Quantum Circuits and Optimization

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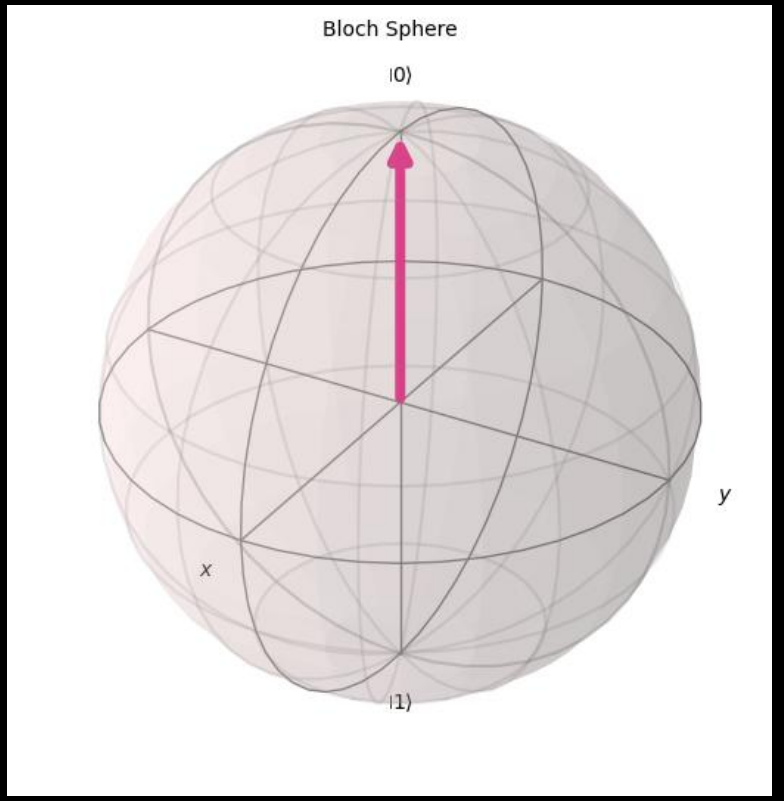
What is Quantum Computing?

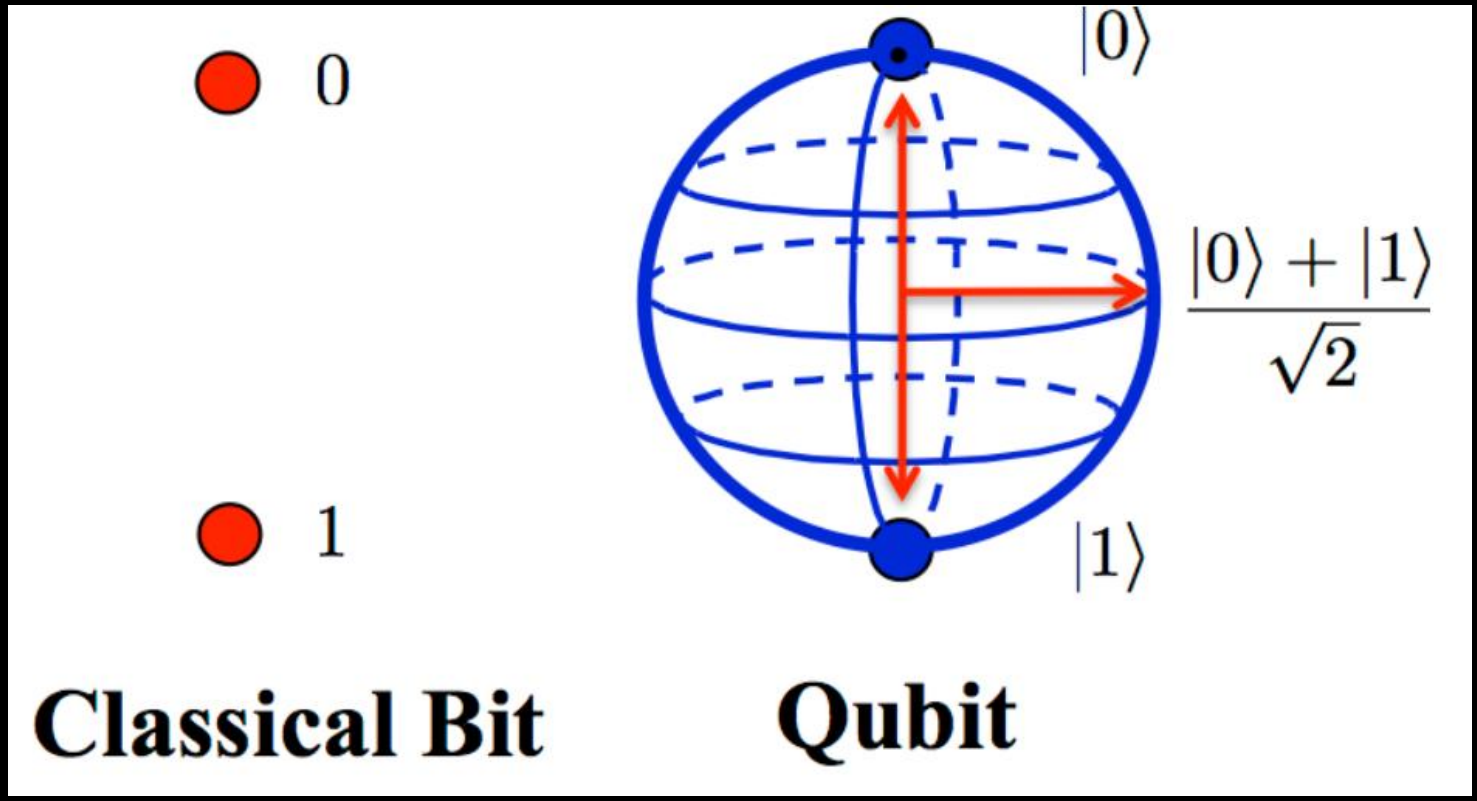
1) Quantum Computing Is a novel Scientific Discipline which uses concepts of Quantum Mechanincs and Computer Science.
2) The fundamental information unit is the Qubit, that can exist as a superposition of states as long as it is not classically measured.
3) Quantum Algorithms leverage these objects to perform opertations using properties of Quantum Mechanics, looking for advantages on the classical counterparts.
4) Quantum Computers have to be built with the idea of being able to manifest these operations and manipulate Qubits.



The Qubit

The Fundamental Concepts used to build the Qubit:

1) Entanglement.
2) Superposition.



Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy.

— Richard P. Feynman —

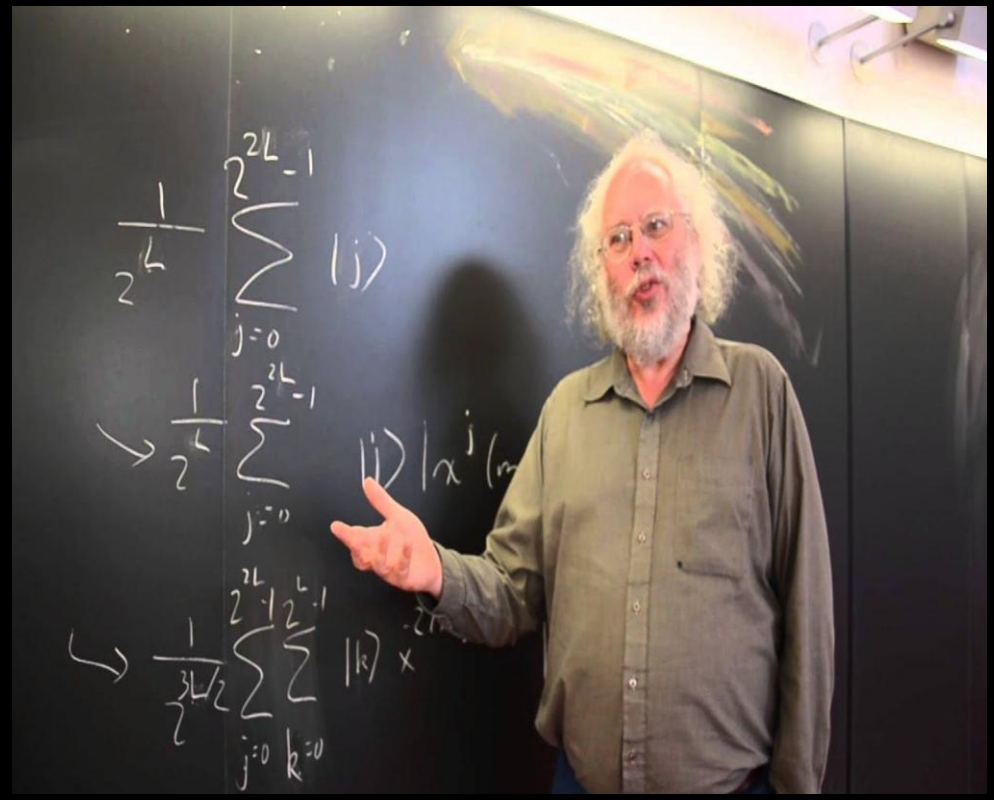
AZ QUOTES

Quantum History

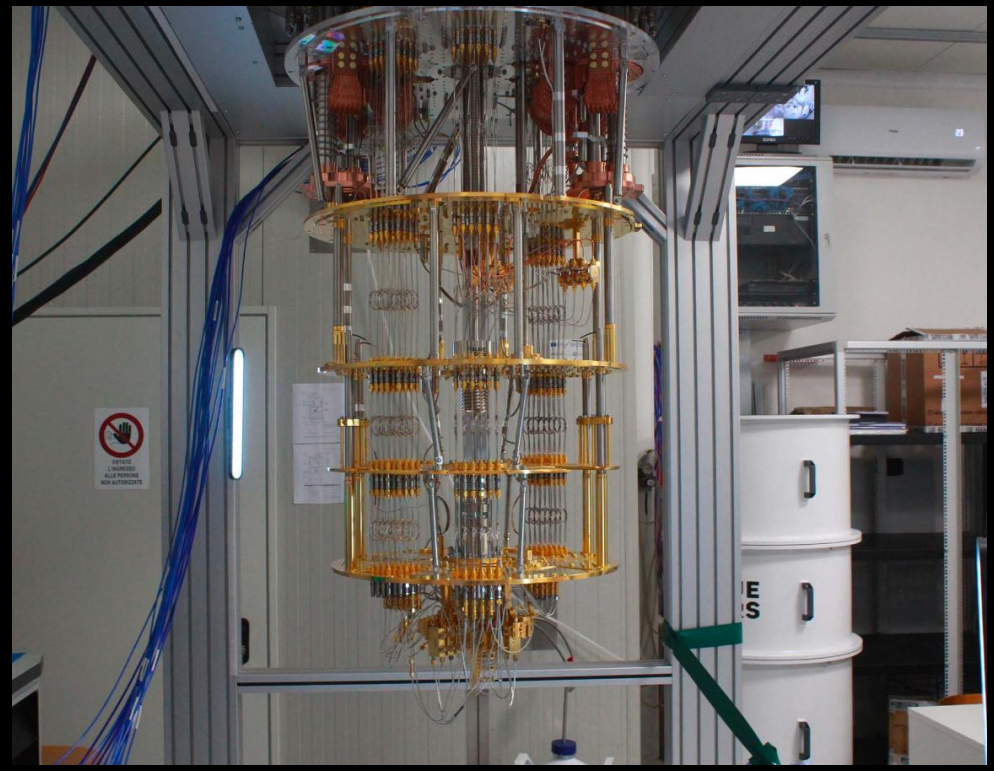
After the first idea from Feyman (1982), theorethically, Quantum Computing has been extensively studied since the 80s.

Two very famous Quantum Algorithms are Shor's (1994) for factorization of numbers, and Grover's (1996) for quantum search in a database.

These two algoritms present an exponential and polynomial speed-up with respect to classical counterparts, respectively.

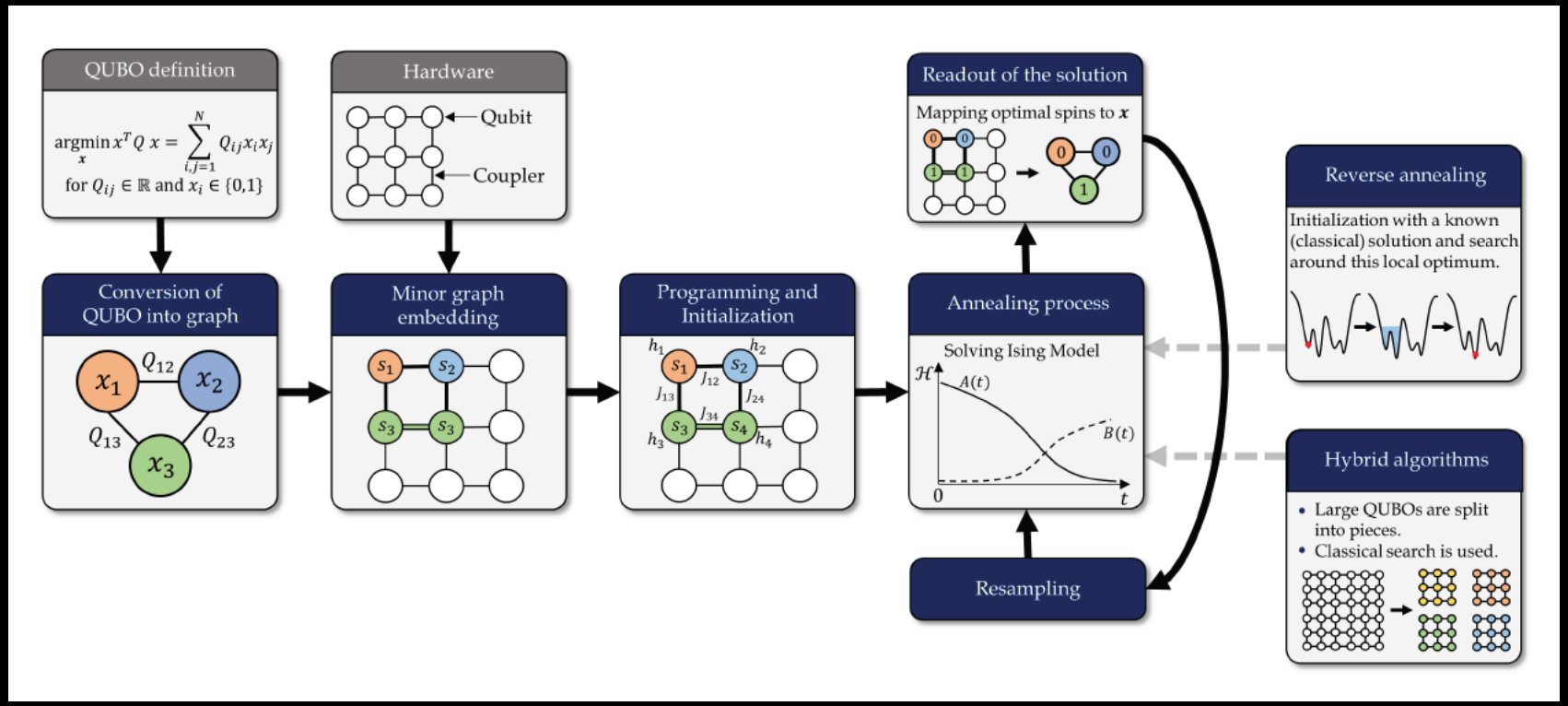


Quantum Hardware



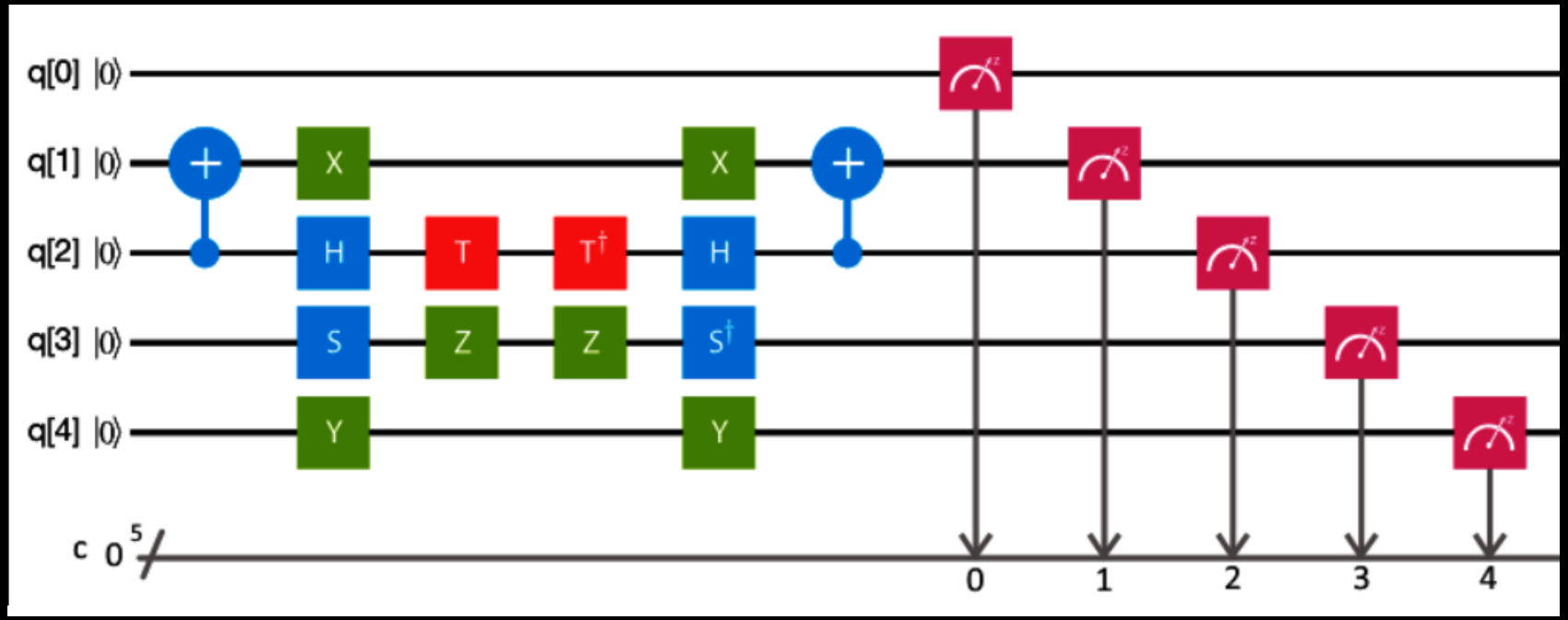
Quantum Annealing

1) Very High number of «Qubits».
2) Scope limited to the minimization of Ising-like Hamiltonians
3) Very Stable and with low errors, but less user-friendly and sometimes acts as a black box.

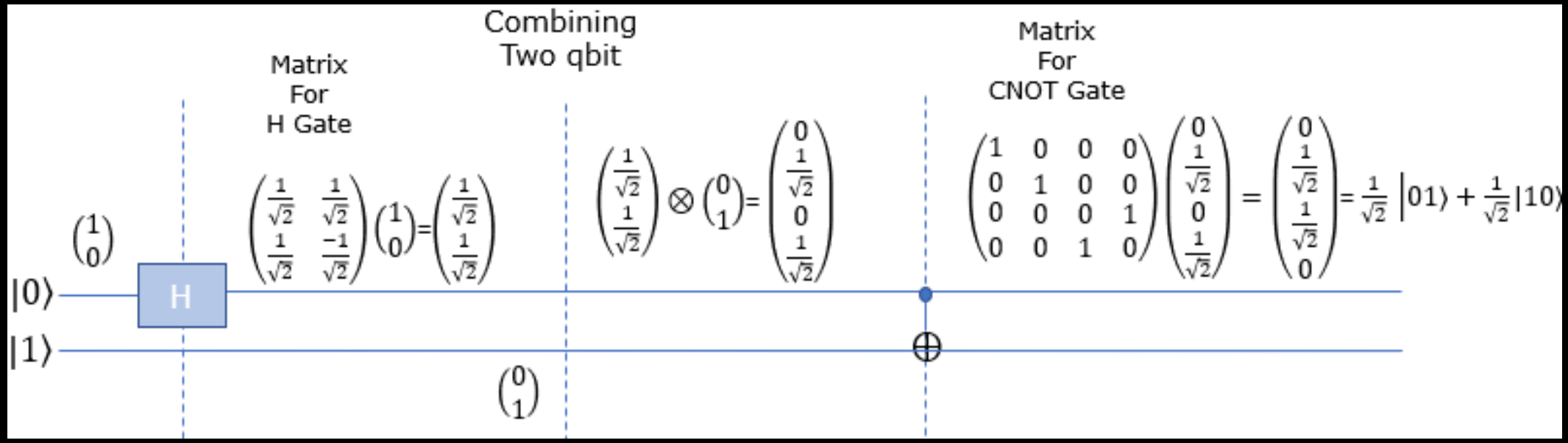


Quantum Circuits

1) Limited number of Qubits.
2) Very general scope.
3) Less stable, and the errors can become problematic with deep circuits
4) User-friendly and clear.

