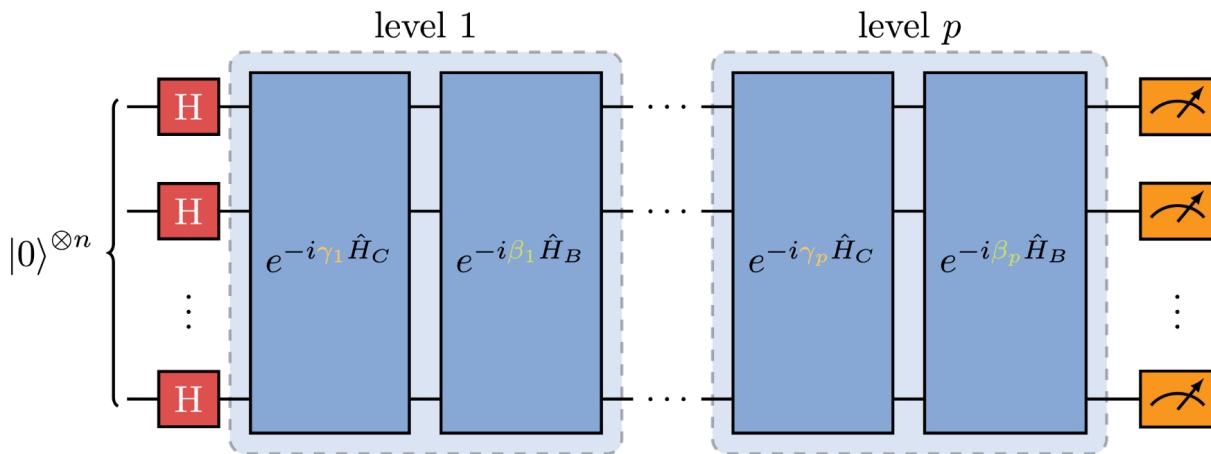
Cost Function Hamiltonian: SparsePauliOp(['IIIIIZZ', 'IIZIIIIZ', 'IZIIIIIZ',
'ZIIIIIZ', 'IIIIIZZI', 'IIIIIZIZI', 'IIIZIZIZI', 'IIZIIIZI', 'IZIIIZIZI',
'ZIIIIIZI', 'IIIZIZIZI', 'IIZIZIZII', 'IZIIIZIII', 'ZIIIZIII', 'IIZZIIIZI',
'IIZIZIII', 'IZZIIIZII', 'ZIZIIIZII', 'ZZIIIZII', 'IIIIIZZ', 'IIIIIZIZI',
'IIIIIZII', 'IIIZIZIZI', 'IIIZIZIZII', 'IZIIIZIII', 'ZIIIZIII', 'IIZIZIII'],
coeffs=[ 1. +0.j, 1.5+0.j, 2.5+0.j, 1.5+0.j, 1.5+0.j, 4.5+0.j, 2.
+0.j,
1.5+0.j, 2.5+0.j, 1. +0.j, 1.5+0.j, 2.5+0.j, 3. +0.j, 3.5+0.j.,
2.5+0.j, 3. +0.j, 1. +0.j, 6. +0.j, 1.5+0.j, 2. +0.j, 0.5+0.j.,
2. +0.j, -5. +0.j, 4.5+0.j, -4. +0.j, -1.5+0.j, -5. +0.j, -4.5+0.j.,
-3.5+0.j]).
```

## Hamiltonian → quantum circuit

The Hamiltonian  $\langle H_C \rangle$  contains the quantum definition of your problem. Now you can create a quantum circuit that will help sample good solutions from the quantum computer. The QAOA is inspired by quantum annealing and applies alternating layers of operators in the quantum circuit.

The general idea is to start in the ground state of a known system,  $|0\rangle^{\otimes n}$  above, and then steer the system into the ground state of the cost operator that you are interested in. This is done by applying the operators  $\langle \exp\{-i\gamma_k H_C\} \rangle$  and  $\langle \exp\{-i\beta_k H_B\} \rangle$  with angles  $\langle \gamma_1, \dots, \gamma_p \rangle$  and  $\langle \beta_1, \dots, \beta_p \rangle$ .

The quantum circuit that you generate is parametrized by  $\langle \gamma_i \rangle$  and  $\langle \beta_i \rangle$ , so you can try out different values of  $\langle \gamma_i \rangle$  and  $\langle \beta_i \rangle$  and sample from the resulting state.



In this case, you will try an example with two QAOA layers that contains four parameters:  $\langle \gamma_1 \rangle, \langle \beta_1 \rangle, \langle \gamma_2 \rangle, \langle \beta_2 \rangle$ .

```
from qiskit.circuit.library import QAOAAnsatz

circuit = QAOAAnsatz(cost_operator=cost_hamiltonian, reps=2)
circuit.measure_all()

circuit.draw("mpl")
```

circuit.parameters

## Step 2. Optimize circuits for quantum hardware execution

The circuit above contains a series of abstractions useful to think about quantum algorithms, but not possible to run on the hardware. To be able to run on a QPU, the circuit needs to undergo a series of operations that make up the **transpilation** or **circuit optimization** step of the pattern.

Transpilation may involves several steps, such as:

- Initial mapping of the qubits in the circuit (such as decision variables) to physical qubits on the device.
- Unrolling of the instructions in the quantum circuit to the hardware-native instructions that the backend understands.
- Routing of any qubits in the circuit that interact to physical qubits that are adjacent with one another.
- Error suppression by adding single-qubit gates to suppress noise with dynamical decoupling.

The following code transforms and optimizes the abstract circuit into a format that is ready for execution on the specified backend. For simplicity we will use a simulator backend, but this could easily be swapped out for a real quantum computing backend.

```
from qiskit_aer import AerSimulator
from qiskit_ibm_runtime import QiskitRuntimeService
from qiskit.transpiler.preset_passmanagers import generate_preset_pass_manager

# Choose backend (this can either be a simulator or a real qc backend.)
backend = AerSimulator()

# Create pass manager for transpilation
pm = generate_preset_pass_manager(optimization_level=0, backend=backend)

candidate_circuit = pm.run(circuit)
candidate_circuit.draw("mpl", fold=False, idle_wires=False).
```

## Step 3. Execute using Qiskit primitives

In the QAOA workflow, the optimal QAOA parameters are found in an iterative optimization loop, which runs a series of circuit evaluations and uses a classical optimizer to find the optimal  $(\beta_k)$  and  $(\gamma_k)$  parameters. This execution loop is executed via the following steps:

1. Define the initial parameters.
2. Use a classical optimizer to minimize the expectation value of the cost Hamiltonian,  $(H_C)$ , by iteratively adjusting  $(\beta_k)$  and  $(\gamma_k)$ .
3. Once the optimizer converges on a set of optimal parameters, execute the circuit one last time to sample the final distribution. The sampled states represent candidate solutions for the optimization problem.

### Step 3.1: Define circuit with initial parameters

We start with an initial guess for the parameters.