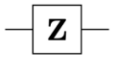
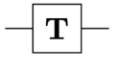
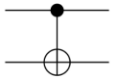
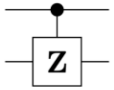
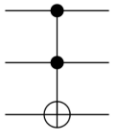


Quantum Gates: Hadamard and CNOT

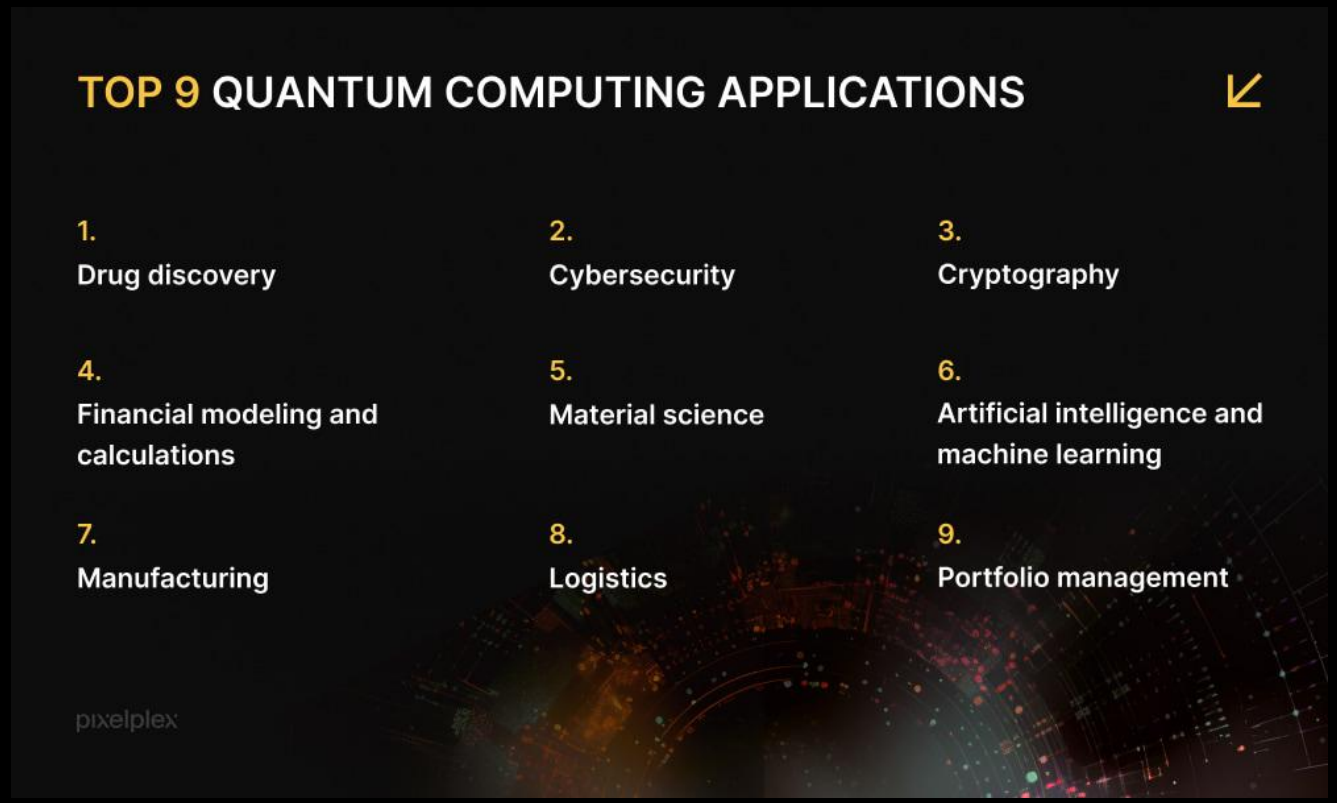


Quantum Gates: Glossary

A Quantum Circuit is a combination of these gates which act on a given number of qubits. Then, a classical measurement is performed, which collapse the Qubits into classical configurations.

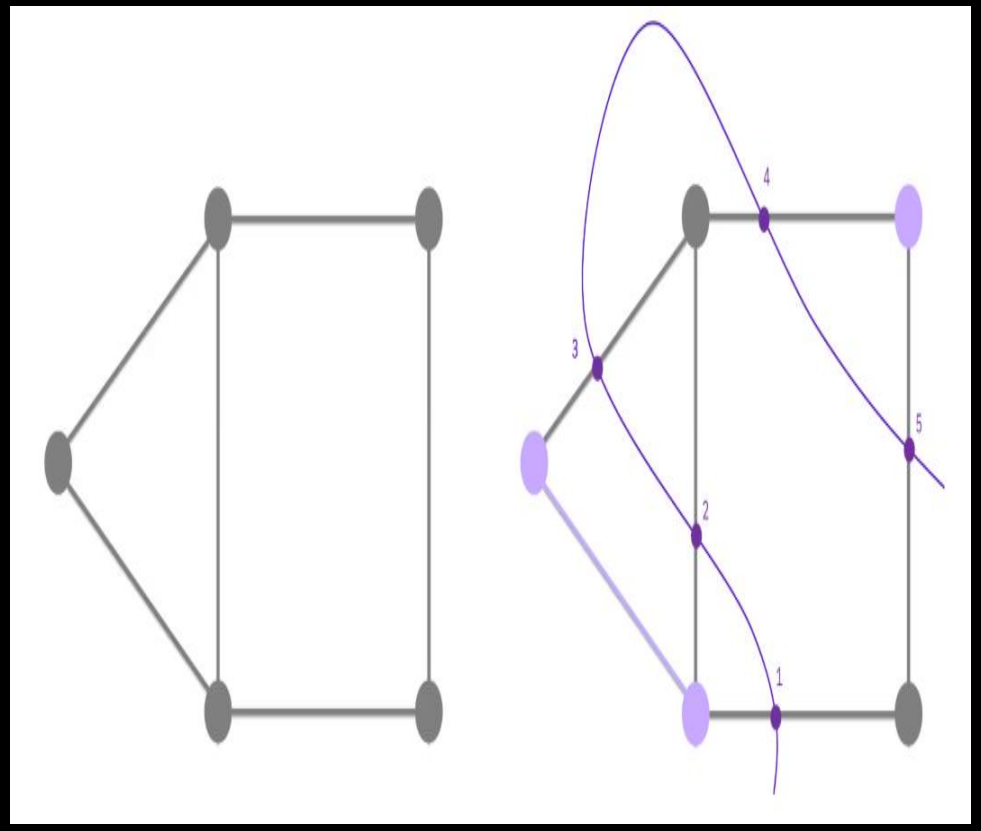
Operator	Gate(s)		Matrix
Pauli-X (X)			$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)			$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)			$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard (H)			$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Phase (S, P)			$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8$ (T)			$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$
Controlled Not (CNOT, CX)			$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
Controlled Z (CZ)			$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$
SWAP			$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$
Toffoli (CCNOT, CCX, TOFF)			$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$

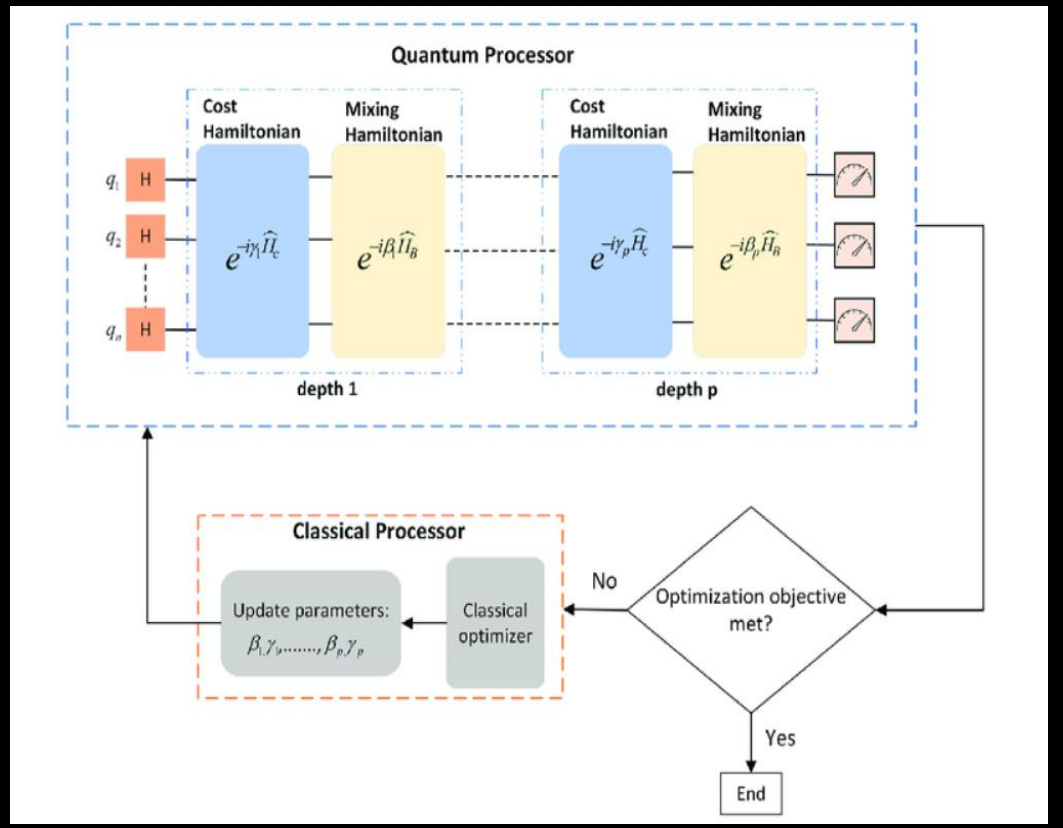
Quantum applications



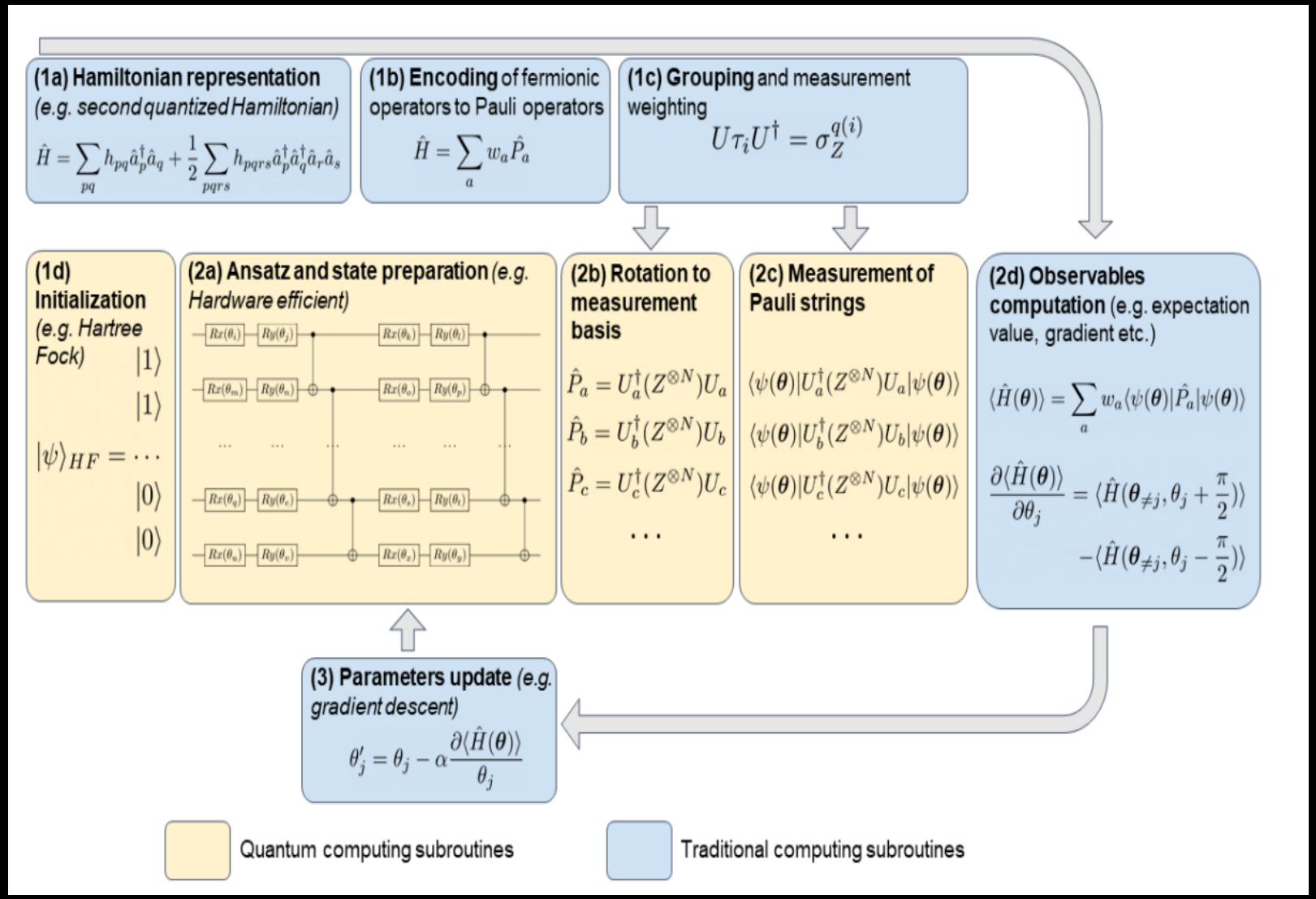
Source: https://pixelplex.io/blog/quantum-computing-applications/

Optimization using Quantum Circuits: QAOA, Hybrid quantum-classical framework





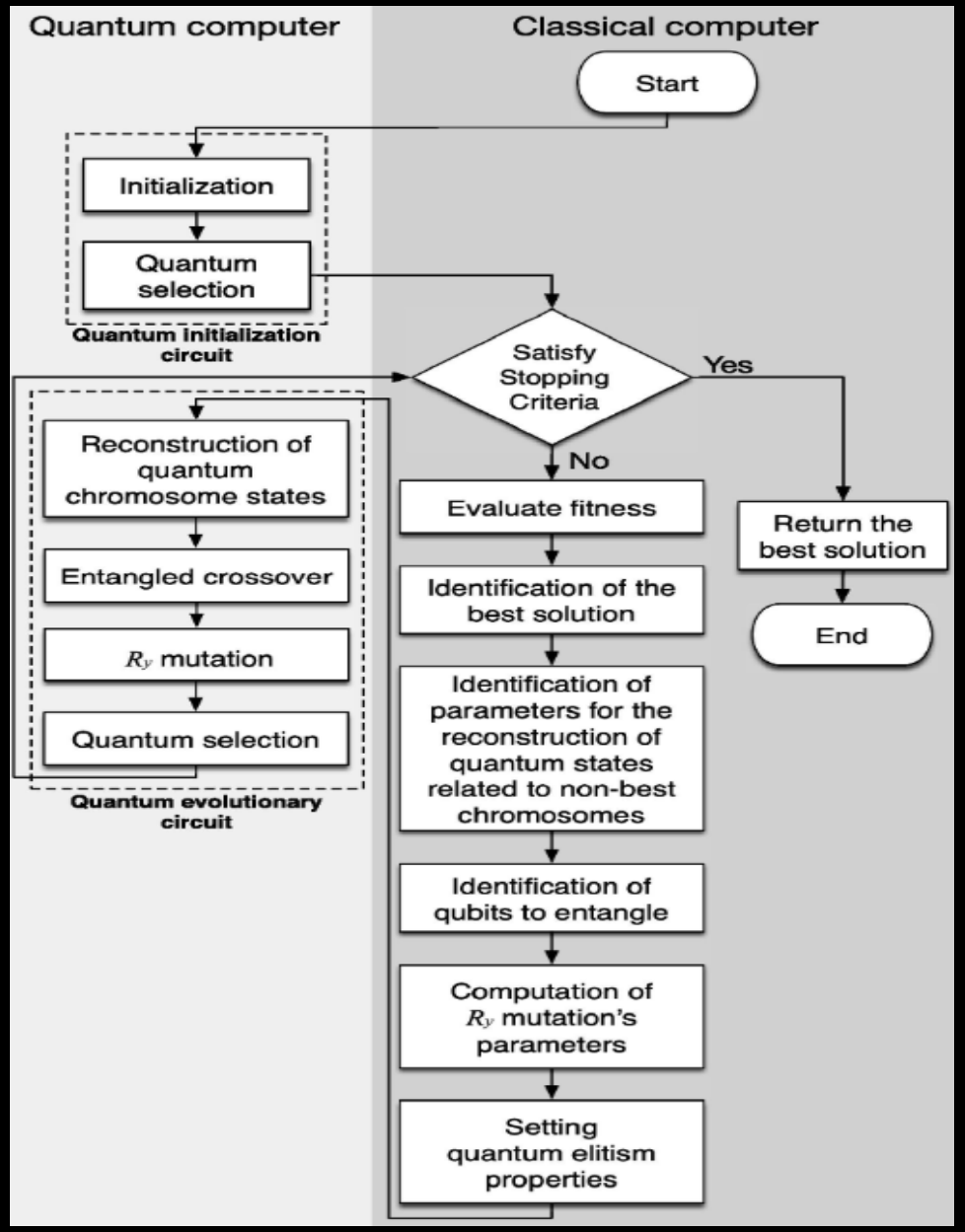
https://quantum.cloud.ibm.com/docs/it/tutorials/quantum-approximate-optimization-algorithm



Variational Quantum Eigensolver (VQE)

https://arxiv.org/pdf/2111.05176

https://quantum.cloud.ibm.com/learning/it/courses/quantum-diagonalization-algorithms/vqe



Quantum Genetic algorithms: another hybrid approach

https://www.sciencedirect.com/science/article/pii/S002002552100640X (Acampora and Vitiello 2021)

Quantum Genetic Algorithm: Workflow

Merit function Evaluation (Classical), evaluation of the chi-squared for the cosmological functions to find the minimization parameters

Individual Selection and Repopulation (Classical, duplication of the selected individuals)

2 quantum circuits, one for the duplicated best data and the other for the rest of the population (random), while keeping the best individuals. Quantum Encoding

Quantum Superposition (already implemented in the encoding)

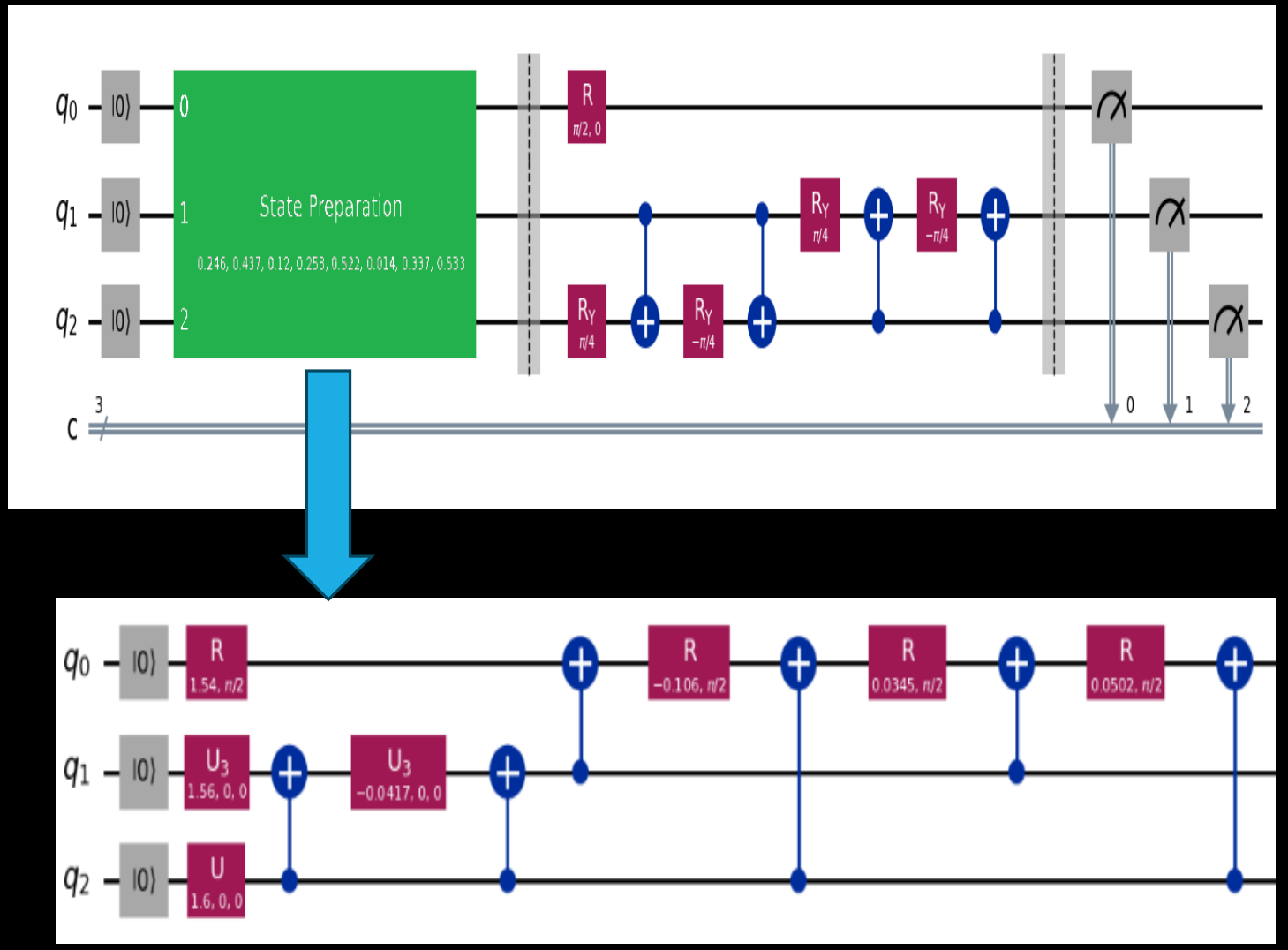
Quantum Crossover + Mutation

Quantum Decoding

Our Quantum Circuit:

$$U_{\text{cross}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{2} & -\frac{1}{2} \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

$$U_{\text{mut}} = R_x\left(\frac{\pi}{2}\right) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix}$$



Some more details on our Quantum Genetic Algorithm

Algorithm 1 Amplitude-Encoded Quantum Genetic Algorithm

Input: Population size n_p, number of generations n_g, crossover probability p_c, mutation probability p_m
Initialize population P with n_p individuals
for $t = 1$ to n_g **do**
    Evaluate fitness of each individual in P
    Select top individuals $P_{\text{elite}} \subset P$ with size $n_p/4$.
    Duplication of the top individuals $P_{\text{elite copy}}$.
    Generate random population P_{rand} so that $P_{\text{rand}}+P_{\text{elite}}+P_{\text{elite copy}}=P$.
    Quantum encode $P_{\text{elite copy}}$ and P_{random} into two different circuits
    for each dimension d **do**
        Apply quantum crossover with probability p_c
        Apply quantum mutation with probability p_m
        Measure circuit to decode updated individuals (two different decoding schemes forP_{random} and $P_{\text{elite copy}}$)
    end for
    Combine: $P \leftarrow P_{\text{elite}} \cup P_{\text{decoded}}$
end for
Return: Best individual in final population

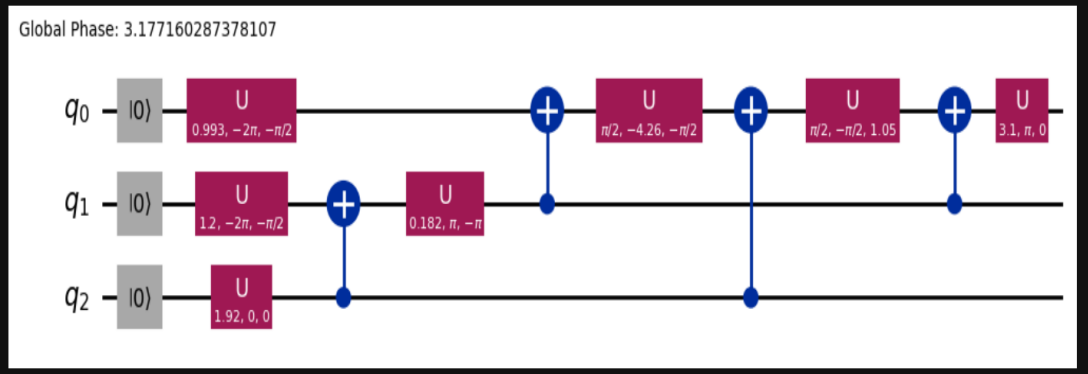
Algorithm 2 AEQGA Decoding from Quantum Measurements

Input: Quantum circuit C (with measurements), number of qubits n_q, decoding flag `flag` $\in$ {`best`, `random`}, interval $[n_{\min}, n_{\max}]$, shots S
Initialize simulator with seed s and run C for S shots to obtain counts
if `flag` = `best` **then** ▷ Restricted box around elites; probability–based decoding
    $C \leftarrow \sum_i c_i$ ▷ total measurements
    $p_i \leftarrow c_i/C$
    $x_i \leftarrow n_{\min} + (n_{\max} - n_{\min}) \cdot \sqrt{p_i}$ ▷ $\sqrt{p_i}$ focuses samples toward box center
else ▷ `random`: full-range min–max decoding
    $c_{\min} \leftarrow \min_i c_i, \quad c_{\max} \leftarrow \max_i c_i$
    $x_i \leftarrow n_{\min} + (n_{\max} - n_{\min}) \cdot \dfrac{c_i - c_{\min}}{c_{\max} - c_{\min}}$
end if
(**Post–process**): if any $x_i = n_{\min}$ exactly, replace it with a draw from $\mathcal{U}(n_{\min}, n_{\max})$
Output: Decoded vector $\mathbf{x}$ of the classical individuals for the populations

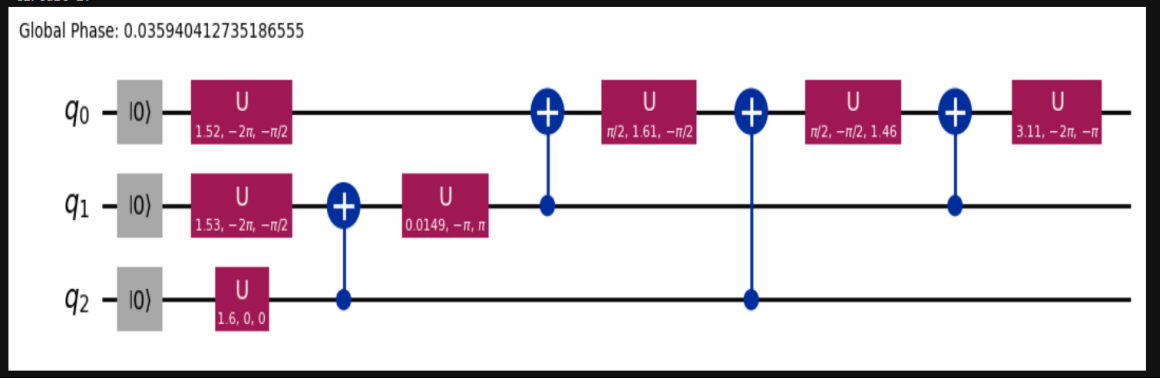
The Quantum Genetic Algorithm Step by step on qiskit: Quantum Encoding

```python
def Quantum_Encoding(population, n_qubit, dimensions):
    i=0
    j=0
    norm_vectors=np.array([])
    population_norm=np.array([])
    while i<dimensions:
        norm_constant = np.linalg.norm(population[i])
        pop_norm=population[i]/norm_constant
        norm_vectors=np.append(norm_vectors,norm_constant)
        population_norm=np.append(population_norm, pop_norm)
        i=i+1
    population_norm=population_norm.reshape(dimensions,2**n_qubit)

    quantum_circuits = []
    while j<dimensions:
        circ_encoding=QuantumCircuit(n_qubit)
        circ_encoding.initialize(population_norm[j])
        quantum_circuits.append(circ_encoding)
        j=j+1
    return quantum_circuits
Initial_Quantum_pops=Quantum_Encoding(initial_population, n_qubit, dimensions)

Initial_Quantum_pops2=Quantum_Encoding(initial_population, n_qubit, dimensions)

for i, qc in enumerate(Initial_Quantum_pops2):
    print(f"Circuit {i+1}:")
    display(qc.decompose(reps = 7).draw('mpl'))
    plt.show()
```

Circuit 1:



Circuit 2:



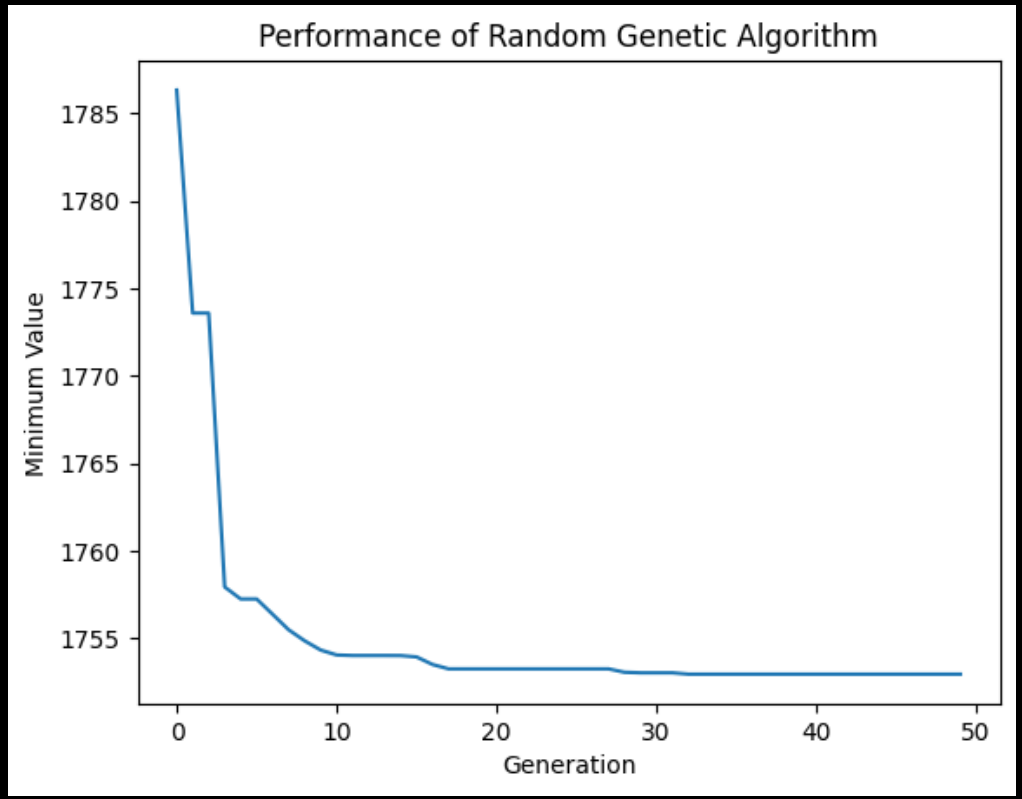
Quantum Genetic Algorithm: Quantum Crossover and mutation

```python
def quantum_crossover(quantum_pop,n_qubit, crossover_probability, flag="new"):
    quantum_pop.barrier()
    if flag=="old":
        for q in range(n_qubit):
            if np.random.rand() < crossover_probability:
                qubit2=(q + 1) % n_qubit
                quantum_pop.swap(q, qubit2)

    elif flag=="new":
        if np.random.rand() < crossover_probability:
            q=random.randint(0, n_qubit-2)
            #theta = np.random.uniform(np.pi/8, np.pi)
            quantum_pop.cry(np.pi/2, q, q+1)
            quantum_pop.cry(np.pi/2, q+1, q)
    return quantum_pop
```

```python
def quantum_mutation(quantum_pop, n_qubit, mutation_probability, flag="one"):
    #np.random.seed(seed_quantum)
    if flag=="all":
        for q in range(n_qubit):
            if np.random.rand() < mutation_probability:
                # Randomly select a gate
                gate_choice = np.random.choice(['rx', 'ry', 'rz'])

                if gate_choice == 'rx':
                    theta = np.random.uniform(0, np.pi)
                    quantum_pop.rx(theta, q)
                elif gate_choice == 'ry':
                    theta = np.random.uniform(0, np.pi)
                    quantum_pop.ry(theta, q)
                elif gate_choice == 'rz':
                    theta = np.random.uniform(0, np.pi)
                    quantum_pop.rz(theta, q)
    elif flag=="one":
        if np.random.rand() < mutation_probability:
            q=random.randint(0, n_qubit-1)
            #theta = np.random.uniform(np.pi/4, np.pi)
            quantum_pop.rx(np.pi/2, q)
    quantum_pop.barrier()
    quantum_pop.measure([k for k in range(n_qubit)], [k for k in range(n_qubit)])
    return quantum_pop
```

Quantum Genetic Algorithm: Quantum Decoding

```python
def quantum_decoding(quantum_pop,n_qubit,n_min, n_max, flag, seed,shots = 500*2**n_qubit):
    aersim = AerSimulator(seed_simulator=seed)
    quantum_popt = transpile(quantum_pop, aersim)
    result = aersim.run(quantum_popt, shots=shots).result()
    counts = result.get_counts(quantum_popt)
    if not counts:
        raise ValueError("No counts found. Check the quantum circuit setup.")
    all_outcomes = [format(i, '0' + str(n_qubit) + 'b') for i in range(2**n_qubit)]
    if flag=="random":
        counts_list = [counts.get(outcome, 0) for outcome in all_outcomes]
        norm = np.linalg.norm(counts_list)
        normalized_counts = counts_list / norm
        population = n_min + (n_max - n_min) * (normalized_counts - np.min(normalized_counts)) /
        (np.max(normalized_counts) - np.min(normalized_counts))
    if flag=="best":
        total_measurements = sum(counts.values())
        percentages = [counts.get(outcome, 0) / total_measurements for outcome in all_outcomes]
        population = [n_min + (n_max - n_min) * (percentage**0.5) for percentage in percentages]

    return population
```



Back up Slides

Talk layout

- What is quantum computing?
- Cosmological parameters: probes and open issues for modern cosmology.
- Overview of the problem we aim to solve: Quantum Genetic Algorithm to optimize cosmological parameters.
- Main results and tests with its hyperparameters.
- Comparison with other algorithms.
- Discussions and Conclusions.

What is MODERN cosmology?

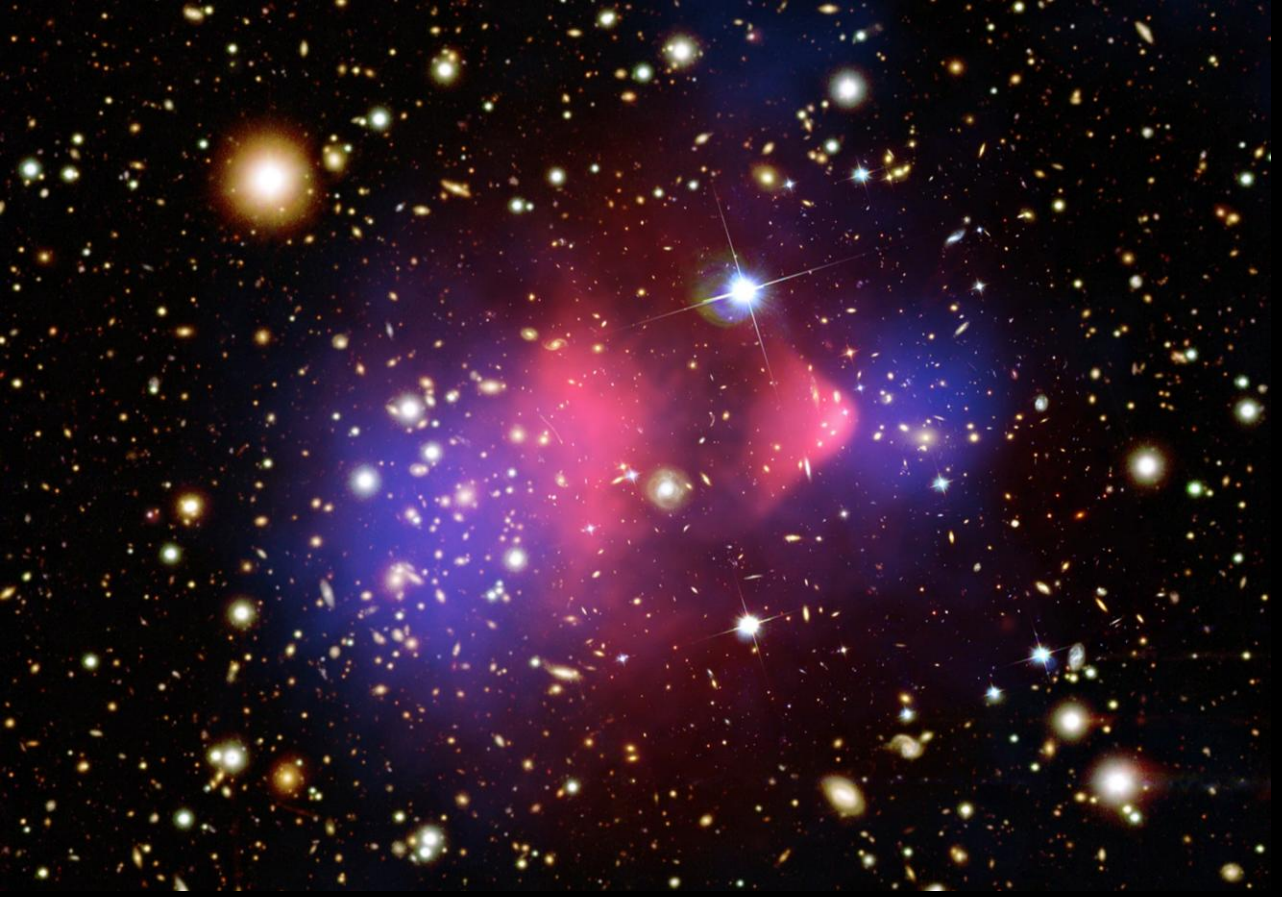
The study of the origin, evolution, overall stucture, and fate of the Universe.

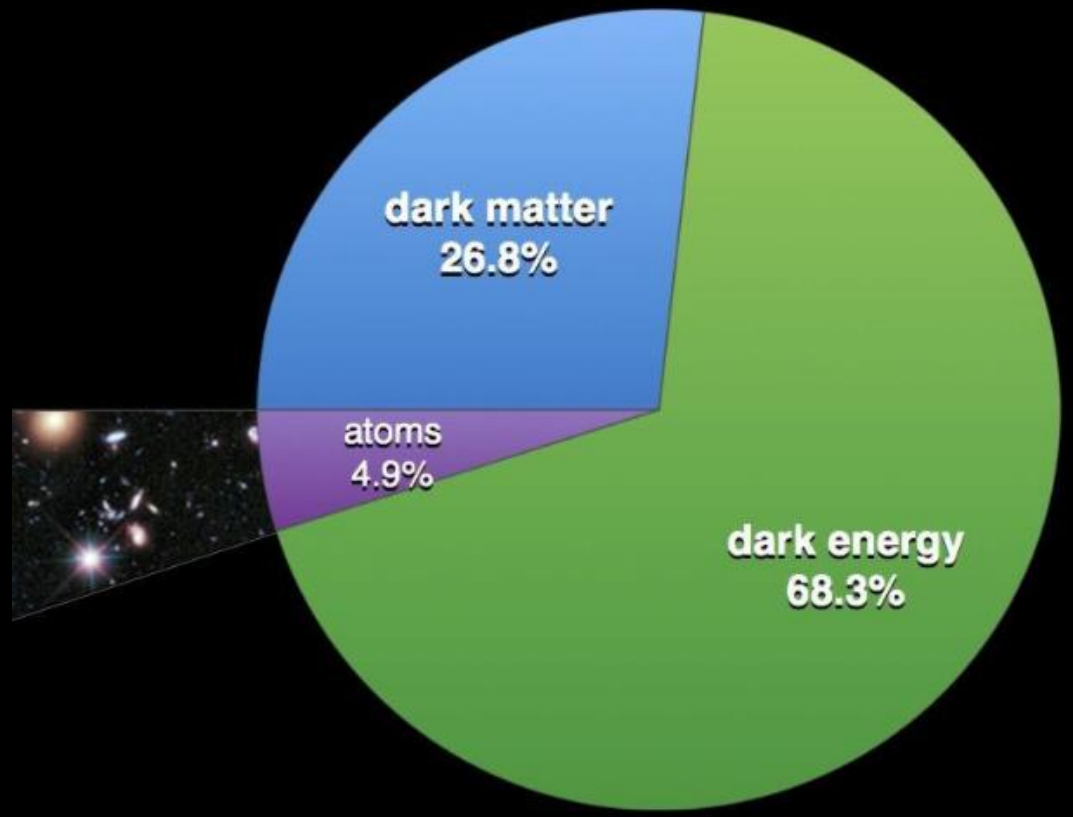
The standard Cosmological scenario is based on two fundamental assumptions:

1) The Cosmological Principle,

2) General Relativity.

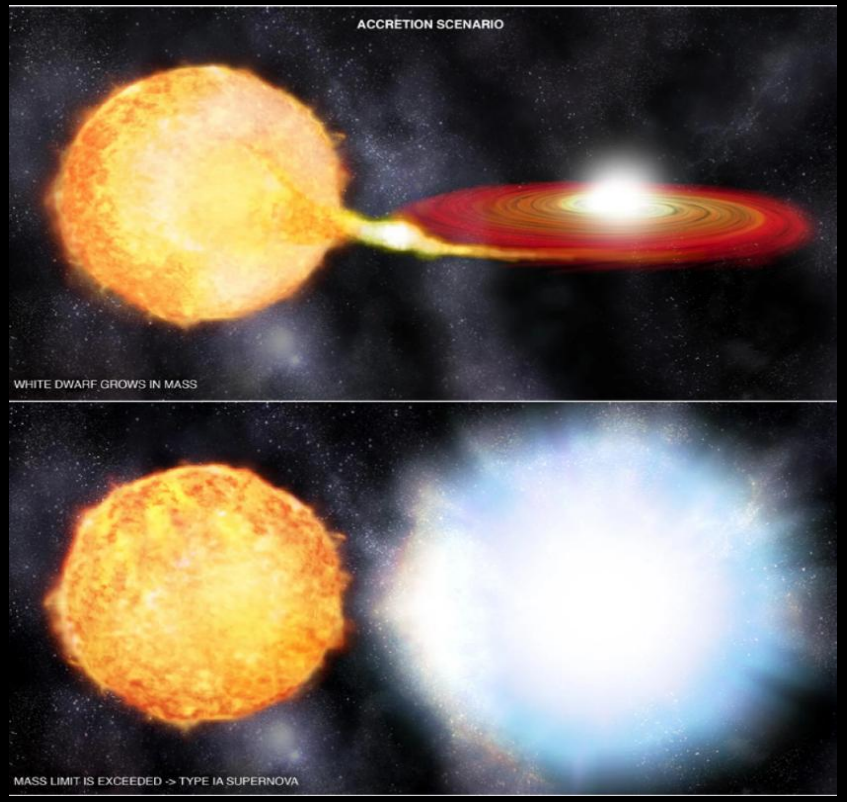
Under these, one can define the so called Λ-Cold Dark Matter (ΛCDM) model, which can allow us to describe the universe using «a small number» of cosmological fundamental parameters.

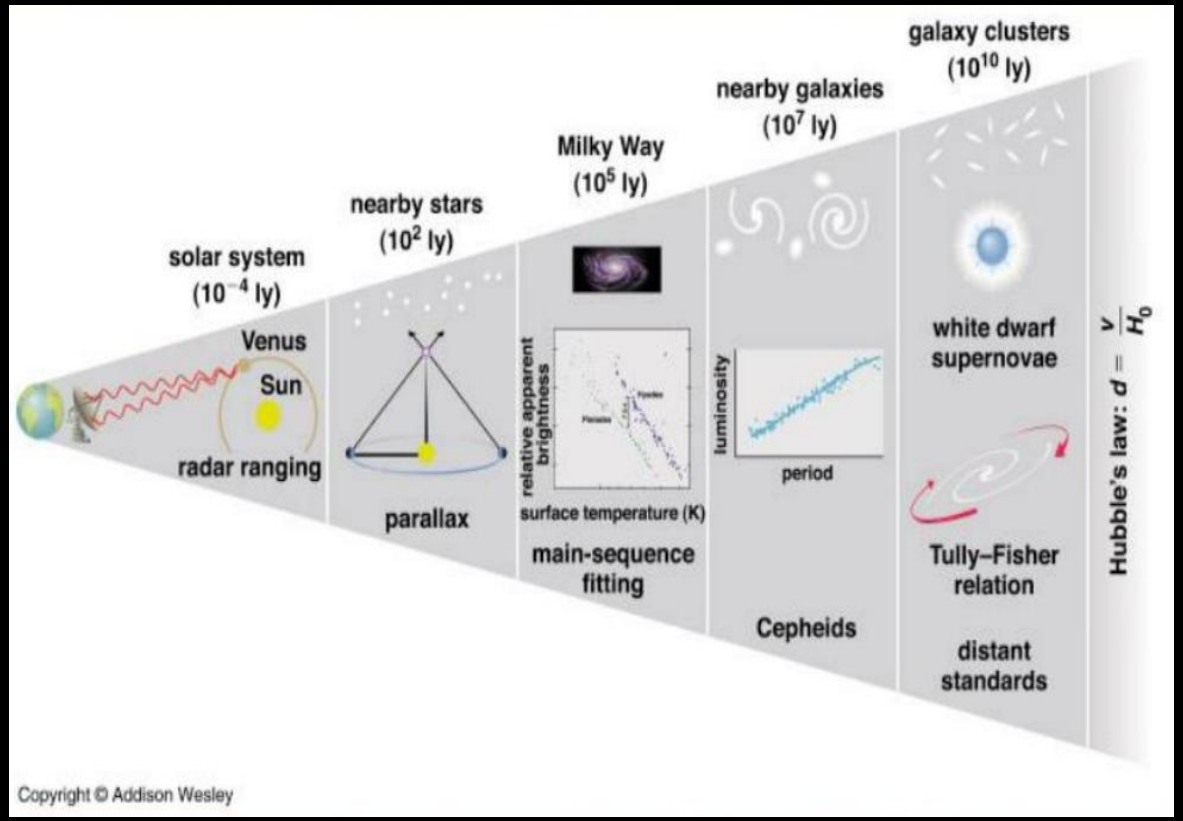




The Cosmic Pie

How to measure cosmological parameters: The cosmic ladder





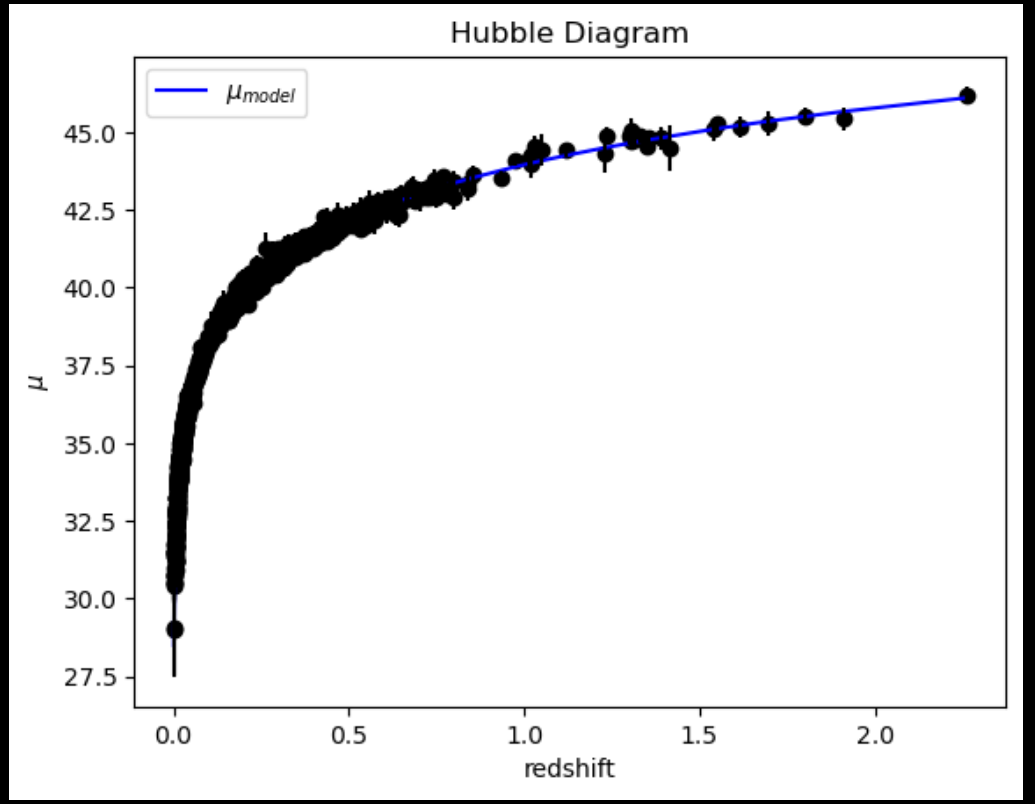
Objective: the Pantheon+ sample of SNe IA