```
init_params = [2.5, 2.5, 0.1, 0.1].  
print(init_params).  
[2.5, 2.5, 0.1, 0.1].
```

## Step 3.2 Run optimizer

The two primitives are Sampler and Estimator, and the choice of primitive depends on what type of measurement you want to run on the quantum computer. For the minimization of  $\langle H_C \rangle$ , use the Estimator since the measurement of the cost function is simply the expectation value of  $\langle \langle H_C \rangle \rangle$ .

```
objective_func_vals = [] # Global variable  
  
def cost_func_estimator(  
    params: list, ansatz: "QuantumCircuit", hamiltonian: "ObservablesArrayLike",  
    estimator: "Estimator"  
) -> float:  
  
    # transform the observable defined on virtual qubits to  
    # an observable defined on all physical qubits for the backend.  
    isa_hamiltonian = hamiltonian.apply_layout(ansatz.layout).  
  
    pub = (ansatz, isa_hamiltonian, params).  
    job = estimator.run([pub]).  
  
    results = job.result()[0].  
    cost = results.data.evs  
  
    objective_func_vals.append(cost).  
  
return cost
```

```
from qiskit_ibm_runtime import EstimatorV2 as Estimator  
from scipy.optimize import minimize  
  
estimator = Estimator(mode=backend, options={"default shots": 4_000}).  
  
bounds = [(0, np.pi), (0, np.pi), (0, np.pi), (0, np.pi)].  
result = minimize(  
    cost_func_estimator,  
    init_params,  
    args=(candidate_circuit, cost_hamiltonian, estimator),  
    method="COBYLA",  
    bounds=bounds,  
    tol=1e-3,  
    options={"rhobeg": 1e-1}.  
)  
print(result)
```

```
message: Optimization terminated successfully.  
success: True  
status: 1  
fun: -23.82091977005749  
x: [ 2.635e+00  2.625e+00  5.093e-02  1.087e-01].  
nfev: 30  
maxcv: 0.0
```

The optimizer was able to minimize the cost and find better parameters for the circuit.

```
import matplotlib.pyplot as plt  
  
plt.figure(figsize=(12, 6)).  
plt.plot(objective_func_vals).  
plt.xlabel("Iteration").  
plt.ylabel("Cost").  
plt.show().
```

Once you have found the optimal parameters for the circuit, you can assign these parameters and sample the final distribution obtained with the optimized parameters. Here is where the `Sampler` primitive should be used since it is the probability distribution of bitstring measurements.

**Note:** This means preparing a quantum state  $\langle \psi \rangle$  in the computer and then measuring it. A measurement will collapse the state into a single computational basis state - for example, `01010100` - which corresponds to a candidate solution  $|x\rangle$  to our initial optimization problem ( $\max f(x)$ ) or ( $\min f(x)$ ) depending on the task).

### Step 3.3: Run circuit once more using optimal parameters

```
optimized_circuit = candidate_circuit.assign_parameters(result.x).  
optimized_circuit.draw("mpl", fold=False, idle_wires=False).
```

```
from qiskit_ibm_runtime import SamplerV2 as Sampler  
  
sampler = Sampler(mode=backend, options={"default_shots": 4_000}).  
  
pub = (optimized_circuit,)  
job = sampler.run([pub]).
```

```
counts_bin = job.result()[0].data.meas.get_counts().  
shots = job.result()[0].data.meas.num_shots  
final_distribution_bin = {key: val / shots for key, val in counts_bin.items()}.  
print(final_distribution_bin)
```

```
{'10010100': 0.00825, '00010111': 0.02375, '00011101': 0.242, '10110110': 0.00225,
'10000101': 0.05525, '01110100': 0.00175, '00110011': 0.00025, '11000110': 0.004,
'10000100': 0.0165, '00000101': 0.03275, '01000000': 0.001, '00010101': 0.067,
'00110111': 0.00475, '11100111': 0.0035, '00101101': 0.00125, '11001111': 0.0025,
'01100011': 0.0015, '11000101': 0.0095, '10100000': 0.0005, '01011111': 0.003,
'10001111': 0.0105, '10100101': 0.01075, '01011100': 0.005, '11100101': 0.0035,
'11011101': 0.00225, '10010101': 0.02625, '00001101': 0.00975, '10000111': 0.02375,
'10000110': 0.011, '00010100': 0.00575, '11000100': 0.01775, '01010000': 0.00225,
'00000111': 0.017, '01100010': 0.00075, '11110100': 0.00475, '01000010': 0.001,
'00111101': 0.0055, '11110101': 0.00175, '11001101': 0.002, '00100101': 0.00775,
'00011111': 0.01975, '01010101': 0.0145, '00011001': 0.0085, '10110101': 0.0045,
'10011101': 0.02675, '00100111': 0.0045, '11100000': 0.0035, '11001101': 0.004,
'00110100': 0.0015, '01000101': 0.0045, '11100110': 0.004, '00110101': 0.00875,
'00010001': 0.00075, '10110111': 0.0055, '11100100': 0.006, '01110101': 0.0025,
'10100011': 0.0005, '10001101': 0.02525, '10100100': 0.00775, '01010001': 0.00375,
'10001001': 0.002, '01101111': 0.001, '11000001': 0.00175, '01111001': 0.00125,
'11100001': 0.00125, '10101101': 0.0055, '10010110': 0.0015, '10101100': 0.00075,
'00010110': 0.00025, '00001111': 0.00175, '10100110': 0.00325, '00111100': 0.0005,
'11110010': 0.00125, '11000111': 0.0045, '11010100': 0.00275, '11001110': 0.001,
'01011001': 0.0055, '00100011': 0.00125, '01000111': 0.0025, '00000110': 0.0025,
'01000110': 0.00125, '10000001': 0.0015, '01110011': 0.00025, '10101110': 0.00175,
'01110111': 0.0015, '10111100': 0.0005, '00100100': 0.00175, '11101110': 0.00025,
'01101110': 0.00075, '11010001': 0.00125, '10101111': 0.00575, '11101111': 0.0005,
'01100100': 0.00175, '01010100': 0.00775, '01100101': 0.00125, '10111001': 0.0005,
'00000100': 0.008, '10110001': 0.00025, '01011101': 0.006, '01001111': 0.0015,
'01000100': 0.006, '10110100': 0.0005, '10111101': 0.00275, '10010111': 0.012,
'11011000': 0.00025, '01010010': 0.0005, '01100000': 0.0015, '01111100': 0.0005,
'11110110': 0.00025, '01101101': 0.00075, '11000000': 0.00075, '10011110': 0.0005,
'11010101': 0.004, '10001011': 0.0005, '00000011': 0.00025, '00001001': 0.00175,
'01100111': 0.00075, '11010111': 0.00275, '11100011': 0.00125, '01010111': 0.005,
'01111110': 0.00075, '11001100': 0.0005, '11101011': 0.0005, '01111011': 0.00075,
'10100111': 0.006, '11110111': 0.00075, '10011111': 0.00475, '10010001': 0.00075,
'01100001': 0.001, '11101100': 0.0015, '11011100': 0.00175, '01001101': 0.00175,
'11010110': 0.00175, '01111101': 0.0005, '10001100': 0.00075, '00111011': 0.00075,
'11000011': 0.0015, '01001100': 0.00125, '00100110': 0.00125, '11011001': 0.001,
'11010000': 0.001, '01011000': 0.00025, '00011100': 0.0005, '11100010': 0.00125,
'10011011': 0.00025, '11011111': 0.00075, '00101011': 0.00025, '01011011': 0.00175,
'001111001': 0.001, '00010000': 0.00075, '00111111': 0.00075, '11110001': 0.00125,
'11111110': 0.002, '01110000': 0.00025, '01000001': 0.00125, '01001000': 0.00025,
'10100001': 0.0005, '10000000': 0.0005, '11000010': 0.002, '00011110': 0.00025,
'00001100': 0.00025, '11111100': 0.0005, '10001110': 0.00075, '11111111': 0.00075,
'11010011': 0.00075, '00100000': 0.001, '01110001': 0.0005, '11111011': 0.0005,
'01101011': 0.00075, '01011110': 0.001, '10010000': 0.0005, '11111101': 0.00025,
'10000010': 0.0005, '10110011': 0.00075, '10100010': 0.00075, '00101100': 0.00025,
'00011000': 0.00025, '11011011': 0.00025, '10111111': 0.00025, '01010110': 0.0005,
'10011001': 0.0005, '11101001': 0.00025, '01000011': 0.0005, '01011010': 0.0005,
'11001001': 0.00075, '00110110': 0.00025, '00110001': 0.00025, '10001000': 0.00025,
'00010011': 0.00025, '01111111': 0.0005, '10010010': 0.00025, '00101111': 0.00075,
'01001001': 0.00025, '01001010': 0.0005, '00000110': 0.00025, '00000000': 0.00025,
'00011011': 0.00025, '11001011': 0.00025, '10110010': 0.00025, '01001011': 0.00025}.
```

## Step 4. Post-process, return result in classical format

The final step involves interpreting the output of the quantum computation and translating it back into a solution for your original problem.

When the quantum circuit is executed, it samples from the probability distribution defined by the final quantum state. The output consists of bitstrings, where each bitstring corresponds to a potential solution to the problem. In this step, we:

- 1. Filter Solutions:** If any of the sampled bitstrings satisfy the constraints of the original problem (e.g.,  $\|f(\vec{x})\|_2^2 = 0$  for the tail-assignment problem).
- 2. Count Occurrences:** Determine the most frequently observed bitstrings and plot a histogram.

## Step 4.1: Filter Solutions

We now process the bit-strings sampled from the quantum circuit to determine if any of them satisfy the constraints of the original optimization problem. For each sampled bitstring, we calculate whether it satisfies the problem constraints using the classical cost function  $|f(\vec{x})|$ . If and only if this function evaluates to  $0$  for a bitstring, a solution exists!