$$\chi^2 = \Delta\vec{D}^T \; C^{-1}_{\text{stat+syst}} \; \Delta\vec{D},$$

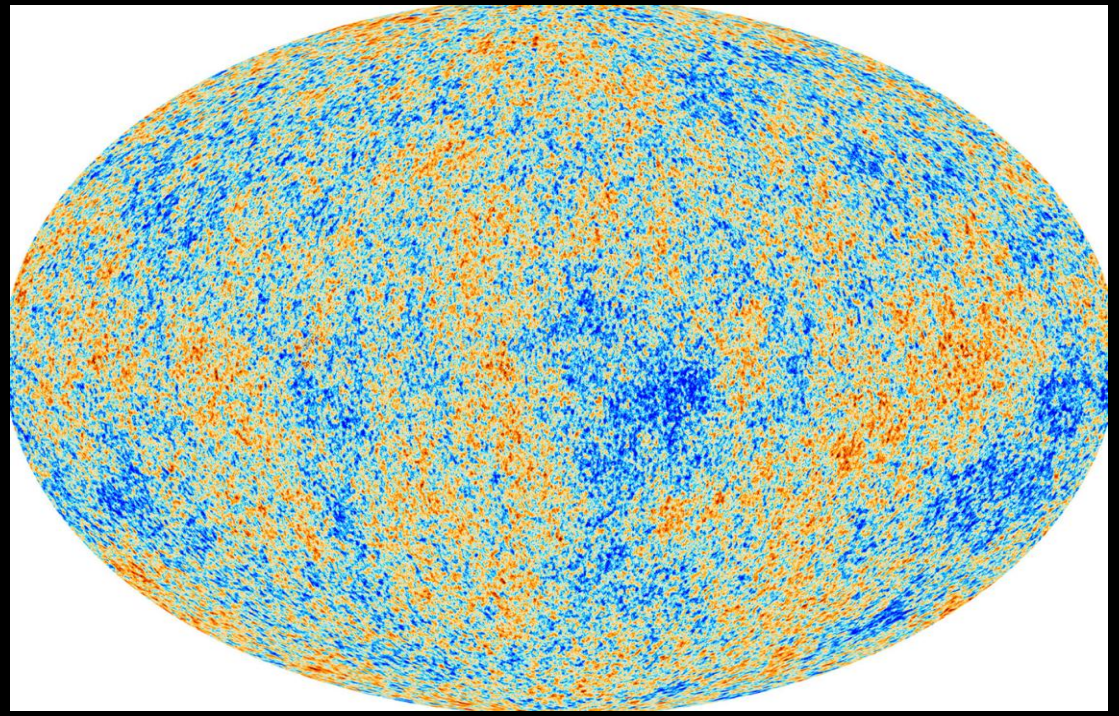
$$\mu_{\text{model}}(z_i) = 5\log(d_L(z_i)/10\,\text{pc}),$$

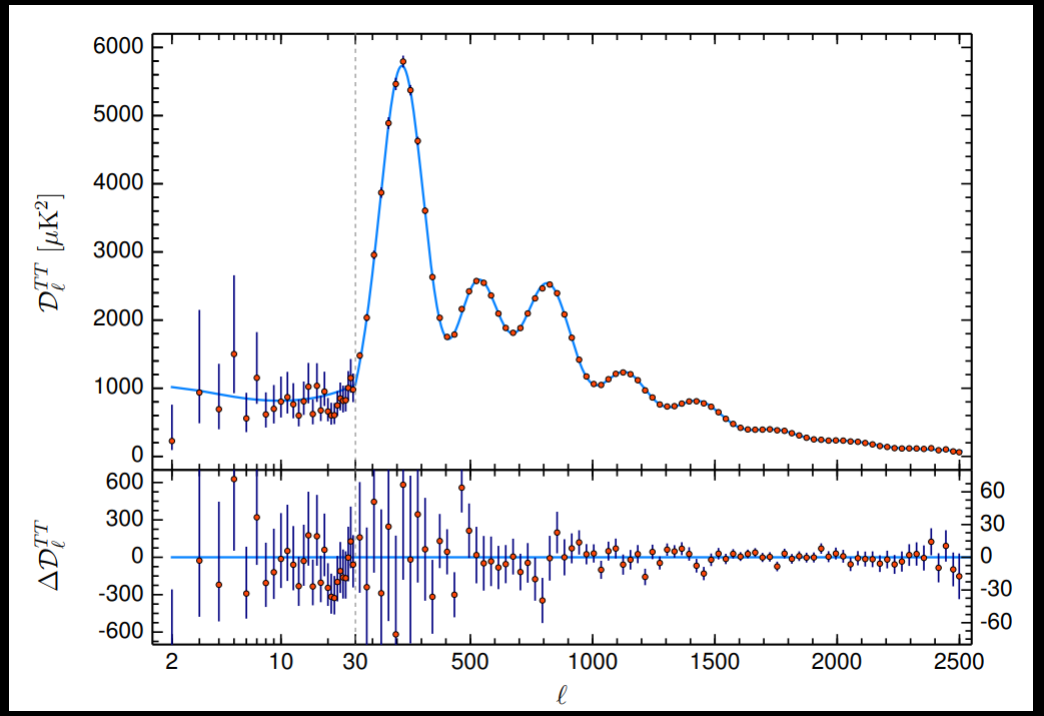
$$d_L(z) = (1+z)c\int_0^z \frac{dz'}{H(z')},$$

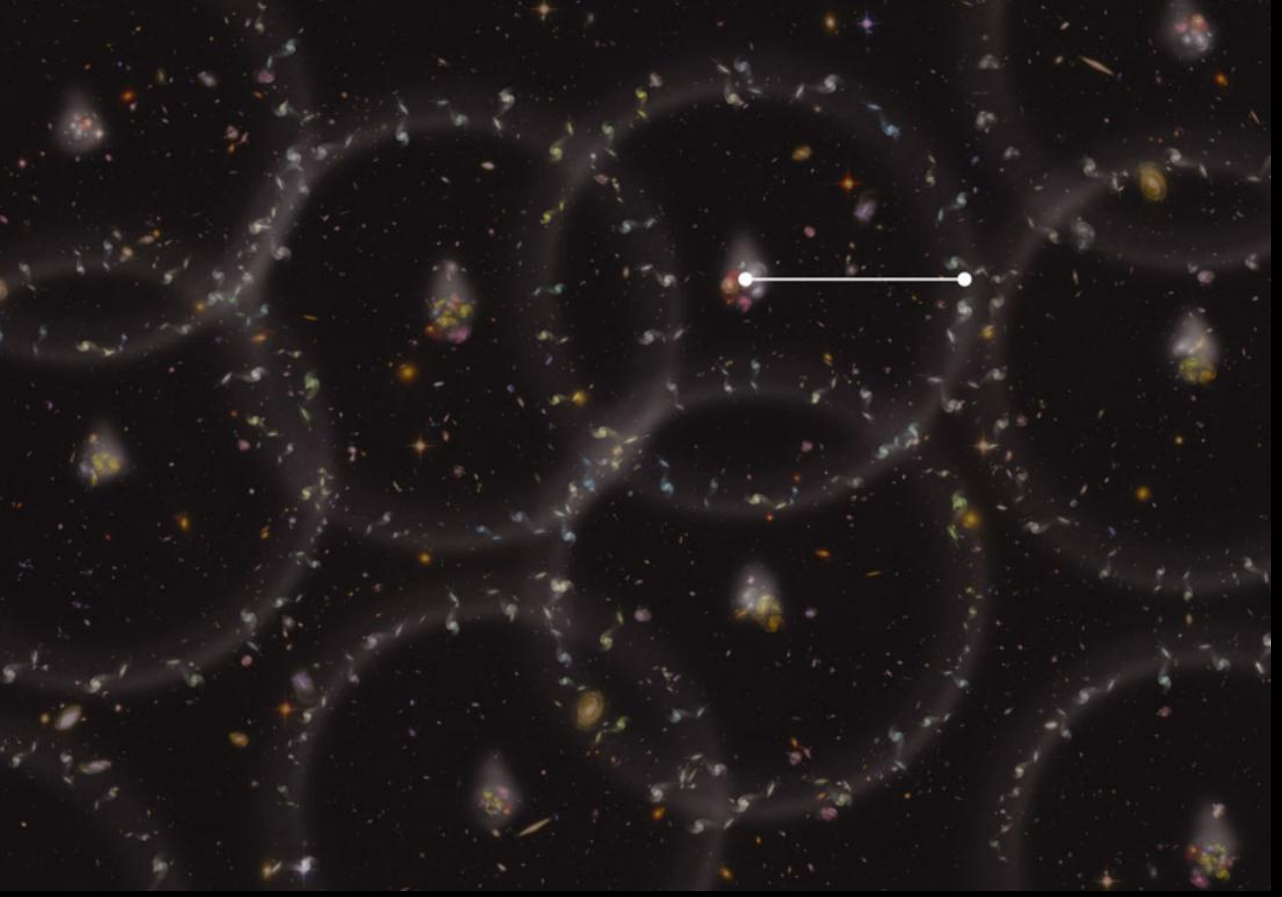
$$H(z) = \text{H}_0\sqrt{\Omega_M(1+z)^3 + \Omega_\Lambda(1+z)^{3(1+w)}}.$$

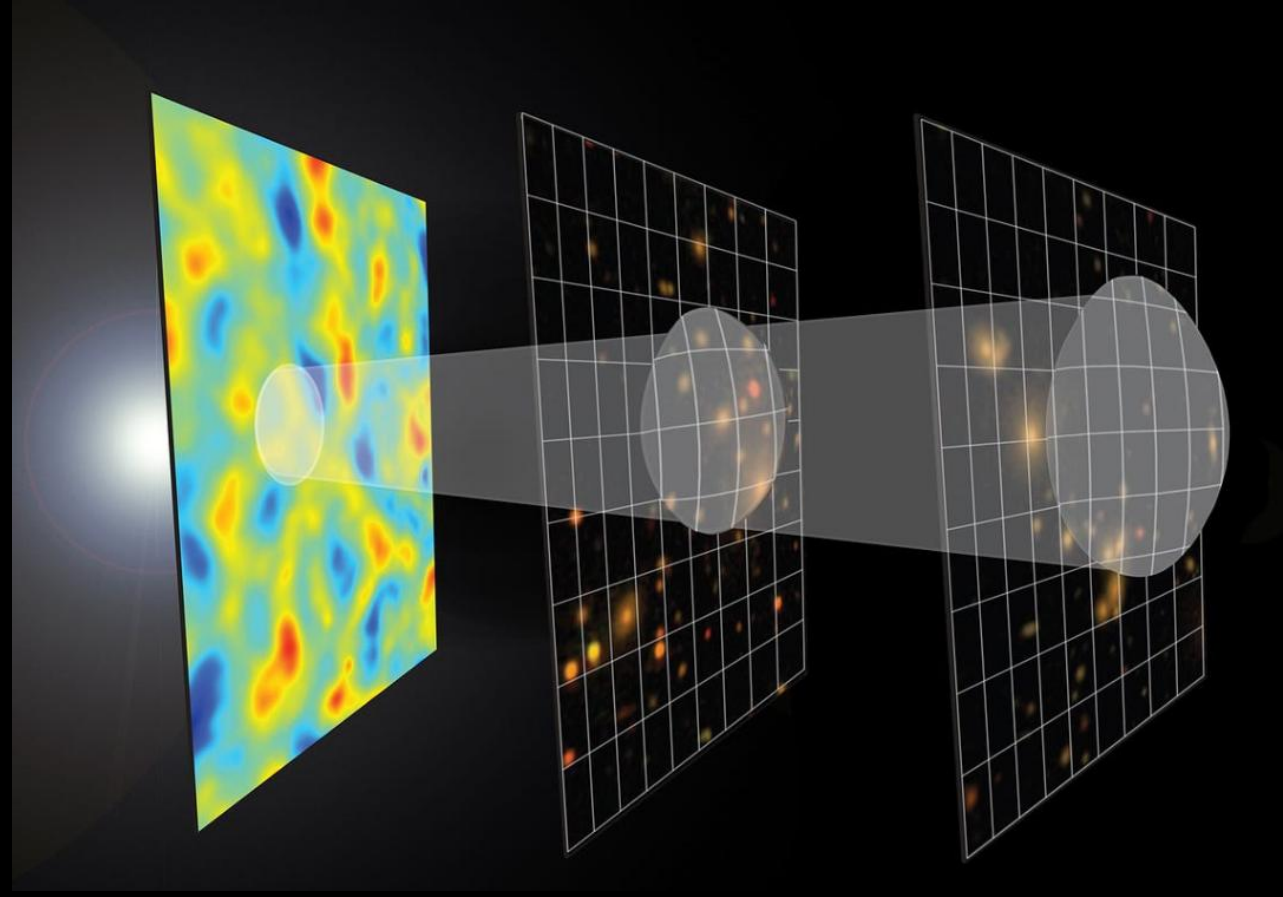


How to measure cosmological parameters: The CMB

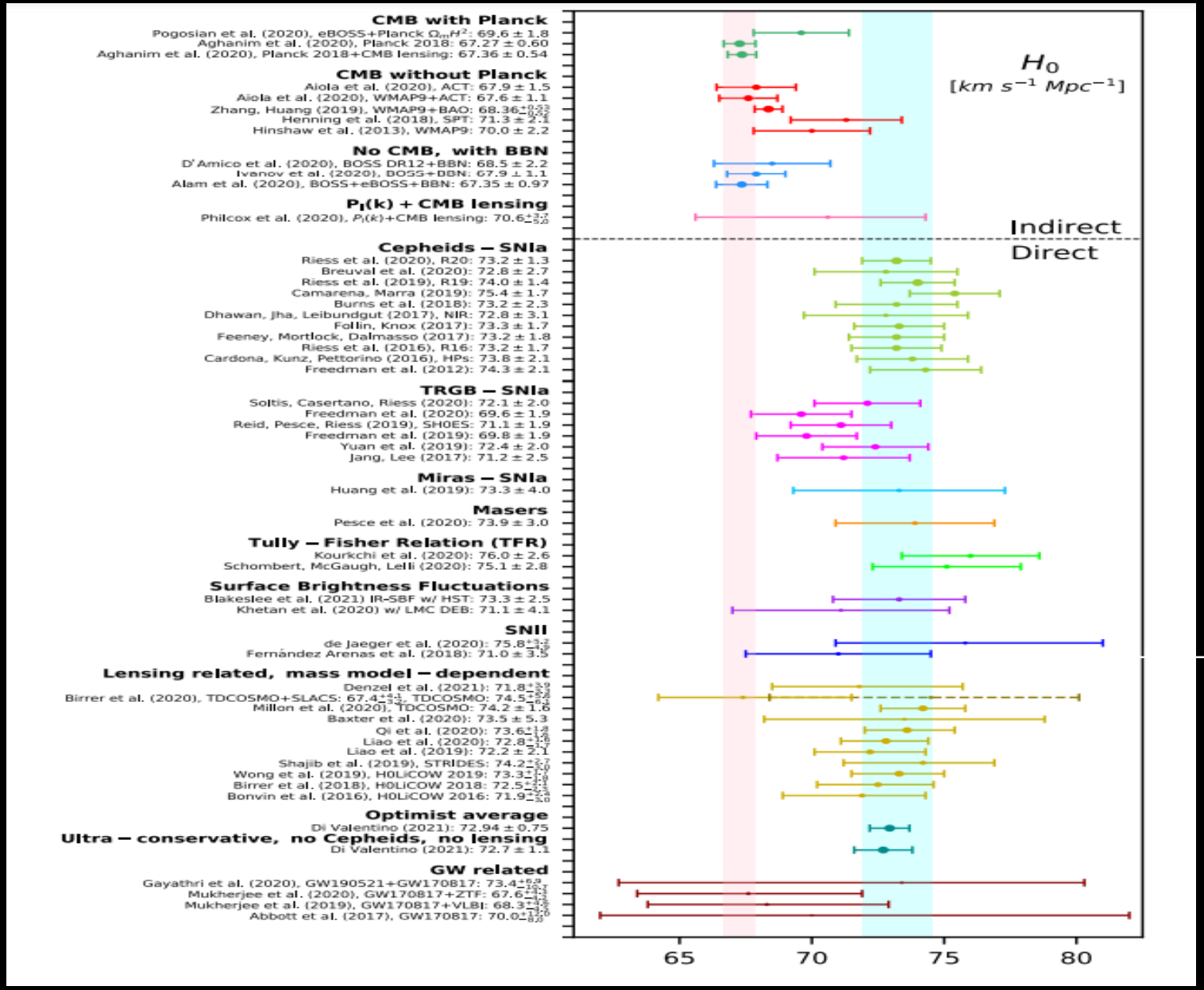






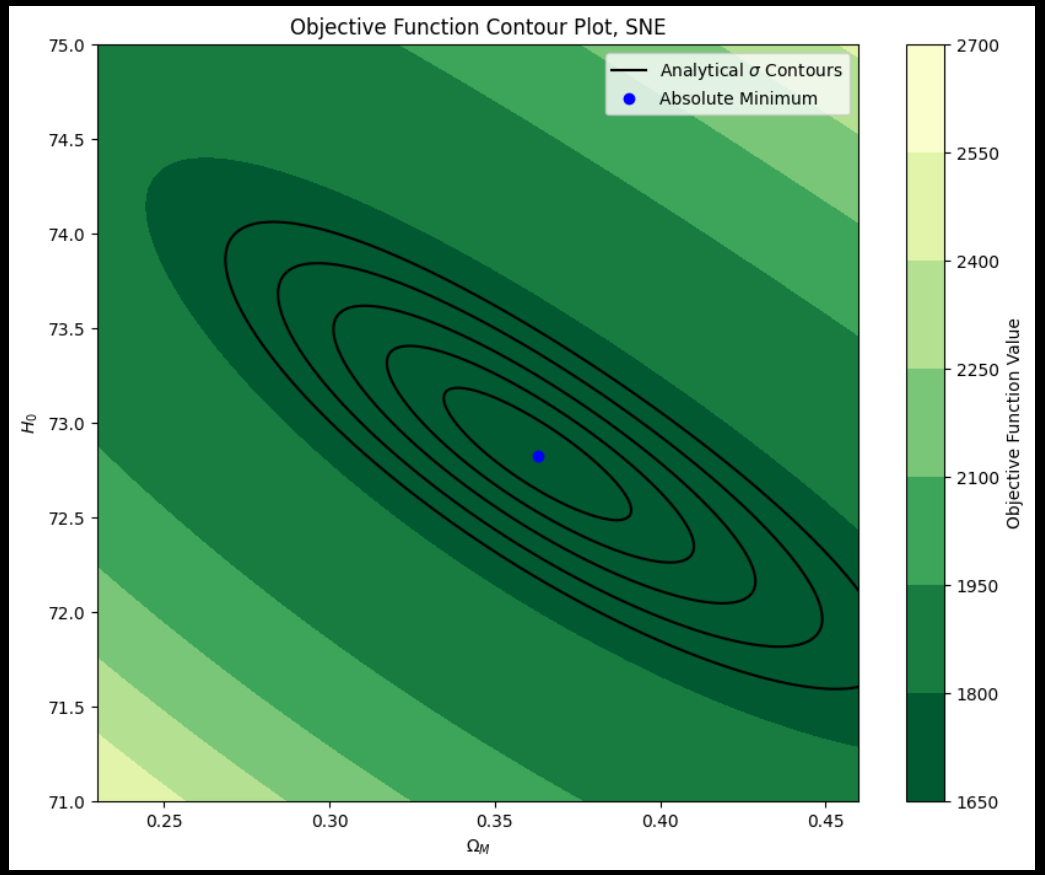


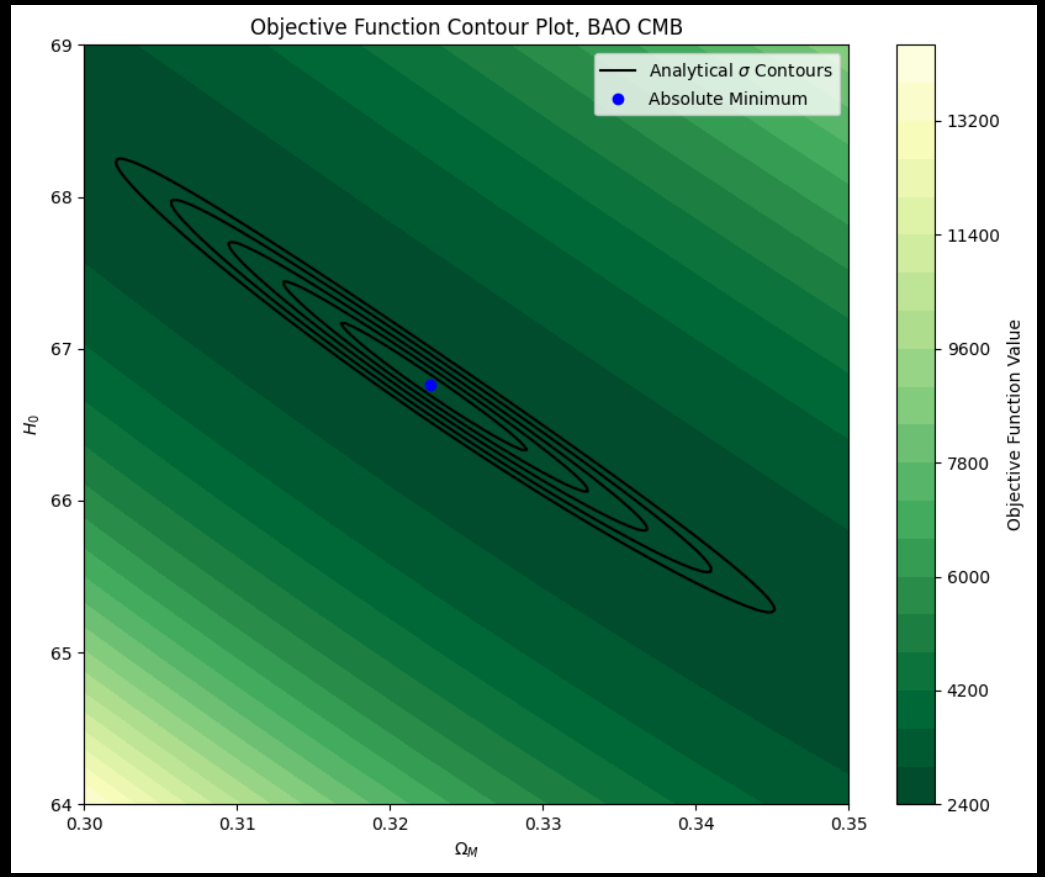
How to measure cosmological parameters: The BAO