```
def classical_cost_fun(bit_str: str, A: np.ndarray) -> float:
    # convert binary string to column vector
    x = np.array([[int(bit)] for bit in reversed(bit_str)])
    id_vec = np.ones((A.shape[0], 1))
    return np.sum(np.square(A @ x - id_vec), axis=0)[0]

# Look through samples to see if any of the bit strings solve the problem
for bit_str in counts_bin.keys():
    if classical_cost_fun(bit_str, A) == 0:
        print("Valid solution found:", bit_str)
        break
```

Valid solution found: 00011101

## Step 4.2 Count Occurrences

```
def highest_probability_bitstring(prob_dict: dict) -> (np.ndarray, float):
    """
    Returns the bitstring with the highest probability as a column vector and
    corresponding probability.
    """

    Args:
        prob_dict (dict): A dictionary where keys are bitstrings (str) and values are
        probabilities (float).

    Returns:
        (np.ndarray, float): The bitstring with the highest probability and the
        corresponding probability.
    """

    # Find the key with the highest value
    highest_key = max(prob_dict, key=prob_dict.get)
    highest_value = prob_dict[highest_key]
    return highest_key, highest_value

bit_str, prob = highest_probability_bitstring(final_distribution_bin)

print(f"Most Likely bitstring is {bit_str} with probability {prob*100}%")
```

Most Likely bitstring is 00011101 with probability 24.2%

We see that QAOA return the solution bit-string with the highest probability. This can be compared to random-guessing, where the probability of obtaining the solution in this case is  $\sqrt{1/2^8} \approx 0.004$ .

```
# Compute the classical cost function for all binary bitstrings
costs = []
probabilities = []

for bit_str, prob in final_distribution_bin.items():
    cost = classical_cost_fun(bit_str, A)
    costs.append(cost)
    probabilities.append(prob)

costs = np.array(costs)
probabilities = np.array(probabilities)

# Plot the histogram
colors = ['purple' if cost == 0 else 'black' for cost in costs]
plt.bar(costs, 100*probabilities, width=0.5, color=colors, alpha=0.7, edgecolor=colors)
plt.xlabel(r'Classical Cost Function $f(x)$')
plt.ylabel(r'Probability %')
plt.title('Histogram of Classical Cost Function vs. Probability')
plt.show()
```

## (Extra): Running a smaller problem on actual quantum computer

In this section, we demonstrate how to run a smaller version of the tail-assignment problem on a real quantum computer. To accommodate the 5-qubit Helmi quantum computer, we load a simplified 2-qubit toy problem.

- Load a Toy Problem: We initialize a smaller version of the tail-assignment problem, ensuring it fits within the qubit limits of the hardware.
- Simulate Performance: Before running the problem on the real hardware, we test the circuit on a simulator to evaluate its behavior under ideal conditions.
- Execute on a Real Backend: Finally, we execute the problem on the Helmi quantum computer to compare results and assess the impact of quantum noise.

By exploring this smaller-scale problem, we get insights into real-world quantum hardware performance and its limitations, while preparing for scaling up to larger problems in the future.

```
A = np.loadtxt(url + "instance_2.csv", delimiter=',') # load problem data
num_rows, num_cols = A.shape
print(f"Number of flights equals {num_rows}, and number of routes equals {num_cols}.")
```

Number of flights equals 2, and number of routes equals 2.

```
Q = QUBO(A)
b = -sum(Q[i,:] + Q[:,i] for i in range(Q.shape[0]))._
pauli_terms = generate_pauli_terms(Q, b)
cost_hamiltonian = SparsePauliOp.from_list(pauli_terms)
cost_hamiltonian
```

```
circuit = QAOAAnsatz(cost_operator=cost_hamiltonian, reps=2).
circuit.measure_all()

# Create pass manager for transpilation
pm = generate_preset_pass_manager(optimization_level=0, backend=backend)
candidate_circuit = pm.run(circuit)

# Theoretical pre-calculated optimal parameters
optimal_params = [2.3562, 2.3562, 1.5708, 1.5708]
optimized_circuit = candidate_circuit.assign_parameters(optimal_params)
```

```
optimized_circuit.draw("mpl").
```

```
sampler = Sampler(mode=backend, options={"default_shots": 4_000}).
pub = (optimized_circuit,).
job = sampler.run([pub]).
```

```
counts_bin = job.result()[0].data.meas.get_counts()
shots = job.result()[0].data.meas.num_shots
final_distribution_bin = {key: val / shots for key, val in counts_bin.items()}
final_distribution_bin
```

```
# Look through samples to see if any of the bit strings solve the problem
for bit_str in counts_bin.keys():
    if classical_cost_fun(bit_str, A) == 0:
        print("Valid solution found:", bit_str)
        break
x, prob = highest_probability_bitstring(final_distribution_bin)
```

```
Valid solution found: 01
```

```

# Plot distribution of bit-strings.
bins = list(final_distribution_bin.keys())
probabilities = list(final_distribution_bin.values())

# Plot the histogram
plt.bar(bins, probabilities, width=0.5, alpha=0.7)
plt.xlabel(r'bit-strings')
plt.ylabel(r'Probability %')
plt.title('Histogram of bit-strings vs. Probability')
plt.show()

```

For the 2-qubit toy problem, the QAOA algorithm correctly identifies the optimal solution bit-string with 100% probability in the simulation using 2-layers. This result is under ideal conditions, where noise and hardware imperfections are absent.

## Running QAOA on the HELMI quantum computer

```

import os
from iqm.qiskit.iqm import IQMProvider

HELMI_CORTEX_URL = os.getenv('HELMI CORTEX URL') # This is set when loading the module
provider = IQMProvider(HELMI_CORTEX_URL)
backend = provider.get_backend()

```

```

from qiskit.compiler import transpile
from iqm.qiskit.iqm_transpilation import optimize_single_qubit_gates

transpiled_circuit = transpile(circuit, backend, optimization_level=3)
optimized_transpiled_circuit =
optimize_single_qubit_gates(transpiled_circuit.assign_parameters(optimal_params))
optimized_transpiled_circuit.draw("mpl")

```

```
job = backend.run(optimized_transpiled_circuit)
```

```
job.status()
```

```

counts_bin = job.result().data()["counts"]
shots = job.result().results[0].shots
final_distribution_bin = {key: val / shots for key, val in counts_bin.items()}
final_distribution_bin

```

```

# Plot distribution of bit-strings.
bins = list(final_distribution_bin.keys())
probabilities = list(final_distribution_bin.values())