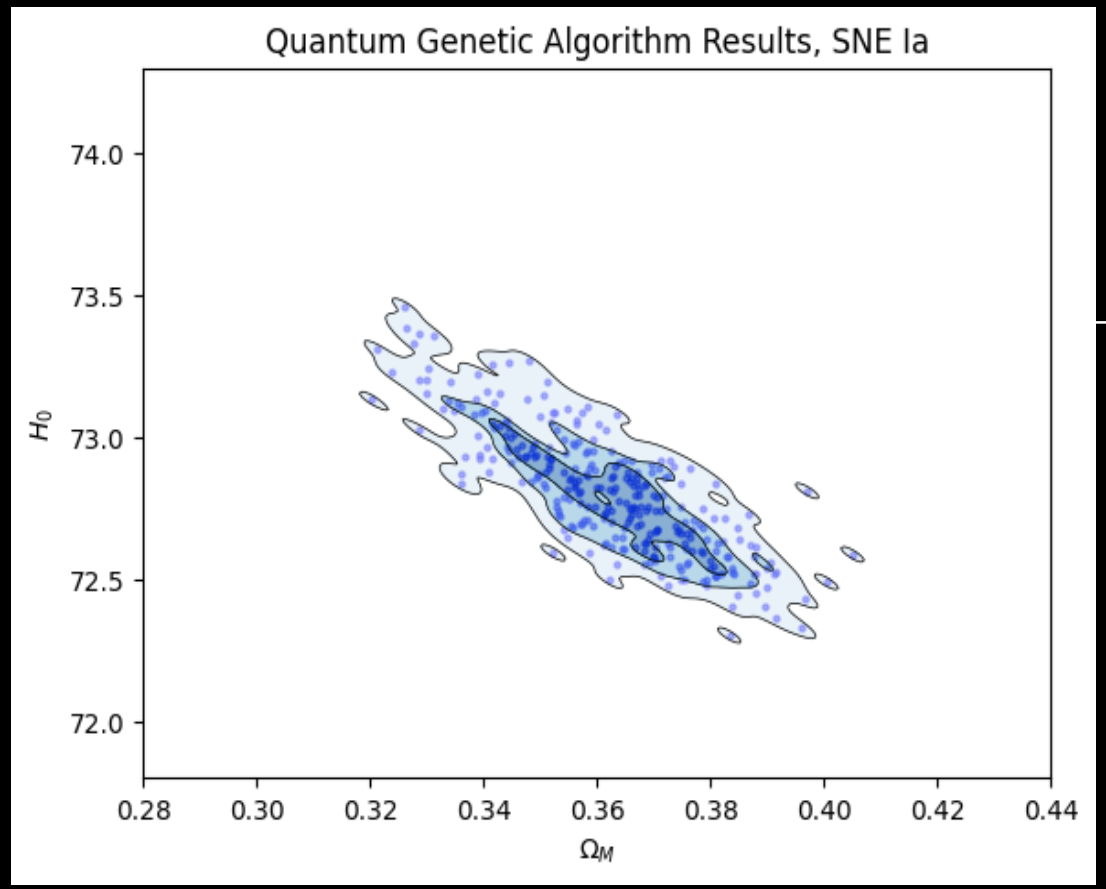


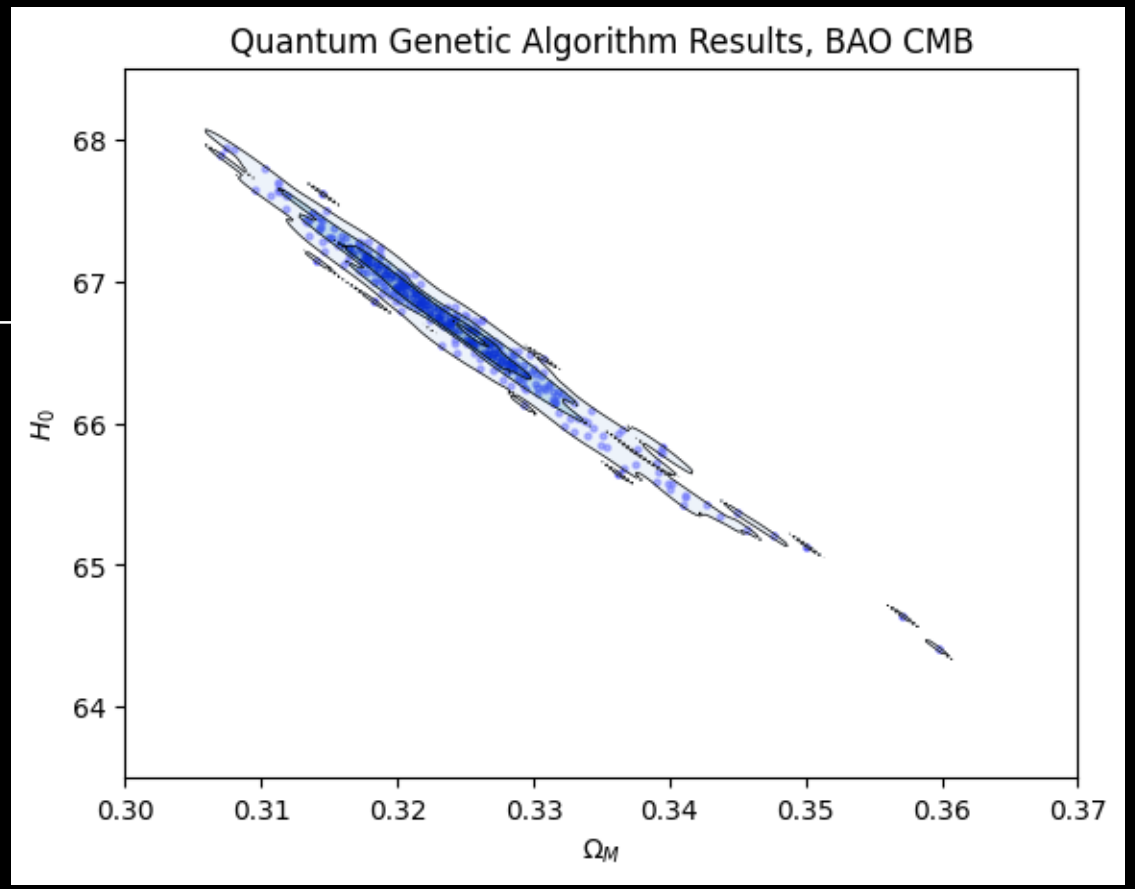
The Hubble Tension

Contour Maps for the Cosmological Objective functions

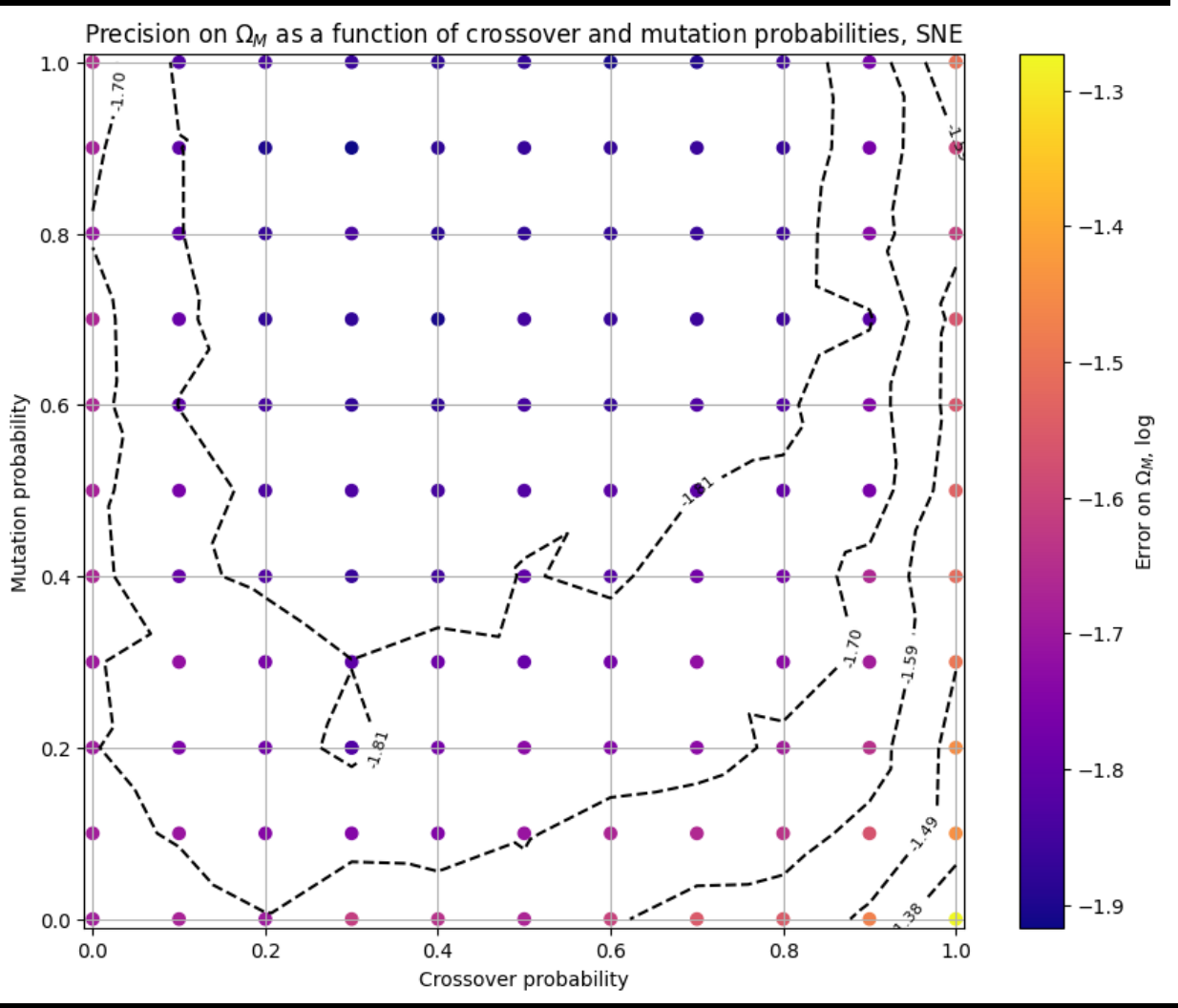


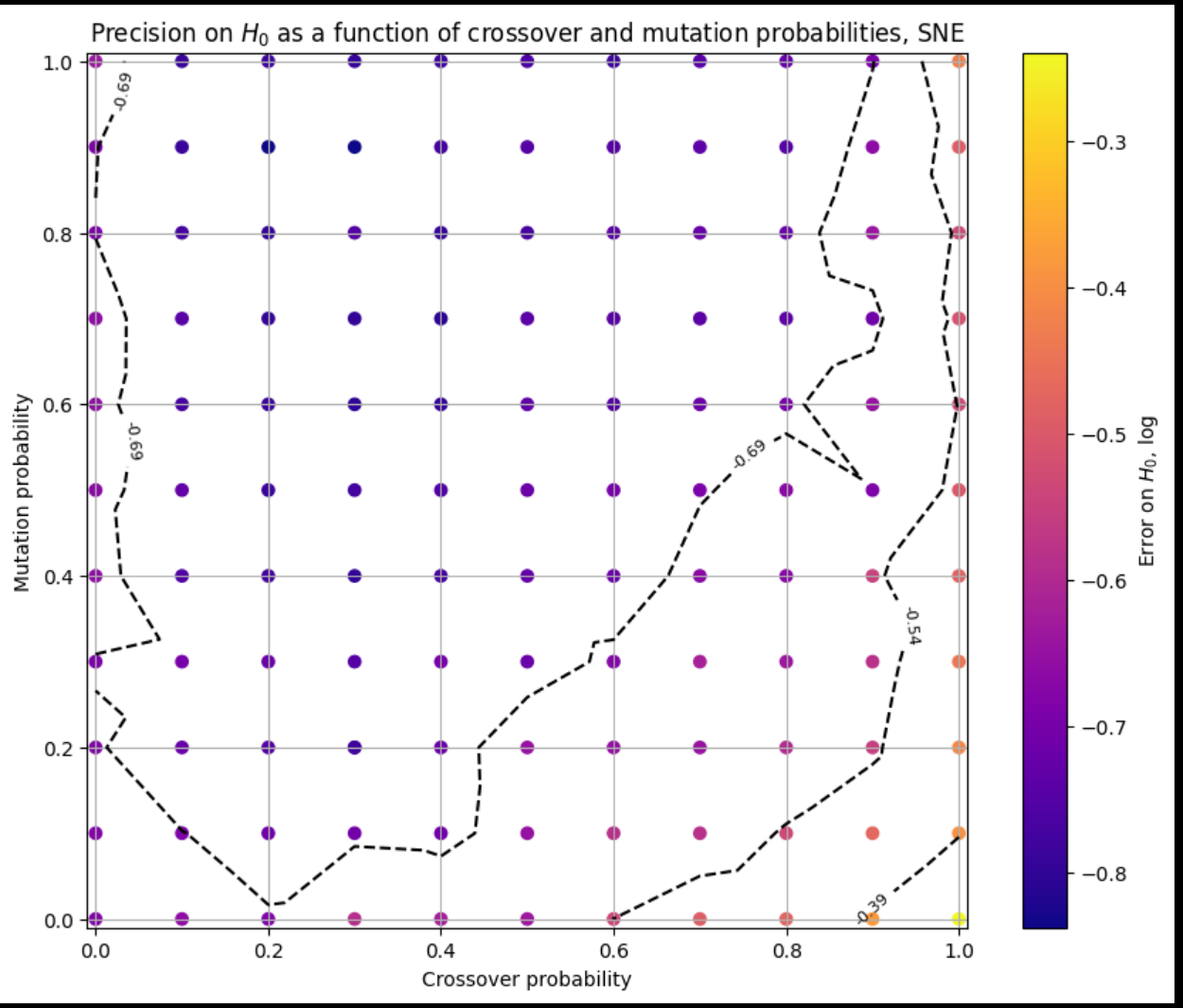






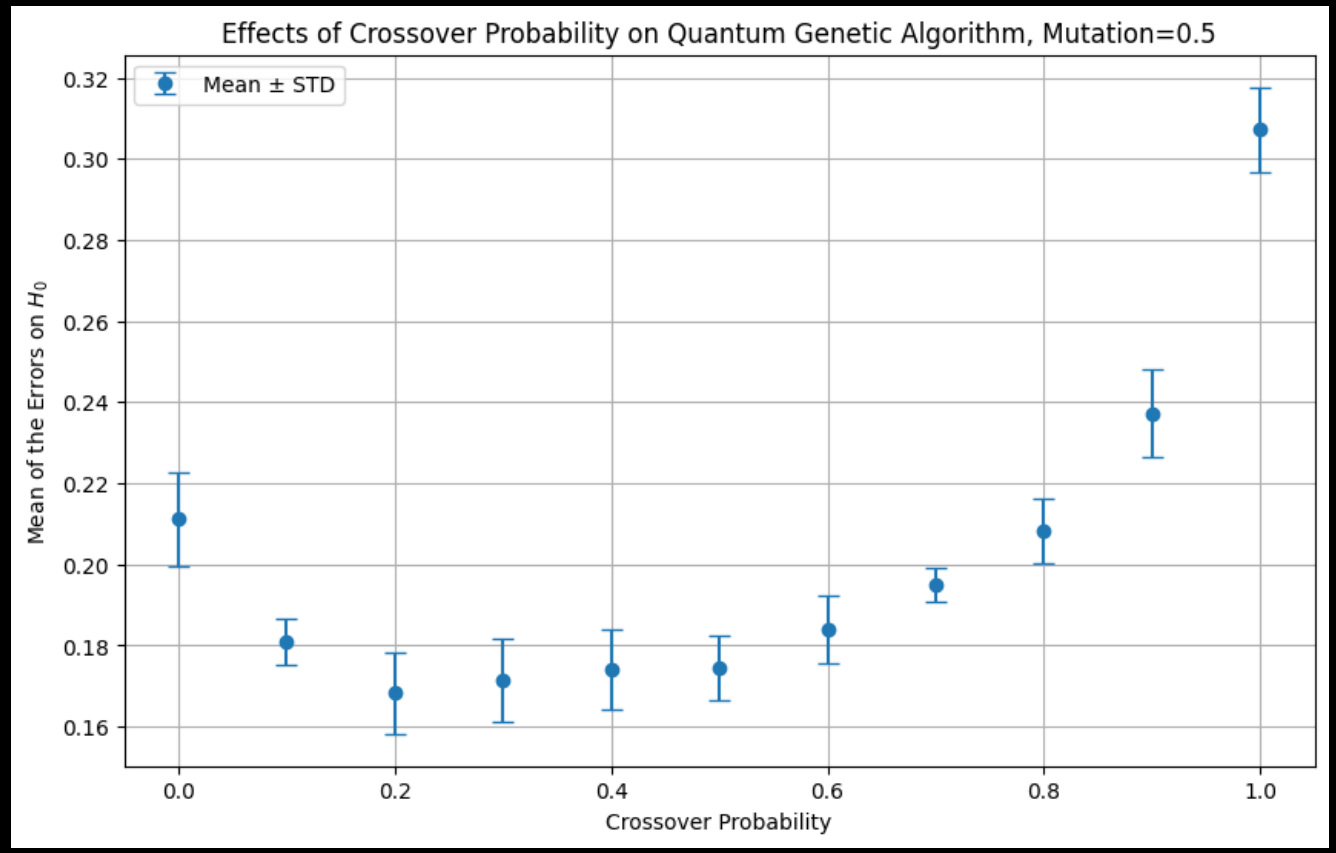
Results (SNe IA left, CMB+BAO right)