# Plot the histogram
plt.bar(bins, probabilities, width=0.5, alpha=0.7)
plt.xlabel(r'bit-strings')
plt.ylabel(r'Probability %')
plt.title('Histogram of bit-strings vs. Probability')
plt.show()

```

## Conclusion

This tutorial demonstrated how to solve the tail-assignment problem using Qiskit. While quantum computers currently do not outperform classical computers for combinatorial optimization tasks—primarily due to noise and hardware limitations—progress in this field is advancing rapidly.

The hardware is steadily improving, with new algorithms continually being developed. Many of these quantum heuristics are currently tested on classical simulators, which are limited to small problem sizes (typically around 20 qubits).

In the near future, as quantum computers with more qubits and less noise, it will become feasible to benchmark quantum heuristics on larger, real-world problem instances. This progress holds the potential to unlock new capabilities in solving challenging optimization problems that are intractable by classical methods.

## Quantum walks on quantum computers

 [Slides](#)

## Tergite overview

 [Overview slides](#)

## Contents

- [What is Tergite?](#)
- [Why is Tergite necessary?](#)
- [What can I do with Tergite?](#)
- [How does Tergite work?](#)
- [Test out Tergite](#)

## What is Tergite?

Let's take a walk down memory lane to the time when classical computers were large expensive machines that could only be afforded by large corporations. Back then, batch processing enabled multiple users in a given company to share a single computer.



An operator working on an old mainframe

Quantum computing is at a similar stage today. Quantum computers are large expensive machines that can only be operated by a select few. There is need for specialized software to give multiple users simplified access to a single quantum computer.

Tergite is one such collection of software that enables a quantum computer experimentalist to:

- Submit experiments to the quantum computer's queue.
- Retrieve results of completed experiments
- Monitor the device parameters of the quantum computer

Just like in the batch processing of old, the quantum computer requires an operator.

Through Tergite, an operator of a quantum computer can do the following:

- (Re)calibrate the quantum computer
- Turn on/off the quantum computer
- Manage experimentalists' access to the quantum computer

## Why is Tergite necessary?

1. Operation of a quantum computer requires a highly specialized skillset.

Most quantum computers of today are very complex machines that require specialized care in a lab environment. The skillset required to operate such machines takes many years of postgraduate studies to master.

Tergite gives experimentalists, who don't have this skill, access to the quantum computer to run experiments on it.

## **2. Quantum computers need frequent recalibration**

One characteristic of today's quantum computers is the fact that their device parameters drift with time. Temperature changes, cosmic radiation, aging of electronics, mechanical vibrations etc. cause the device parameters of the quantum computers to change with time.

Tergite autocalibration is library used to recalibrate quantum computers. It is part of the Tergite stack.

## **3. Idle time on a quantum computer is very expensive.**

A typical quantum computer today costs more than half a million euros (€500,000). Every second a quantum computer lies under-utilized, a lot of money is being thrown down the drain. Batching experiments from multiple experimentalists is an attempt to make sure the quantum computer is in use at all times.

## **What can I do with Tergite?**

### **1. Access the WACQT quantum computer**

The Wallenberg Center for Quantum Computing (WACQT) is a Swedish national research programme with a focus on quantum technology. One of its major goals is to create a quantum computer that is accessible to Swedish researchers and WACQT industrial partners. The WACQT quantum computer is physically housed at Chalmers University of Technology and is operated by Chalmers Next Labs AB.



The WACQT quantum computer laboratory

In order to access this quantum computer via the internet, one has to go through the Tergite stack running at [QAL 9000](#).

Interacting with the WACQT quantum computer requires the use of the [Tergite software development kit \(SDK\)](#).

## **2. Calibrate superconducting qubit chips**

If one has a superconducting quantum chip with a design similar to the WACQT quantum computer chip, it is possible to calibrate this chip using the [Tergite autocalibration library](#). Doing this requires substantial hardware and software know-how.

[Chalmers Next Labs AB](#) currently offers a service to calibrate such chips for Swedish Small and Medium Enterprises (SMEs).

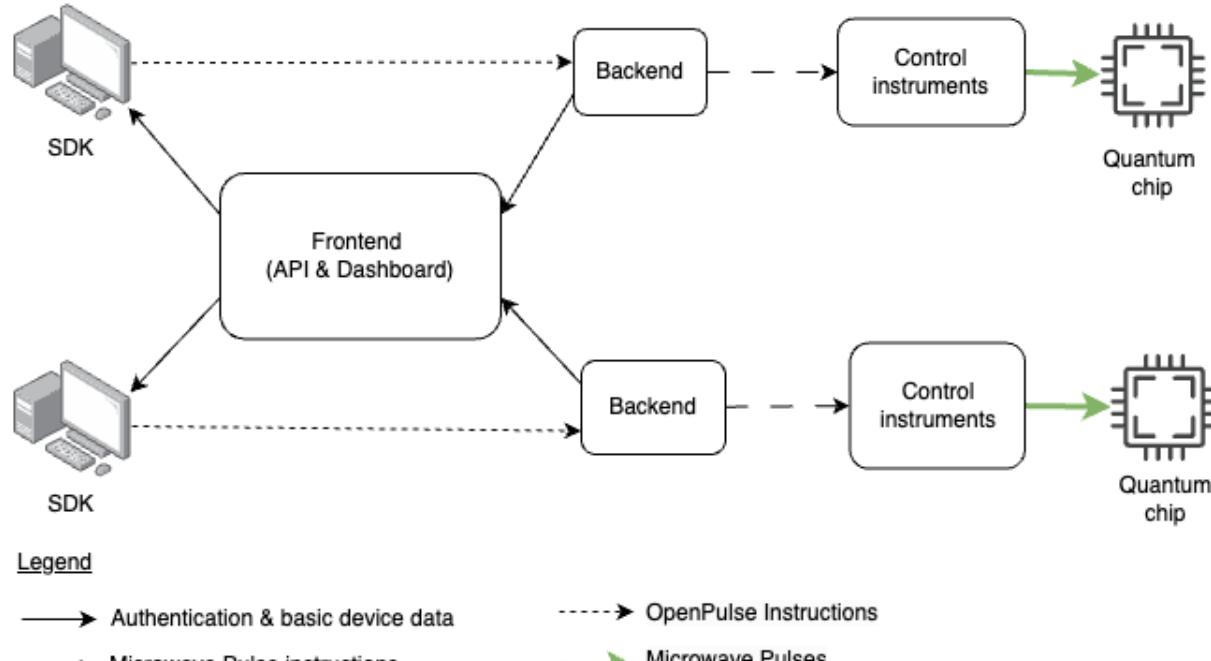
## **3. Expose a physical quantum computer to the internet**

The entire Tergite stack can be run in front of a physical quantum computer to expose it to a select group of experimentalists. It contains Identity Access Management (IAM) to handle authorization of only members of a given organization. Any organization can use Tergite to spin up a cloud offering for their quantum computers. The Tergite stack is open source and free to use or extend under the [Apache 2.0 License](#).

However, there are a few requirements for Tergite to work well:

- The quantum chip should be a superconducting with a similar design to the WACQT quantum computer chip designas described by Kosen et al. in the “[Signal Crosstalk in a Flip-Chip Quantum Processor](#)” article.
- The quantum computer should be controlled by [Qblox instruments](#)

## How does Tergite work?



## Data flows in Tergite

### Components of the stack

Tergite is composed of four main components:

#### Backend

The operating system of the quantum computer. Its basic functions include:

- Transpiling [OpenPulse](#) job definitions to [Quantify Schedules](#) that can be understood by the Qblox control instruments.
- Queuing jobs so that the quantum chip can receive one job at a time.
- Saving the device parameters of the quantum chip, after (re)calibration.

#### Frontend

The public interface through which users on the internet interact with the quantum computer. It consists of:

- [RESTful API](#) : The programmatic interface through which scripts and other computer programs interact with the quantum computer

- Dashboard : The web-based graphical interface through which users interact with the quantum computer

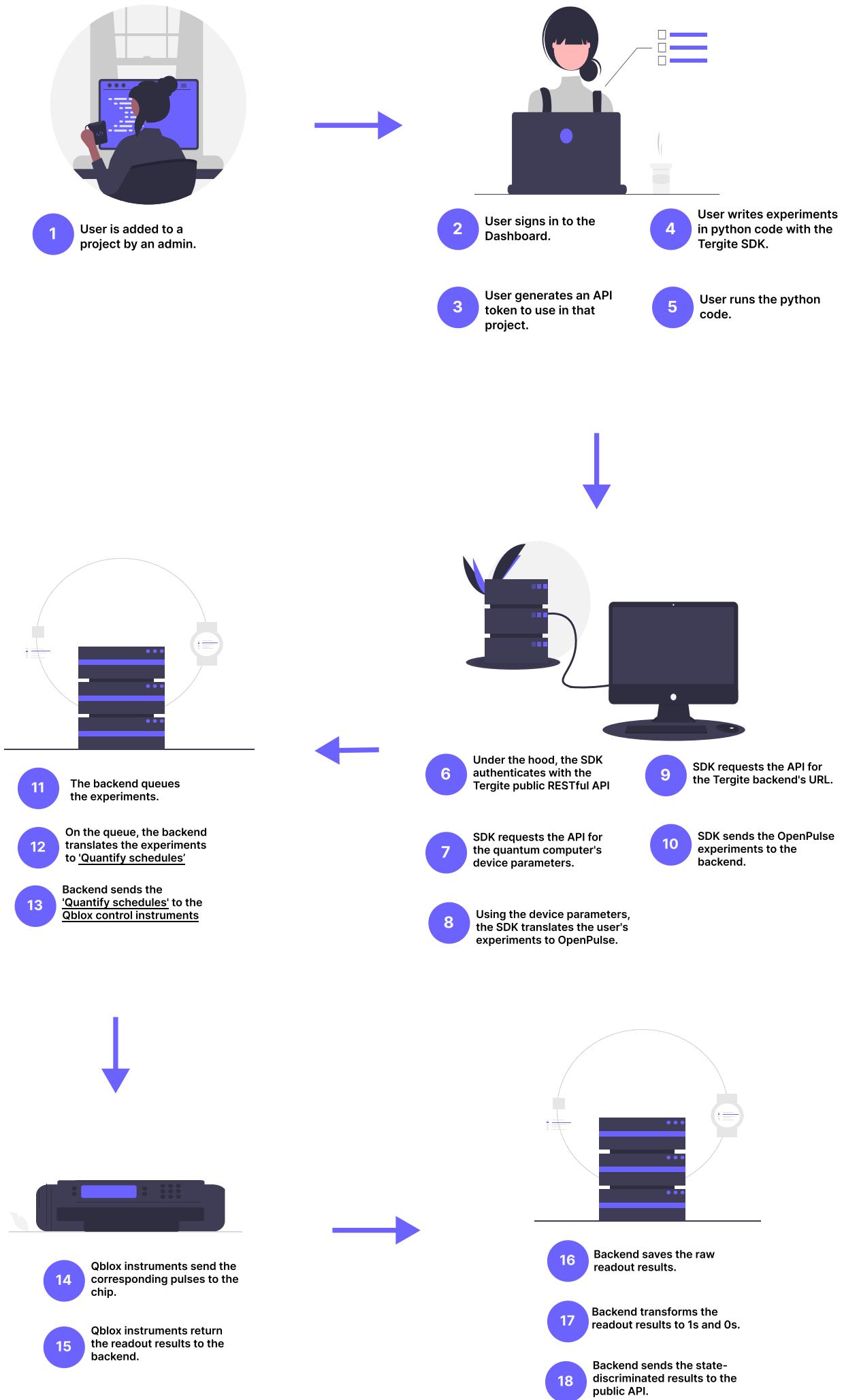
## Software Development Kit (SDK)

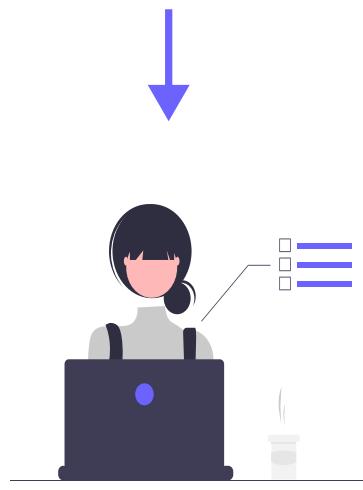
The Library which eases writing of python scripts and programs that interact with the quantum computer. It is based on [Qiskit](#) and communicates with the backend using [OpenPulse](#) sent via HTTP/HTTPS

## Automatic Calibration Tool

The Command Line Interface (CLI) used to determine the device parameters of the quantum computer.

## Basic Flow





- 19 User queries the public API for the results.
- 20 Or user downloads the raw readout results from backend.

## Test out Tergite

It is possible to test out a live instance of Tergite by using the [QAL 9000 quantum computer](#). However, someone from WACQT must have given you permission to use it because it is not open to the general public.

It is also possible to run Tergite on your own computer. The only catch is that you will only be able to run your experiments on simulators. Instructions on how to run Tergite locally are found in the [Tergite quick start tutorial](#).

## Distributed Quantum Computing

Slides

## Quantum extreme learning machine

Slides

## Quantum Computing for Materials Science

**Note:** This tutorial is based on research work available on [arXiv:2412.00951](#). Related codes and input files can be found in the [2024 inhibitQ repository](#).

The slides for the talk related to this tutorial can be found [here](#) (right-click and select “Open in new tab” to view in browser).

The demo files for this tutorial are described and detailed throughout the text here in this page and the associated pages. It should also appear in your LUMI notebooks, otherwise, you can download them from [mat\\_sc\\_on\\_qc](#)

# Contents

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## Introduction

Quantum chemistry calculations are among the most promising early applications of quantum computers. However, materials science simulations, particularly those involving solid-state systems, have not been well covered in the literature. Such calculations are usually associated with periodic system descriptions and can involve a large number of atoms, often in the hundreds. This repository aims to provide a comprehensive guide on how to perform these calculations using quantum computers in a way that aligns with current efforts to introduce quantum-centric supercomputers, where the quantum computer is considered an accelerator for classical calculations, similar to the role of GPUs in various fields. The tutorial here is focusing on simulating the calculation on a quantum computer, some hinders weren't solved when it comes to running the calculation on quantum computer at the time of writing this tutorial.

## Why Quantum Computing for Materials?

The simulation of large solid-state systems typically involves a significant number of atoms, which necessitates approximations in calculating the ground state energy. Methods like Density Functional Theory (DFT) are useful in this context. However, there are important parts of the system that can be described more accurately, especially when they involve interactions of particular interest to scientists. Quantum computing algorithms could be advantageous in focusing on such subsystems of the supercell and communicating the results to the DFT code. In simpler terms, they can correct the energy by accounting for more detailed information from these specific subsystems. This approach is known as quantum embedding<sup>1</sup>. Of course, this is a very simplified description and can be considered analogous to the QM/MM method; again, this is just a simplification of the problem description and not an entirely accurate illustration.