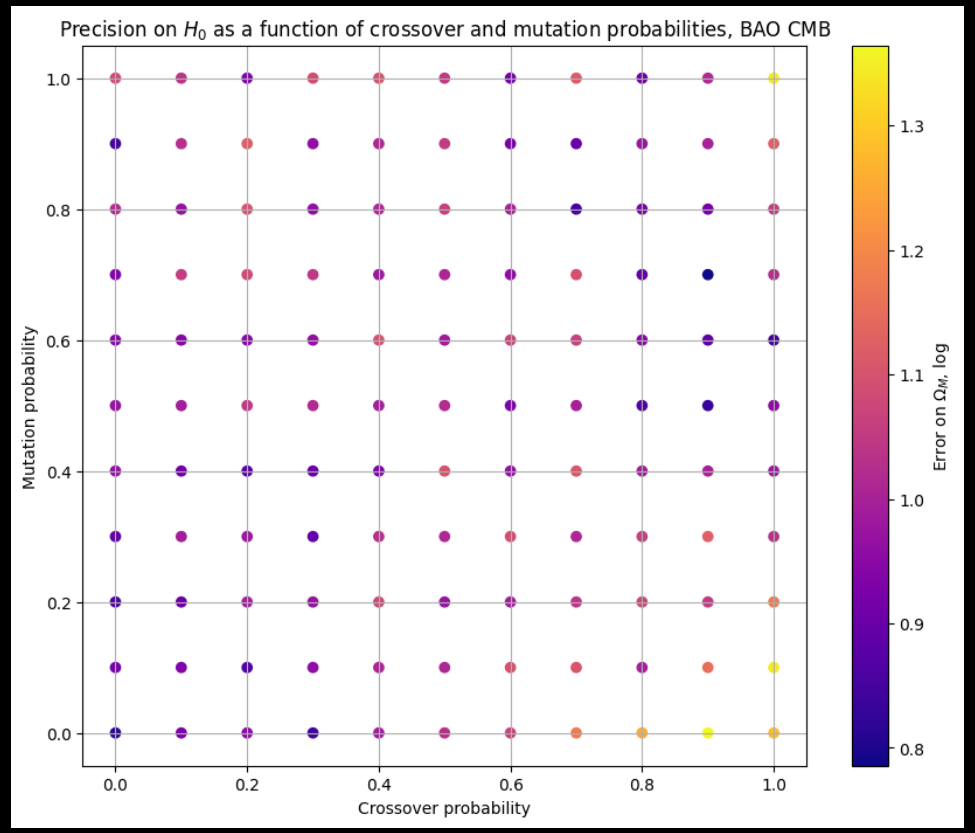


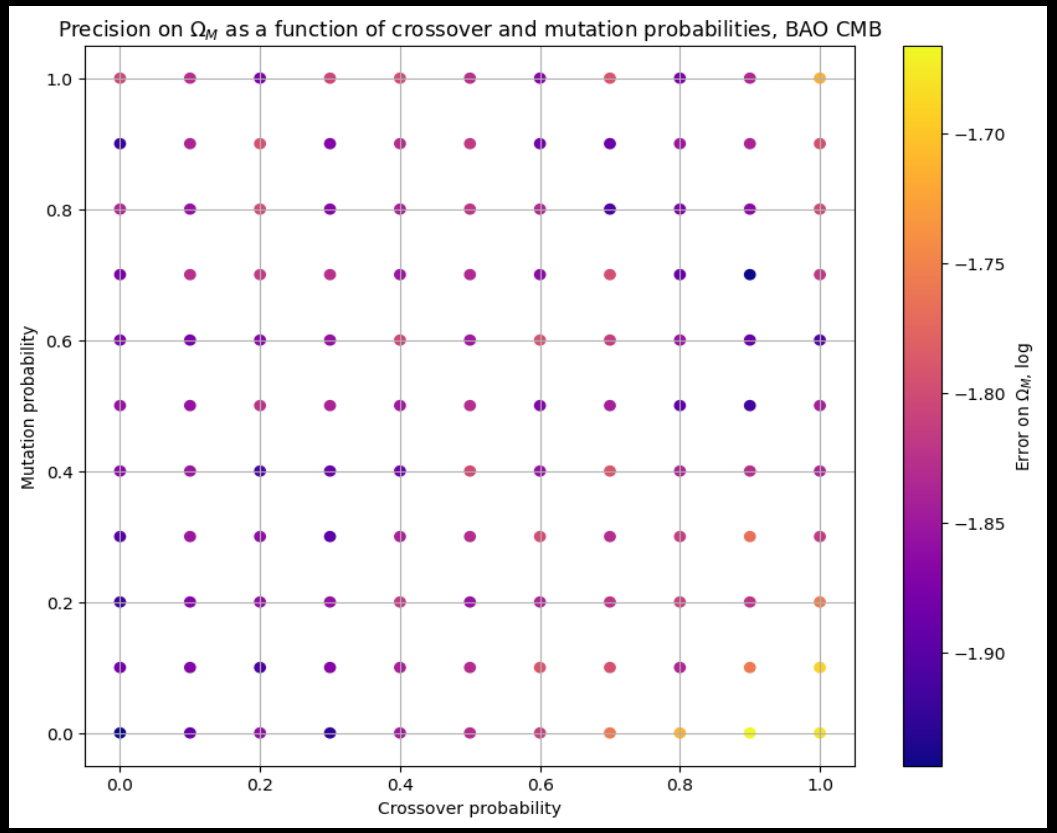


Testing the crossover and mutation effects for the SNe results

Studying the stability of the Algorithm, SNe Ia, error on H0

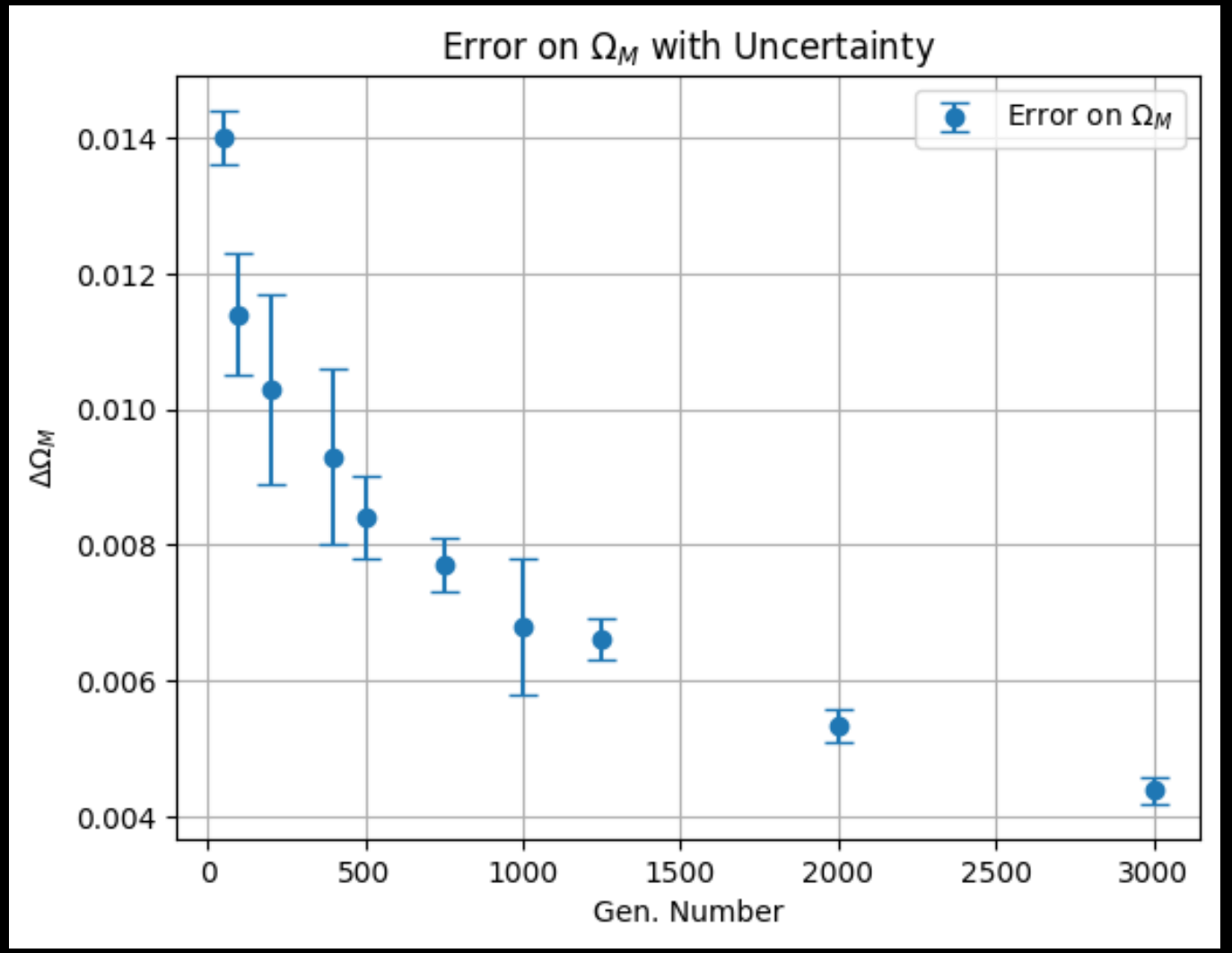




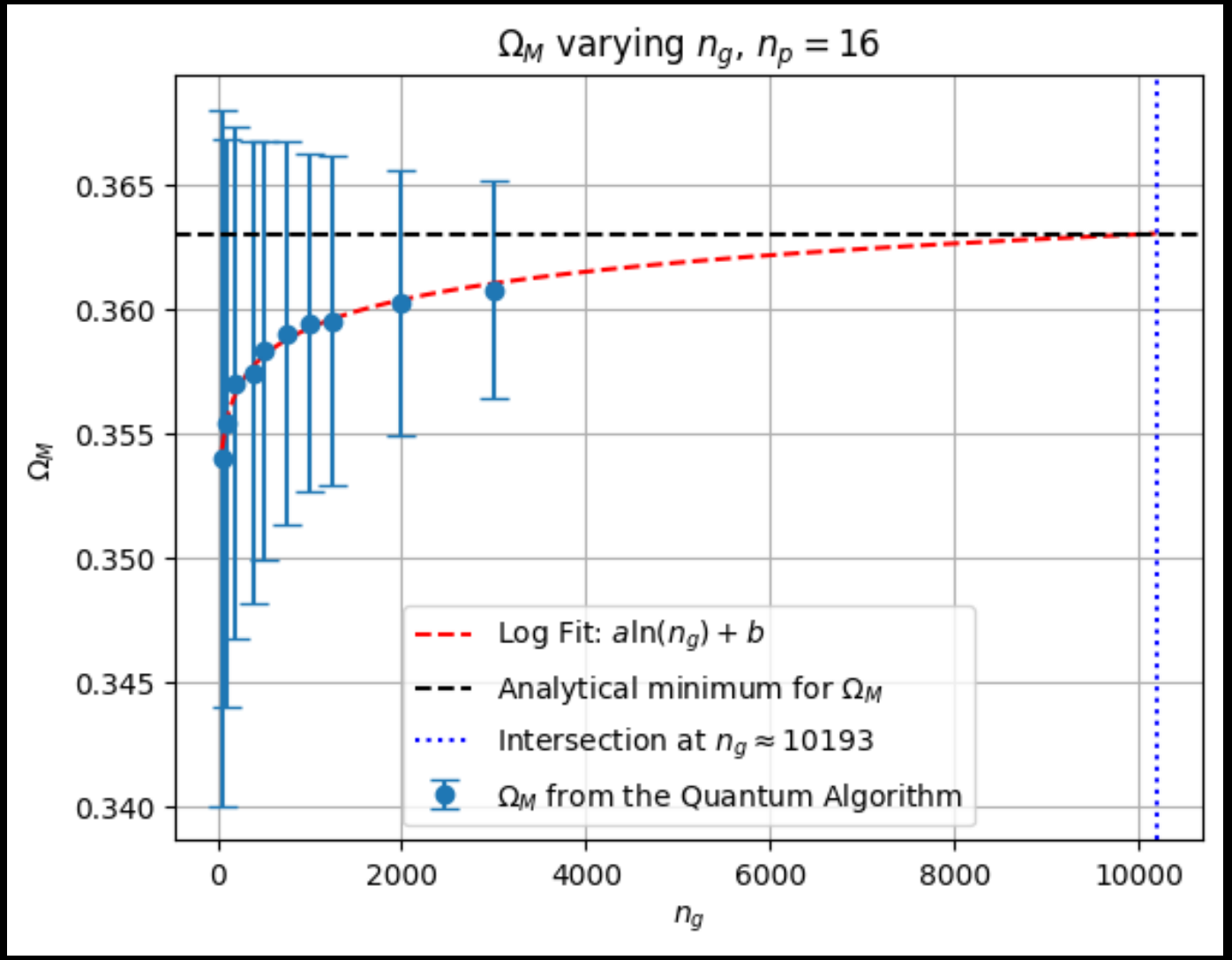


Testing the crossover and mutation effects for the CMB+BAO results

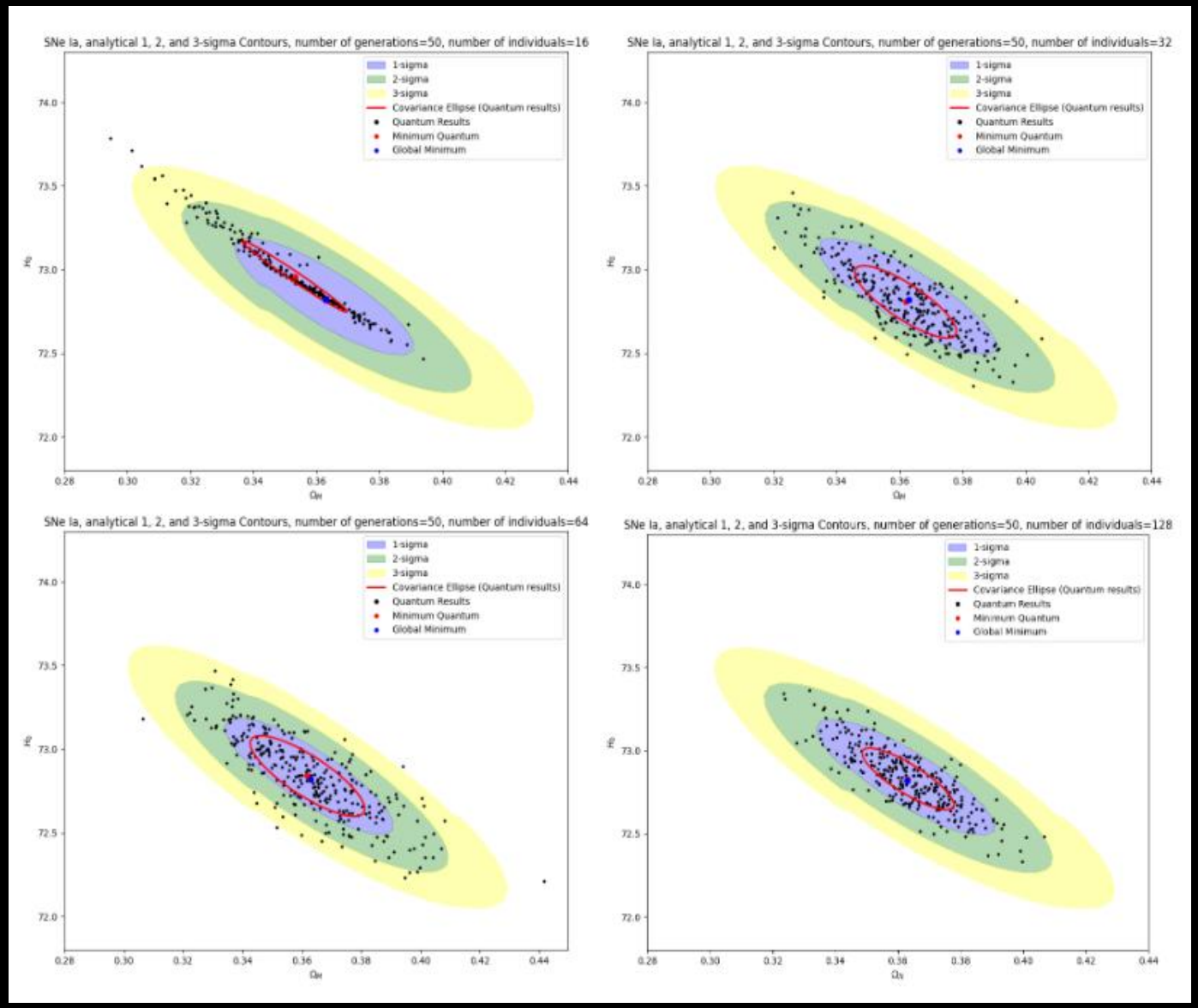
Precision and number of generations, SNE



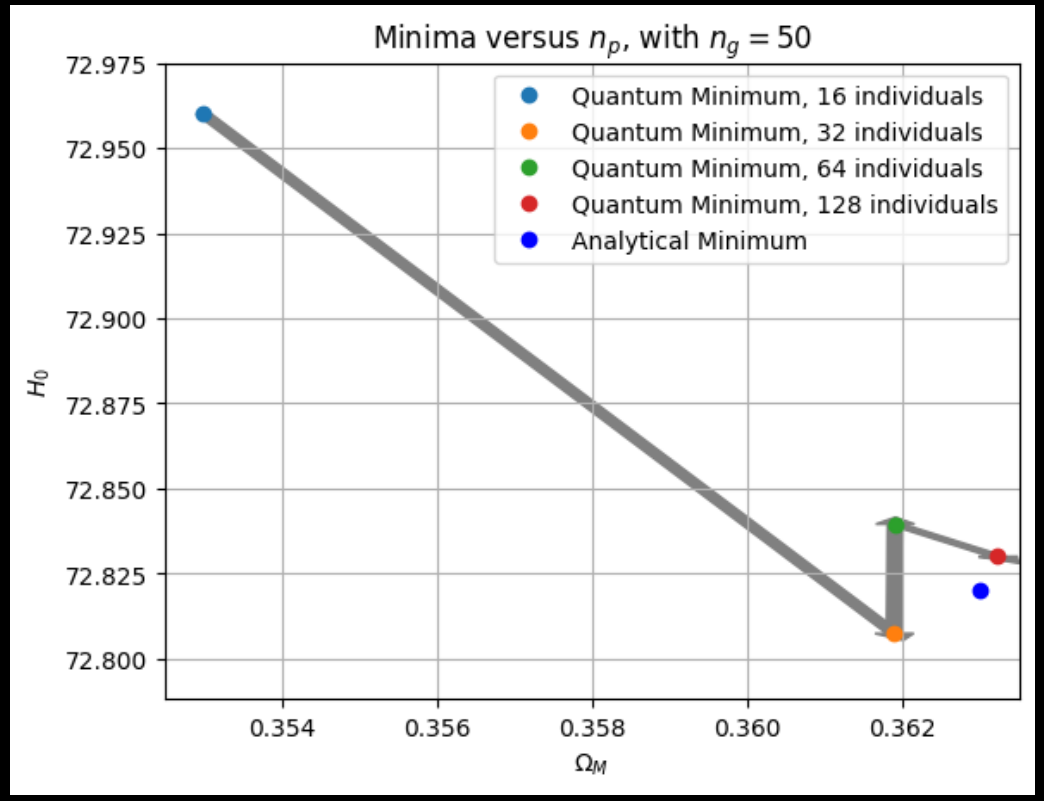
Mean value and number of generations, SNE, with 16 individuals