It is a hot topic now given the quantum centeric supercomputers effort and the rise of hybrid quantum classical approaches. More recent literature to study can be found in those references<sup>2 3 4 5</sup>.

## Prerequisites

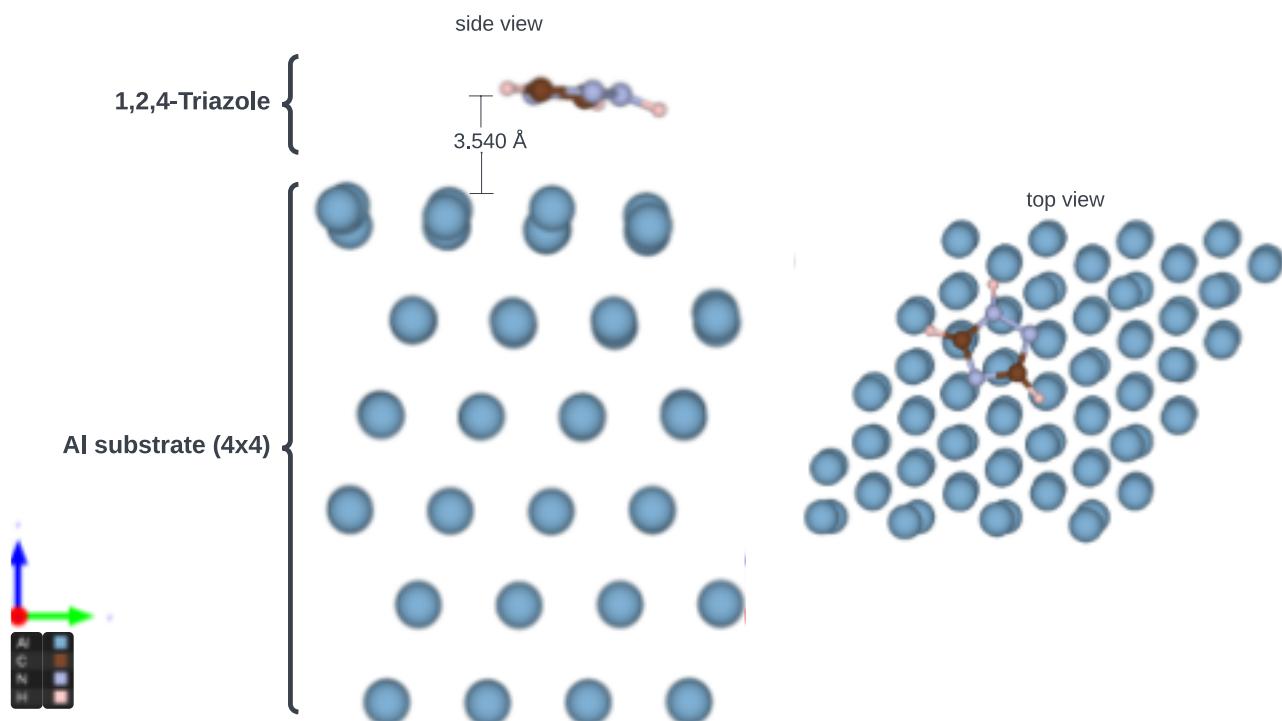
To follow this tutorial, you should have a basic understanding of quantum computing and materials science or quantum chemistry, like simulating the H<sub>2</sub> molecule or LiH tutorials by qiskit for example. Familiarity with quantum chemistry calculations and Density Functional Theory (DFT) will be helpful.

## Hands-on Example

### 1. Classical Calculations

For detailed information about the classical calculations, including supercell generation, geometry optimization, supercell calculations, and binding energy calculation, please see [Classical Calculations](#).

The supercell used in this tutorial is a 4x4x1 Al(111) substrate with a 1,2,4-triazole molecule on top of the Al(111) surface.



### 2. Hybrid Quantum Classical Calculation

This section demonstrates the integration of classical DFT calculations with quantum computing methods through an active space embedding scheme. The implementation combines CP2K for classical DFT calculations with Qiskit for quantum computations, using an active space of 2 electrons in 5 orbitals.

Key components include:

- Classical DFT calculations using CP2K

- Quantum calculations with Active space embedding using ADAPT-VQE algorithm
- Socket-based integration between classical and quantum components

For detailed implementation information, including configuration parameters and workflow structure, see [Hybrid Quantum Classical Calculations](#).

### **3. Calculations Results**

After performing the hybrid quantum-classical calculations, we analyze the binding energy to understand the interaction strength between the surface and the adsorbate. The binding energy is calculated as:

$$E_{\text{binding}} = E_{\text{supercell}} - (E_{\text{substrate}} + E_{\text{inhibitor}})$$

### **Binding Energy Comparison**

<u>Method</u>	<u>Inhibitor</u>	<u>Binding Energy (eV)</u>	<u>Binding Distance (Å)</u>
<u>Classical DFT</u>	<u>1,2,4-Triazole</u>	<u>-0.385512</u>	<u>3.54</u>
<u>AdaptVQE</u>	<u>1,2,4-Triazole</u>	<u>-0.385508</u>	<u>3.54</u>
<u>Vanilla VQE</u>	<u>1,2,4-Triazole</u>	<u>-2.325986</u>	<u>3.54</u>

### **Discussion and Future Work**

The results of this simulations show an agreement between classical DFT and AdaptVQE method. The AdaptVQE implementation proved more robust with its gradient-based operator pool selection compared to the vanilla VQE, which showed significant deviation with notably higher binding energy.

### **Outlook and Discussion**

The calculation employed an active space of 2 electrons in 5 orbitals (10 spin-orbitals) around the Fermi level. For more accurate results, expanding the active space to include more orbitals could lead to different binding energies compared to the classical approach, particularly in better capturing the complex hybridization between molecular orbitals and substrate states. At the time of writing this tutorial, only the assigned number of orbitals and electrons managed the calculation to converge.

### **Conclusion and Future Work**

This work successfully demonstrating a workflow for hybrid quantum-classical calculations for materials science, suitable for running on quantum centric supercomputers like Lumi. A lot of work is still needed to make this method practical for large systems and to improve the convergence of the calculation when using the AdaptVQE algorithm and including more

orbitals in the active space, which will make the calculation worth it on quantum computers.  
Ofcourse, error mitigation techniques will be needed to make this method practical, but that  
is another story.

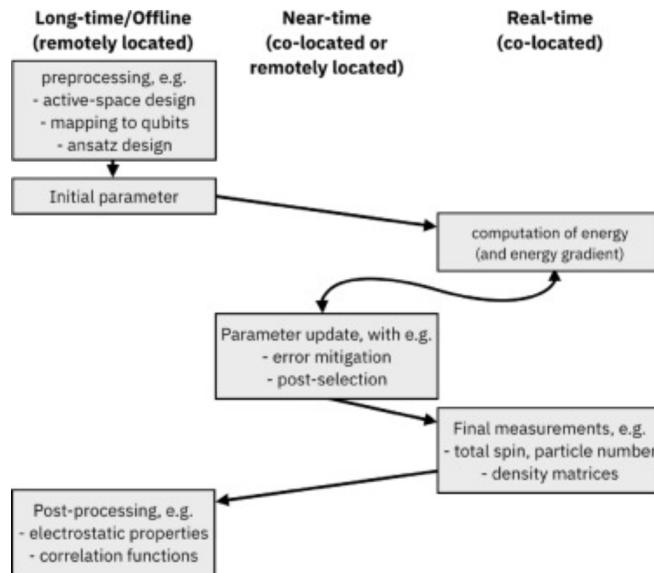
### **Snippets from the slides**

I believe those snippets augment the text and provide a better understanding of the work.  
Ofcourse, the full slides are available [here](#) (right-click and select “Open in new tab” to view in  
browser).

Here comes the snippets from the slides:

## Quantum-centric supercomputing

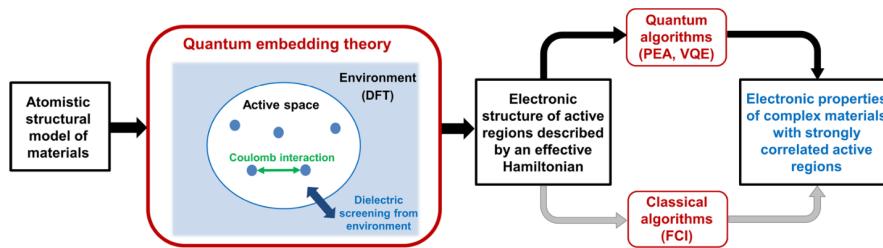
The Quantum-centric supercomputers efforts taking place at the moment using quantum accelerators with current HPC infrastructures can be used to accelerate those materials science simulations