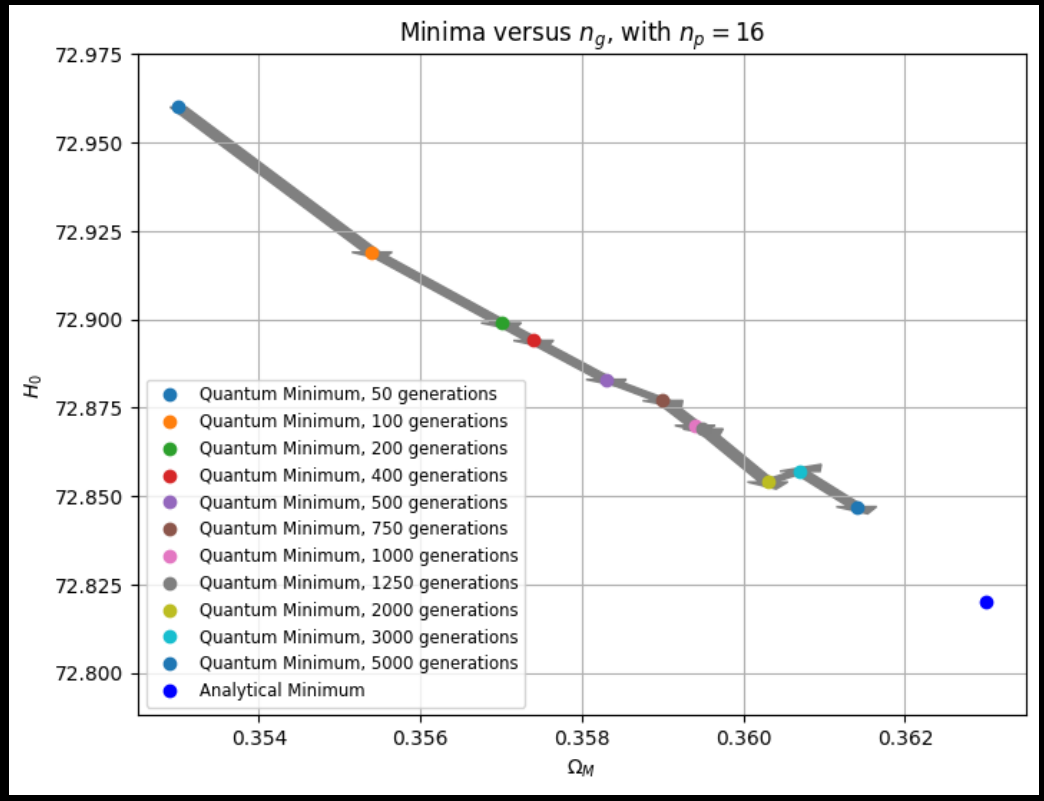


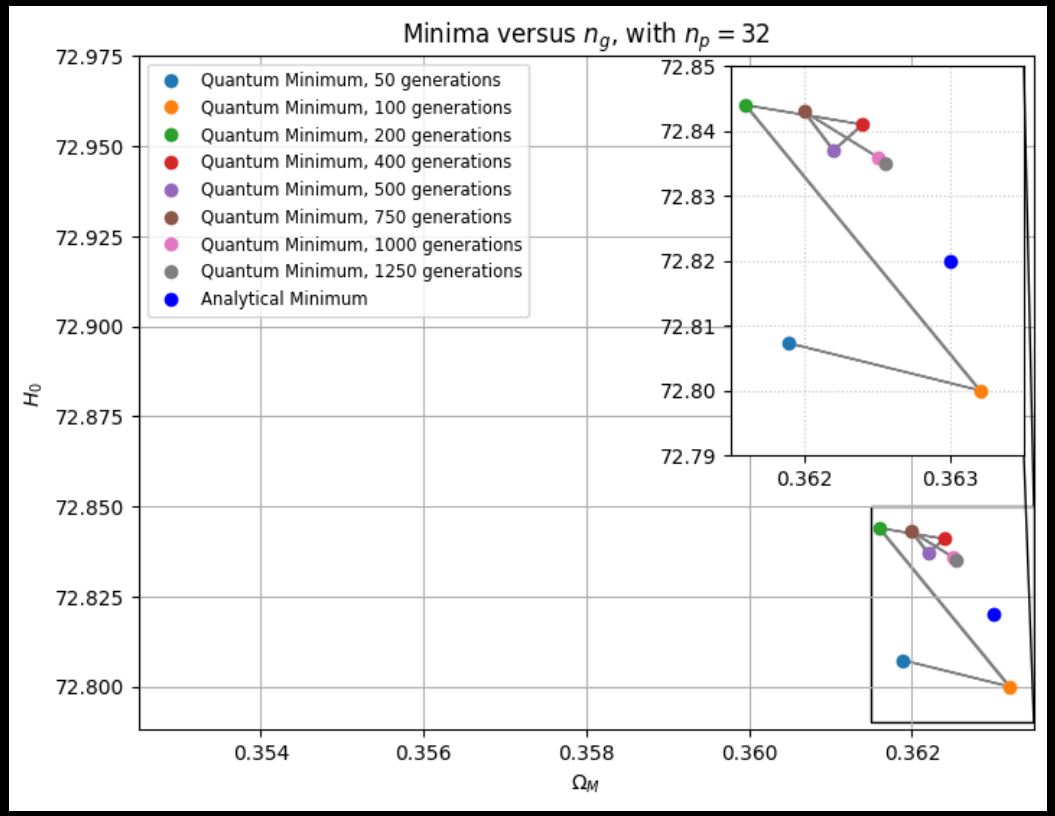
Varying the number of individuals, SNE

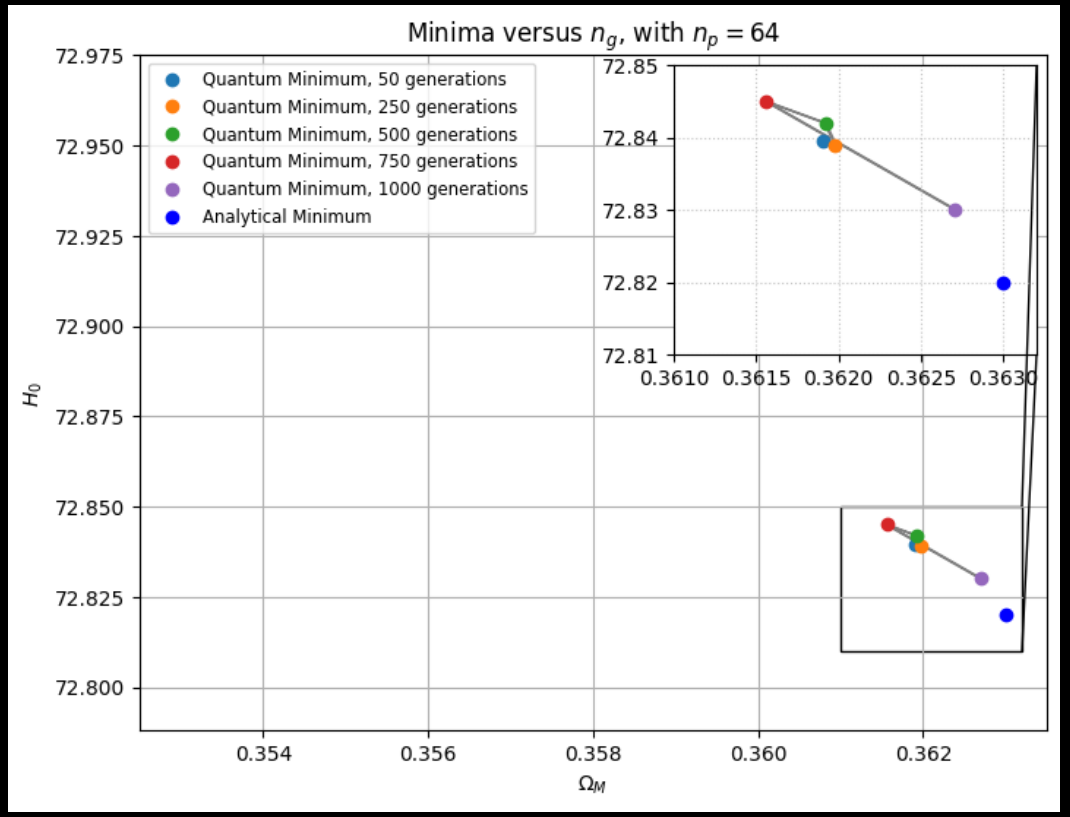


Minima with generations and individuals

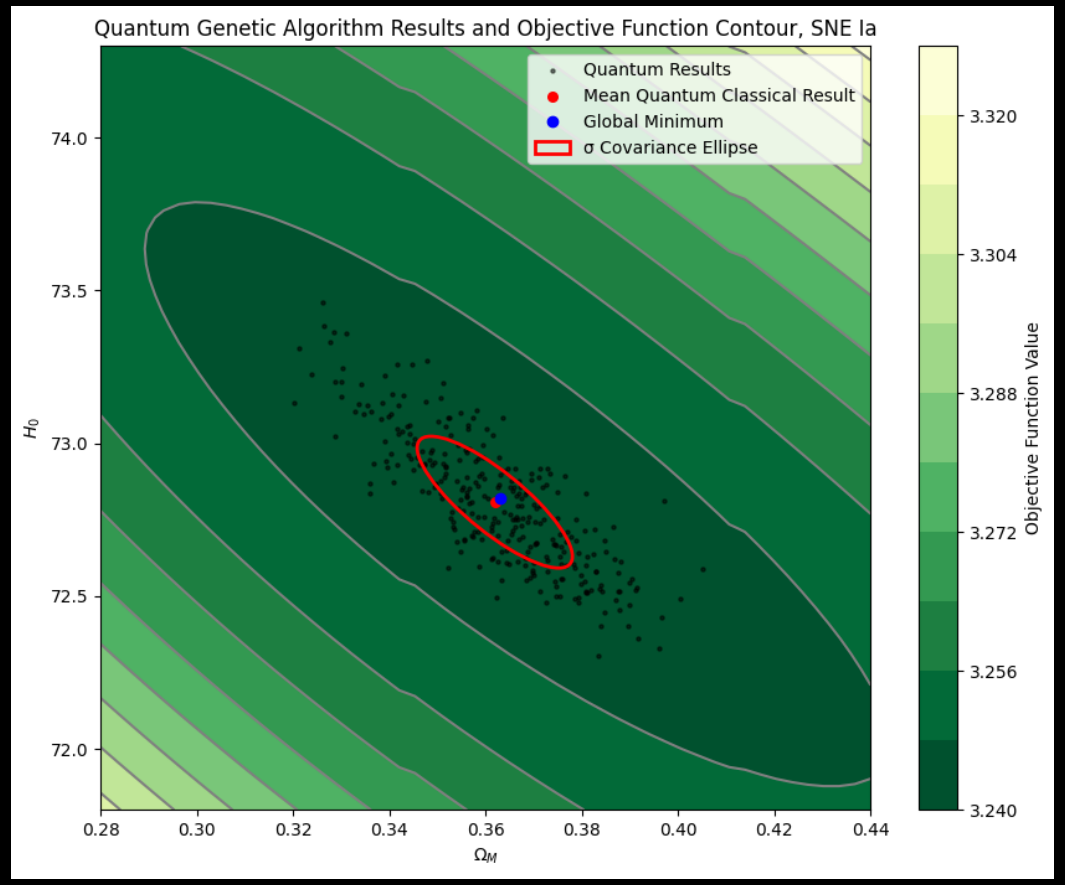


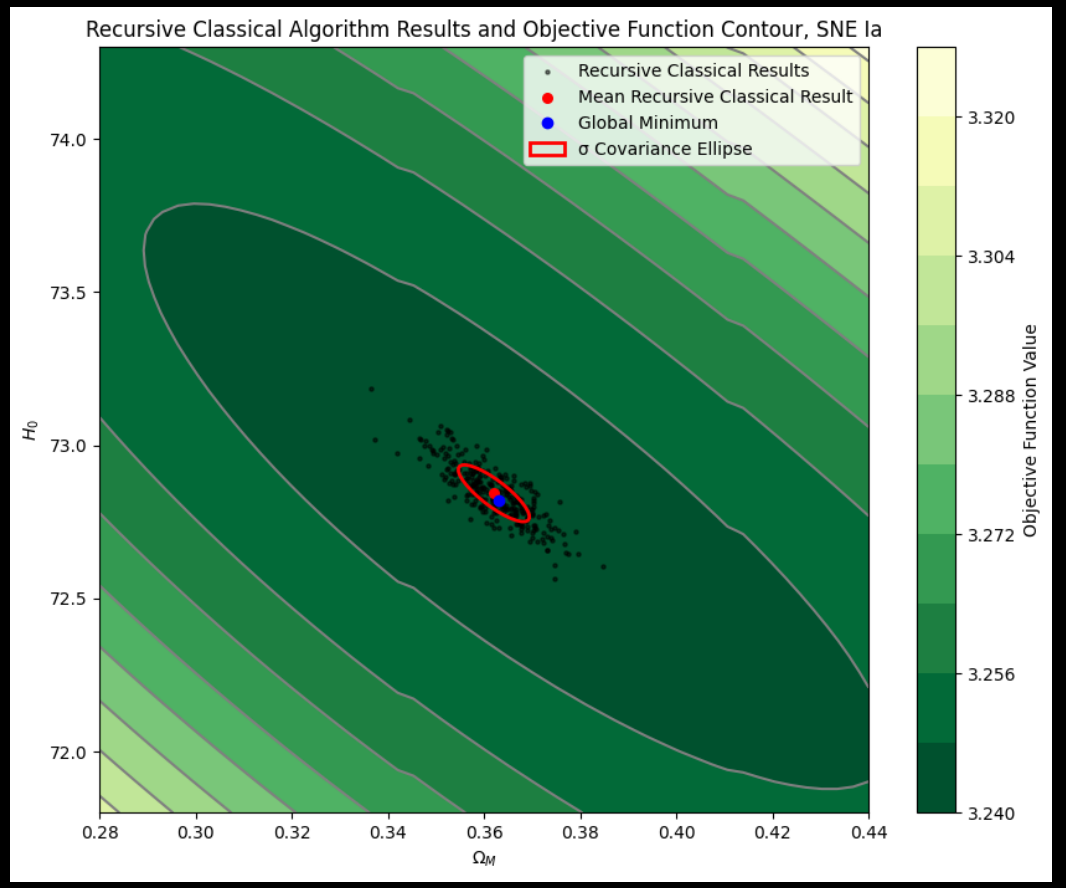




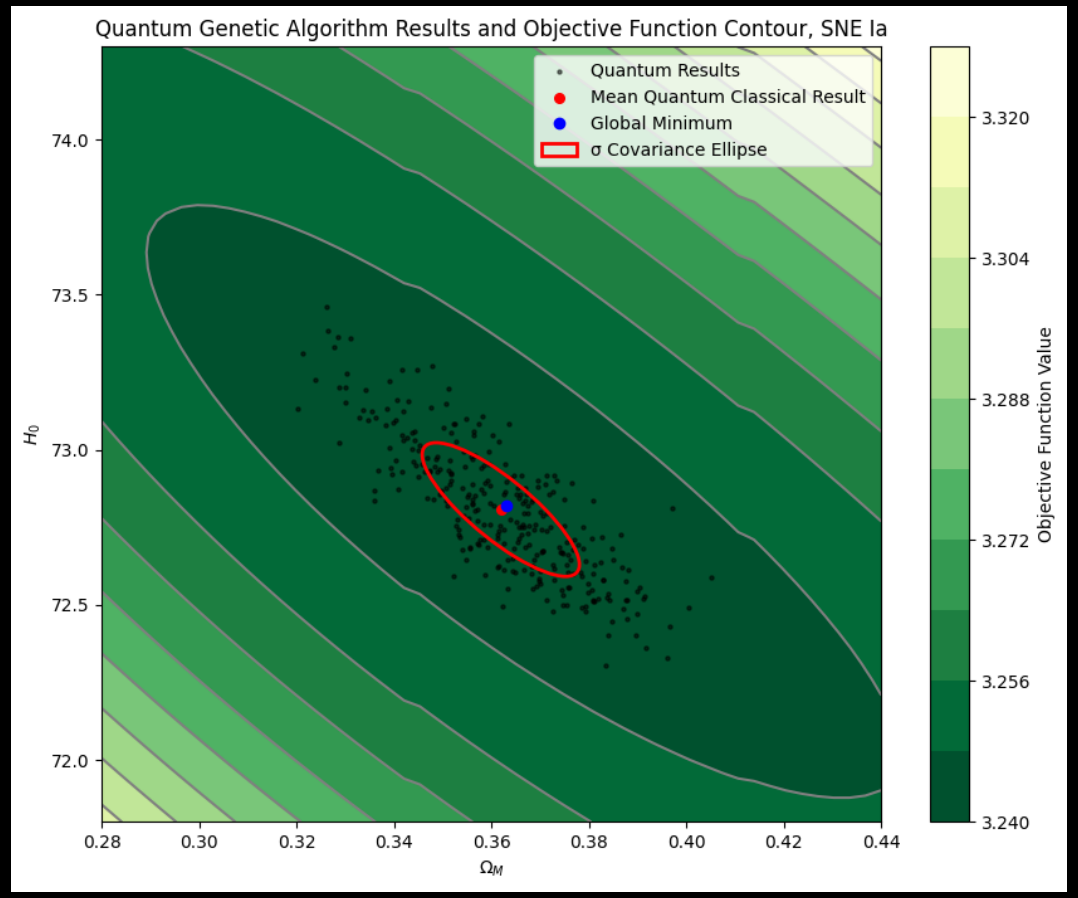


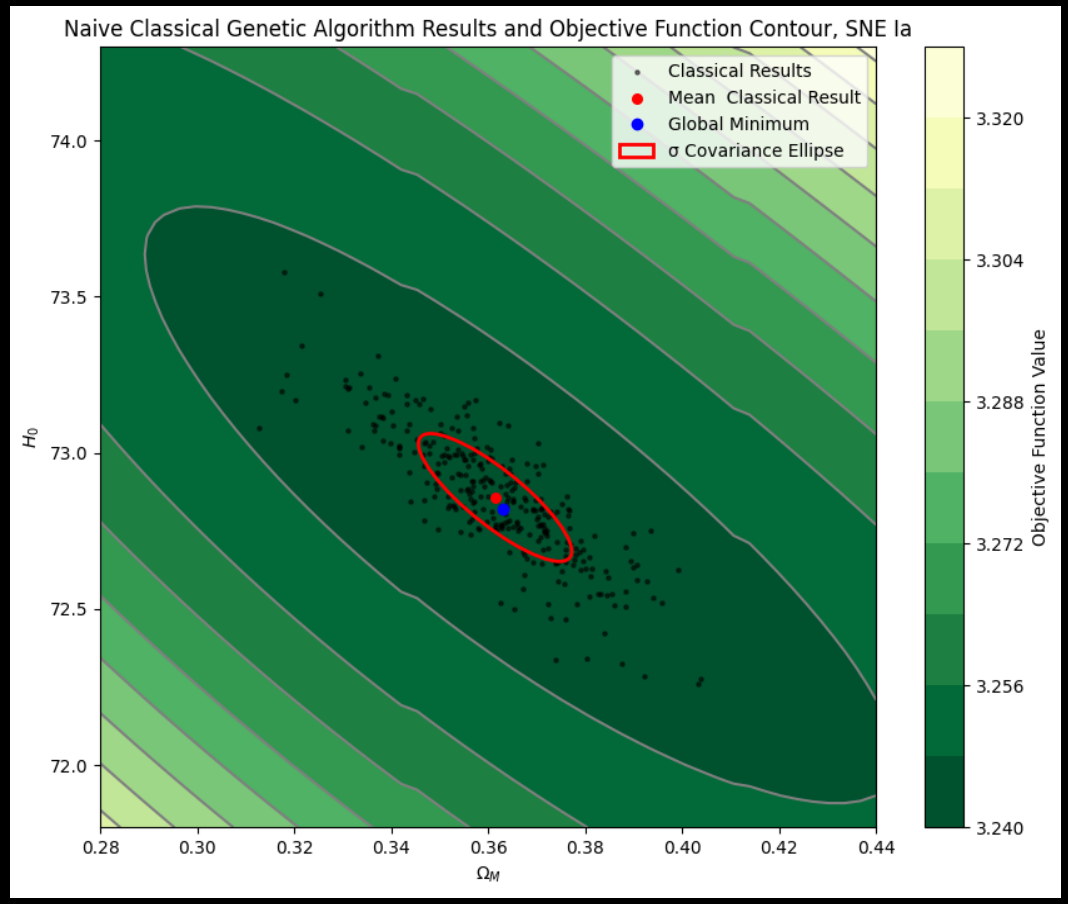
Minima with generations, higher number of individuals





Comparison with classical algorithms (1)

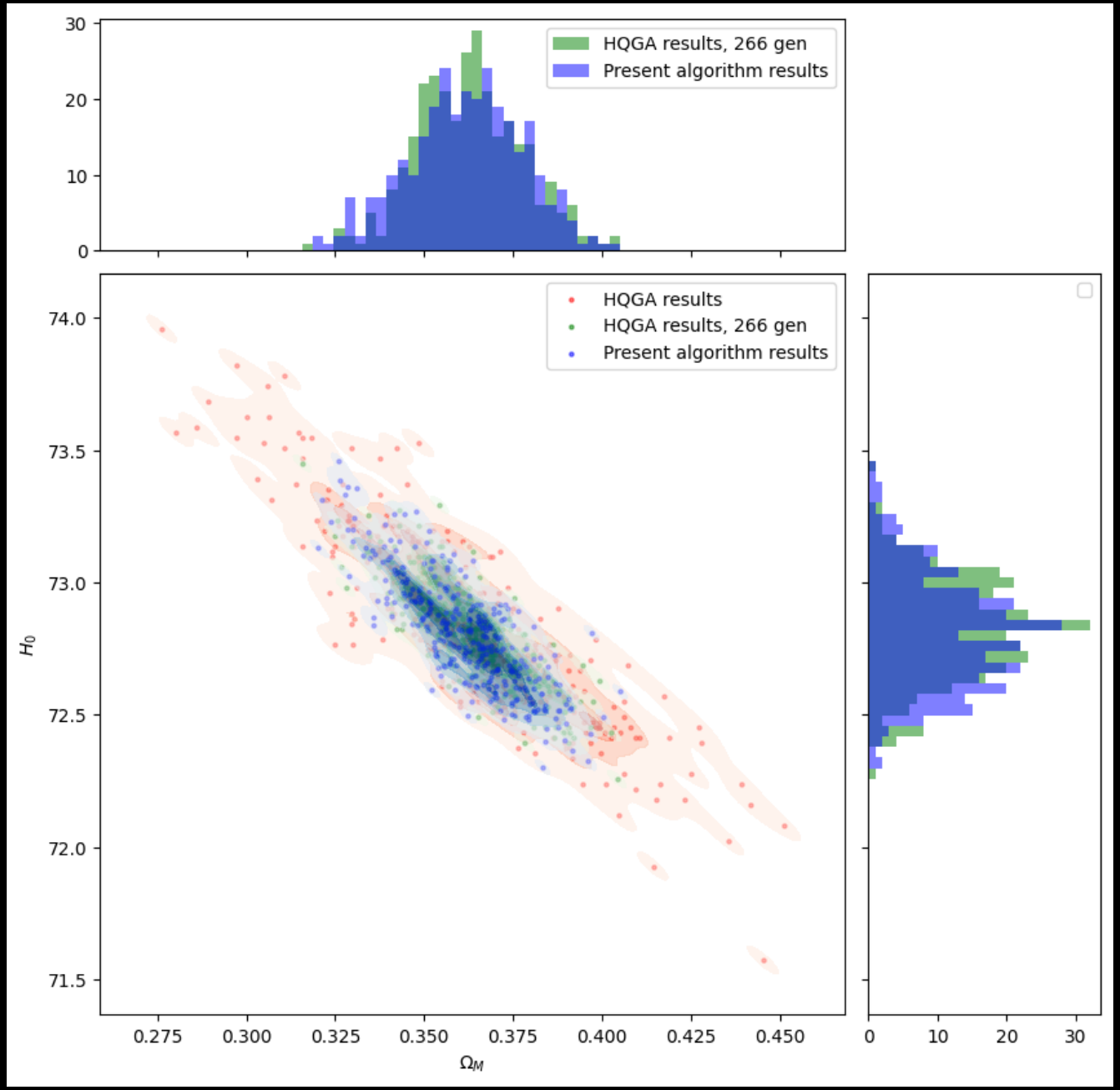




Comparison with classical algorithms (2)

Comparison with HQGA

Hybrid Quantum Genetic Algorithm (HQGA, Acampora et al. 2021) is a quantum genetic algorithm following a different philosophy from ours, but even so the results are comparable if the number of merit evaluation is similar.



Conclusions

1)The algorithm works.

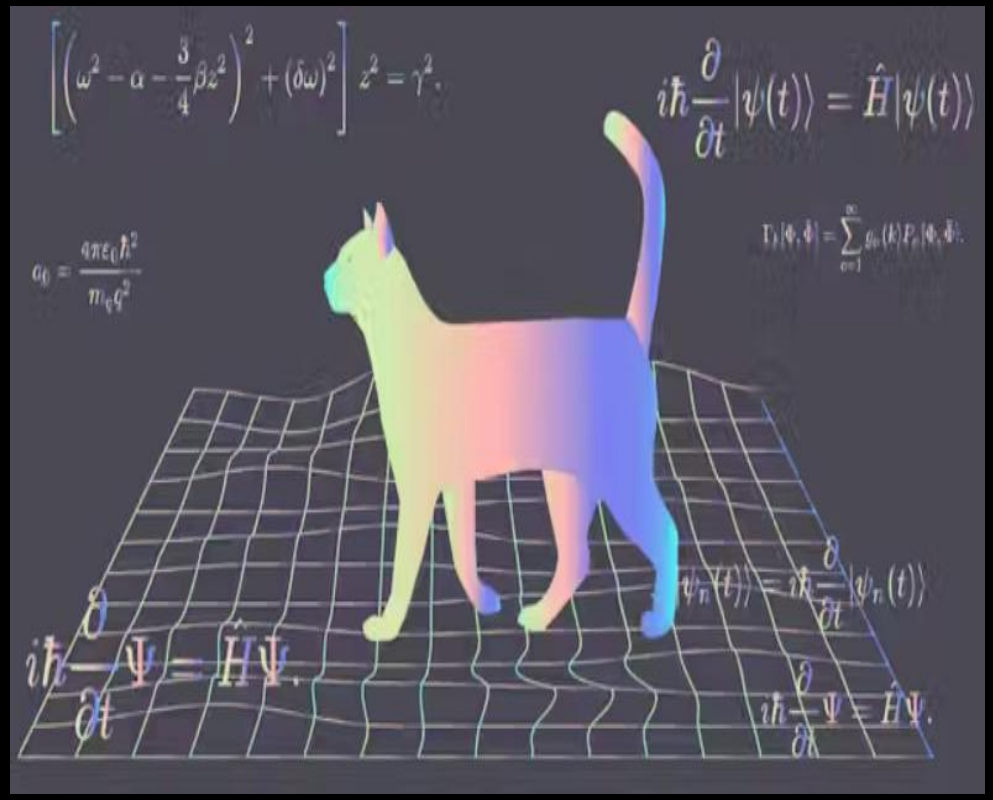
2) An interesting dependence on the crossover and mutation probabilities has been found.