**Figure:** From [6]: Integration between classical (HPC) and quantum computing resources exemplified by the variational quantum eigensolver. The steps of the calculation are represented by gray blocks, connected by arrows describing the flow of operations and arranged left/center/right for operation that require "long-time/near-time/real-time" interaction between HPC and quantum computers

## Workflow for Quantum Simulations of Materials

- Practical-wise, one can use the classical resources to do the calculations as usual and focus the quantum part on the important interactions that can benefit from the quantum algorithms and feed the results back to the classical side



**Figure:** General strategy for quantum simulations of materials using quantum embedding [9]

### quantum embedding and active space

- The figure above shows how to combine the classical and quantum calculations using the quantum embedding method
- Large simulations utilise active space approximation to reduce the resources required to model the system's electronic structure on a quantum workflow

# Quantum Embedding Method for the Simulation of Systems on Quantum Computers I

The energy of the active subsystem A embedded into the environment subsystem B by means of an SCF-in-DFT calculation is given by [10]:

$$E_{\text{SCF-in-DFT}}[\gamma_{\text{emb}}^A; \gamma^A, \gamma^B] = E_{\text{SCF}}[\gamma_{\text{emb}}^A] + E_{\text{DFT}}[\gamma^A + \gamma^B] - E_{\text{DFT}}[\gamma^A] + \text{tr}[(\gamma_{\text{emb}}^A - \gamma^A)\nu_{\text{emb}}[\gamma^A]] + \alpha \text{tr}[\gamma_{\text{emb}}^A \mathbf{P}^B] \quad (1)$$

## Brief Description

This relies on the projection-based wave function-in-DFT (WF-in-DFT) embedding method, where the total KS density matrix,  $\gamma$ , of the molecular system obtained from KS-DFT is partitioned into an active and environment subsystem,  $\gamma_A$  and  $\gamma_B$

## Key Components

- $E_{\text{SCF}}$  is the energy of the embedded subsystem A at SCF level
- $\mathbf{P}^B = S\gamma^B S$  is a projector for orbital orthogonality
- $\alpha$  is a scaling parameter
- $\nu_{\text{emb}}$  includes all two-electron interactions

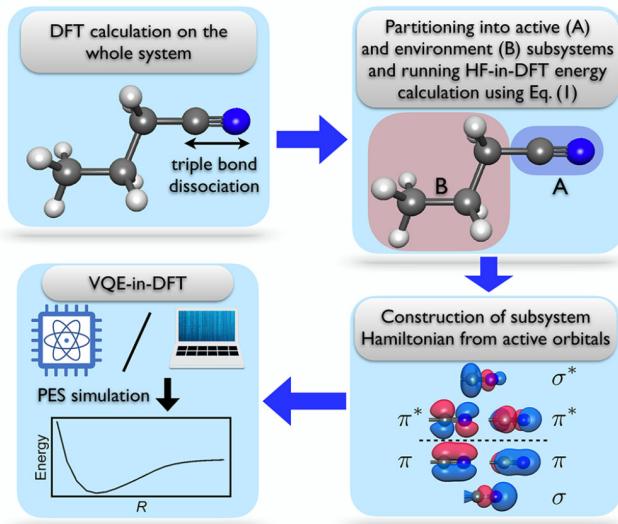


Figure: Quantum embedding in action [10]

## ADAPT-VQE at a glance

Adaptive Derivative-Assembled Pseudo-Trotter VQE (ADAPT-VQE) is a solver technique that builds an ansatz iteratively from a predefined operator pool, which can more efficiently converge to predict the ground state energy [11]

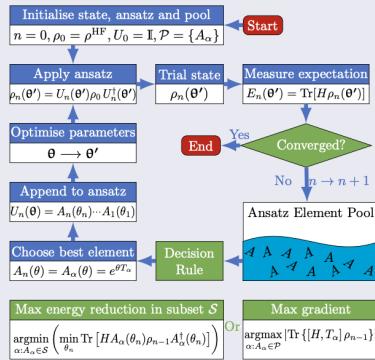


Figure: From [12]:ADAPT-VQE procedure

Then different pool of ansatz offered by UCCSD can be chosen then initial Hartree-Fock state can be formed then build the Hamiltonian

## A practical usecase on Quantum Computing for Materials?

- A practical example of how periodic systems can be important to study is studying corrosion inhibition through examining the adhesion power of few inhibitor molecules on top of metal alloys surfaces that form the body of a car or aeroplane. This can enhance the lifespan and efficiency of the car or aeroplane body, there is research around shifting towards eco-friendly alternatives like smart coatings and organic inhibitors due to environmental concerns, for more information please see [1]
- Such inhibitor molecules can benefit from accurate quantum calculations to study their interactions with the metal surface. Then those calculations can correct for energies computed by the Density Functional Theory (DFT)

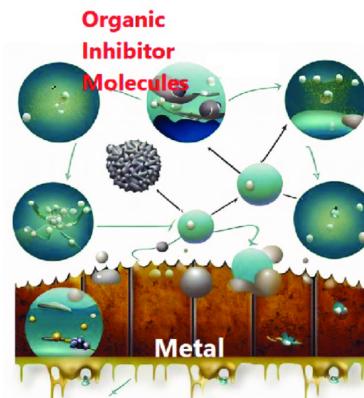


Figure: From [13]: Corrosion inhibition mechanisms of organic inhibitors

## Integration between CP2K and Qiskit

- Socket-based communication between CP2K and Qiskit
- FCIDUMP format for integral transfer

most important article here!

This figure is from [14]

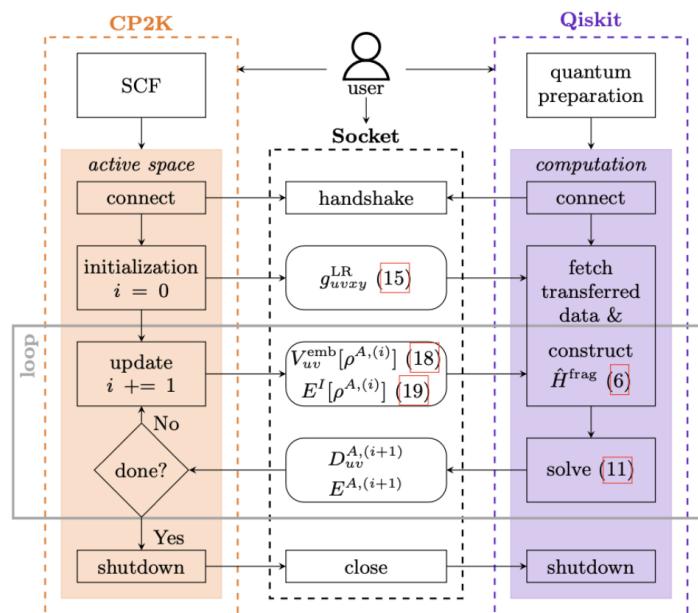


FIG. 2. Workflow diagram depicting the interaction of CP2K and Qiskit Nature. The user configures the two classical processes and the socket for the IPC. Each process then follows the computational steps (rectangular boxes) outlined inside of their respective frames. The data that gets computed and transferred is indicated by the rounded boxes. Numbers in parentheses refer to the respective equations in this manuscript. The self-consistent embedding requires a loop which is highlighted by the gray box. This loop is terminated based on the decision (diamond shape) taken by the CP2K process.

## References

- [1] [Vorwerk, C., Sheng, N., Govoni, M., et al. "Quantum embedding theories to simulate condensed systems on quantum computers." \*Nature Computational Science\* \*\*2\*\*, 424–432 \(2022\). DOI:10.1038/s43588-022-00279-0](#)
- [2] [Multiscale Embedding for Quantum Computing. arXiv preprint arXiv:2409.06813 \(2023\). https://arxiv.org/abs/2409.06813](#)
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- [4] [Quantum Embedding and Quantum Simulations. Galli Group Research. University of Chicago. https://galligroup.uchicago.edu/Research/embedding.php](#)
- [5] [Quantum Embedding Method for the Simulation of Strongly Correlated Systems on Quantum Computers. arXiv preprint arXiv:2302.03052 \(2023\). https://arxiv.org/abs/2302.03052](#)

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 Slides

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