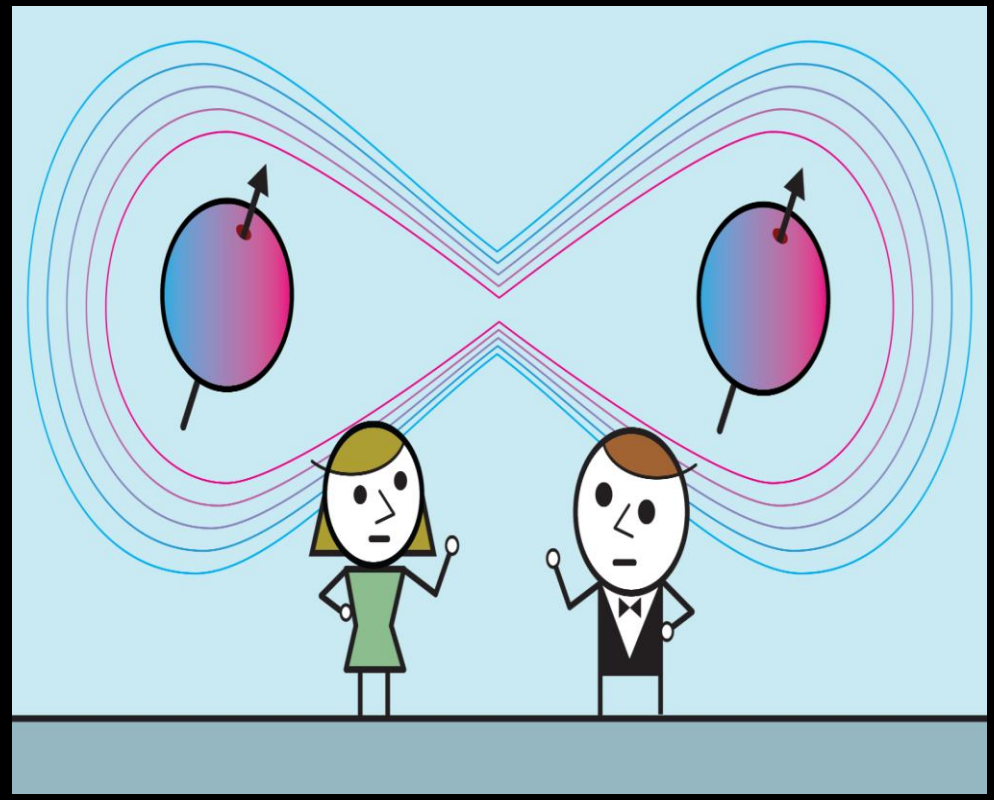
3) The first comparisons with classical results give precisions which are comparable (or even better for a naive application for the classical genetic algorithm), similar conclusion also with another quantum genetic algorithm found in the literature.

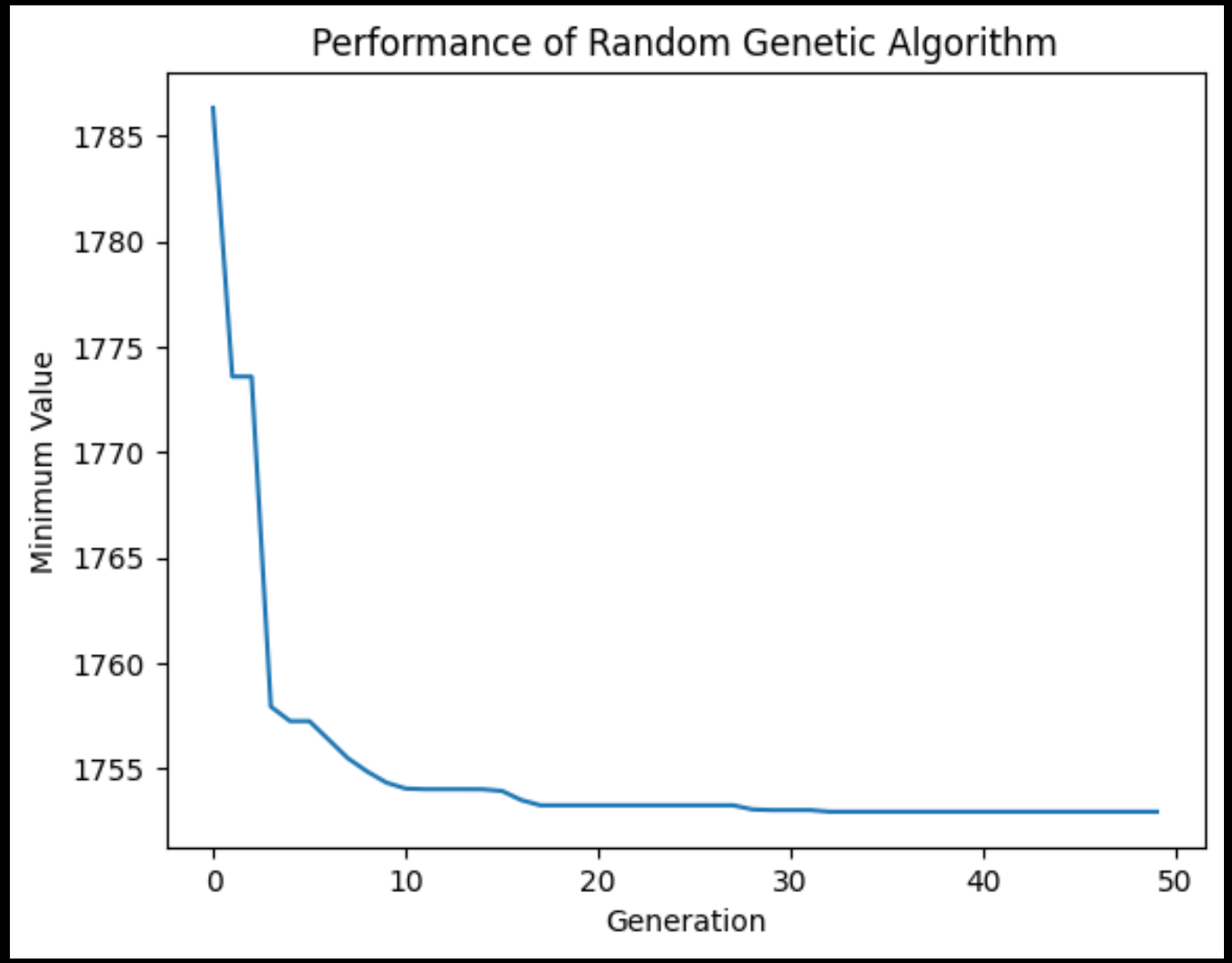
4) Tests on the other hyperparameters (number of population and generation) have also been performed.

5) The speed of the algorithm cannot be better than the classical counterparts given the classical fitness evaluation.

Superposition and Entanglement



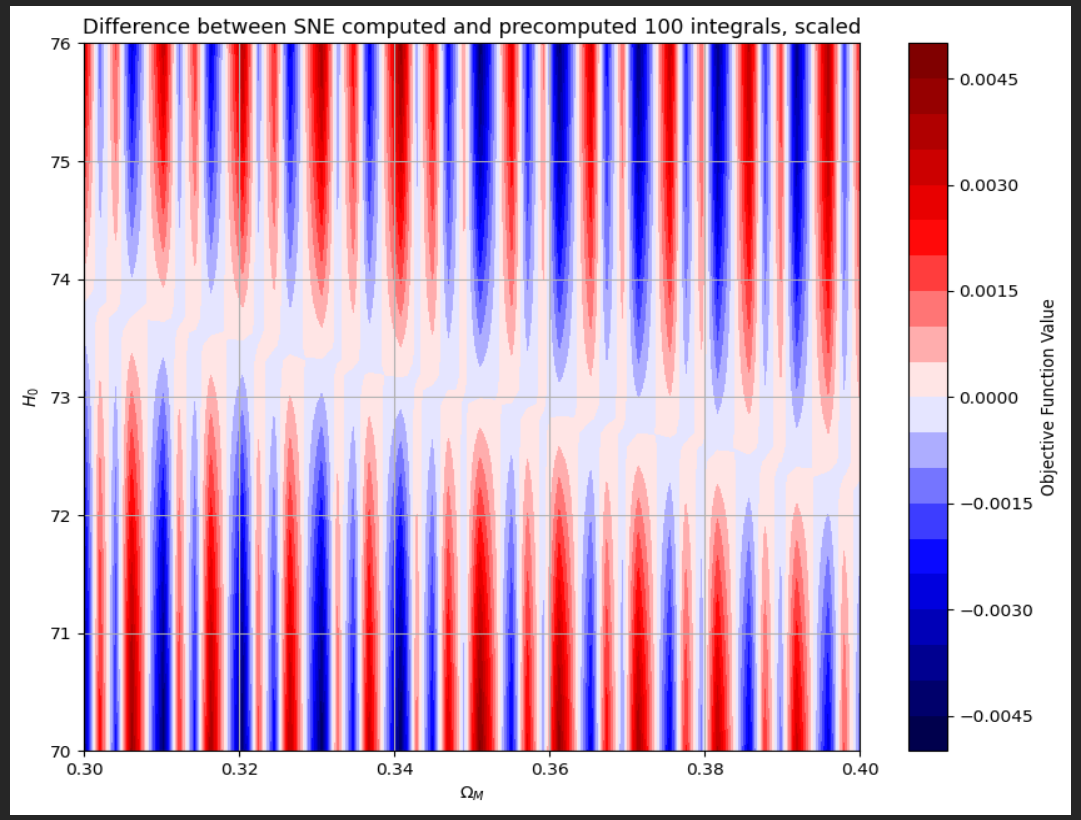


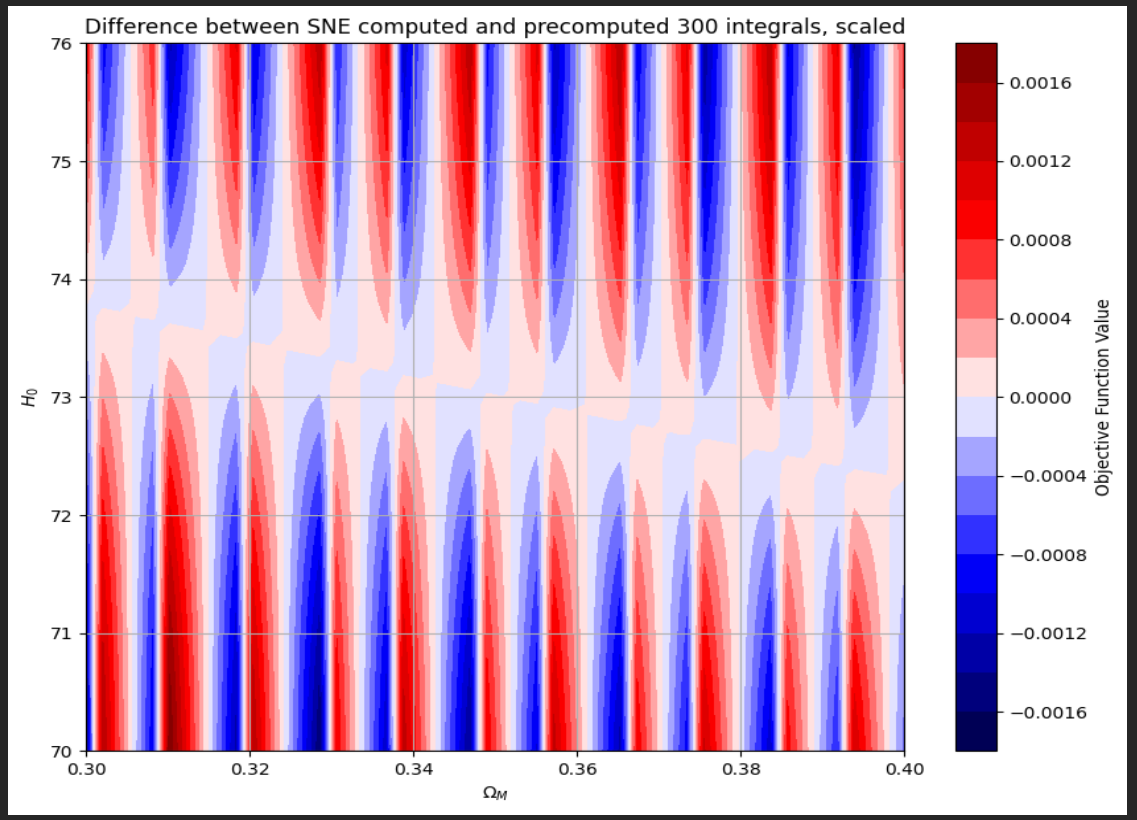


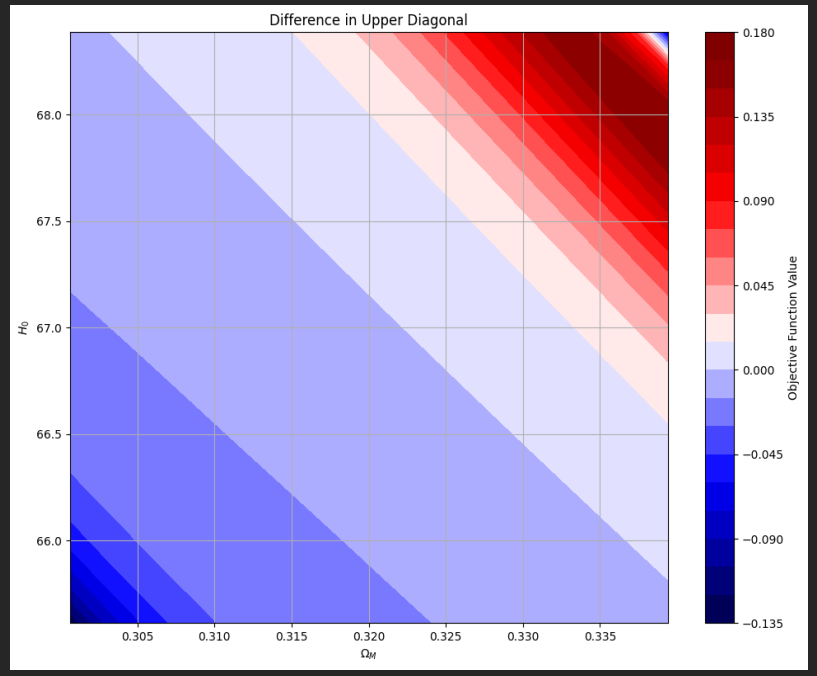
A single iteration of the algorithm for the SNe Ia

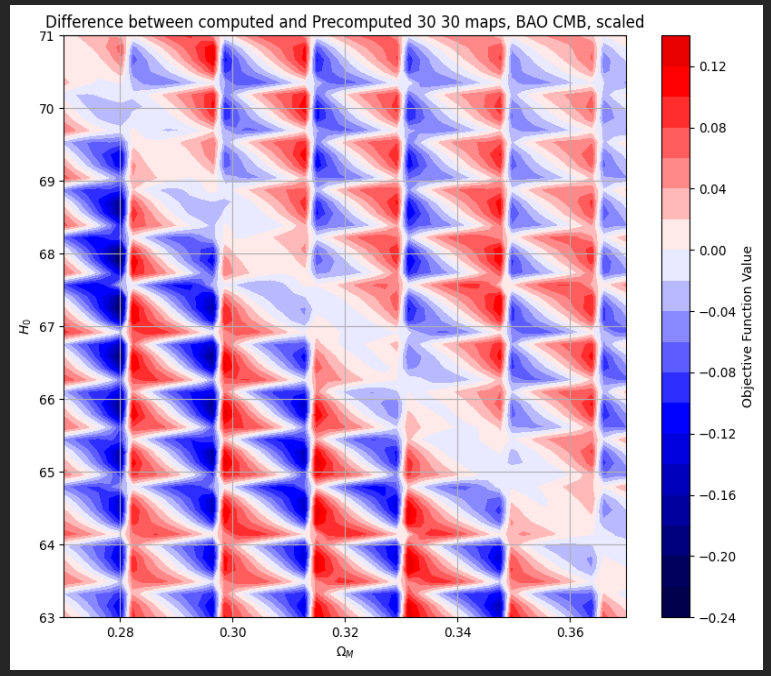
Precomputed Integrals,SNE, confronting the Maps

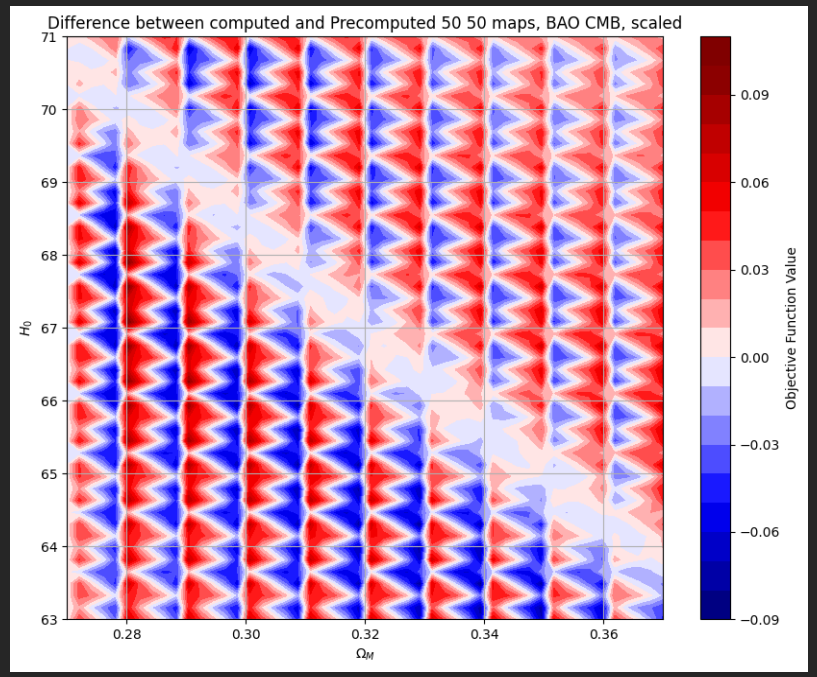
We note the remarkable precision for both the precomputations in the region around the minimum

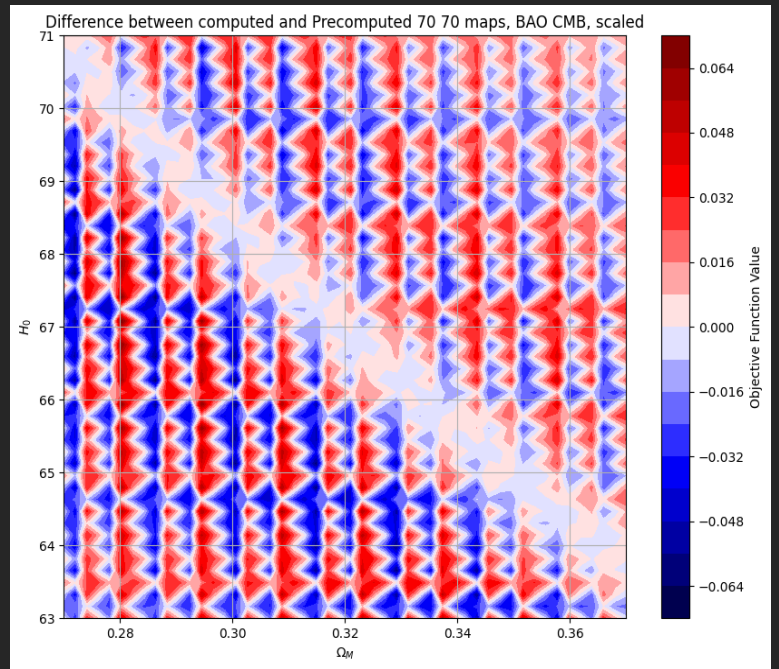






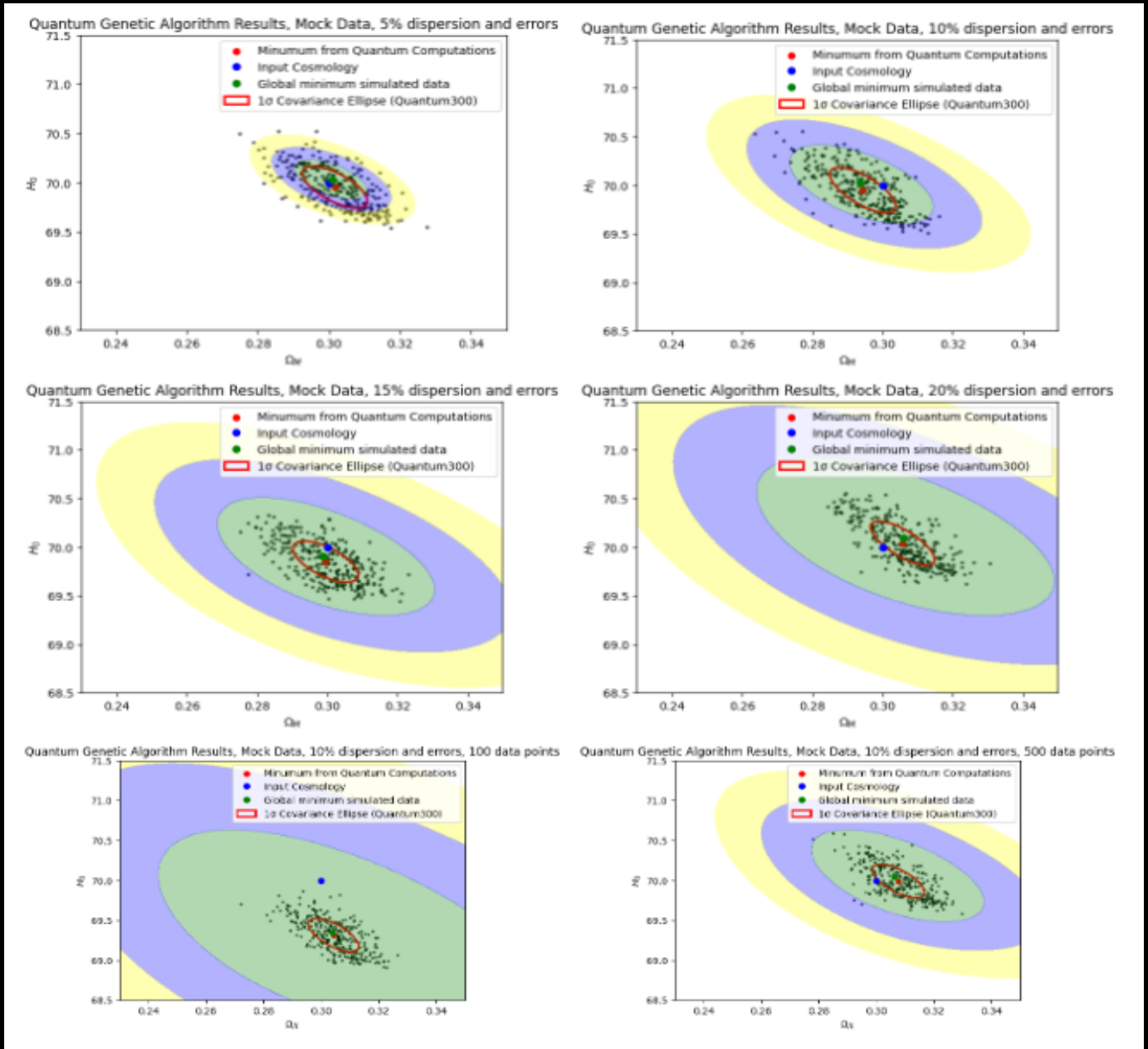




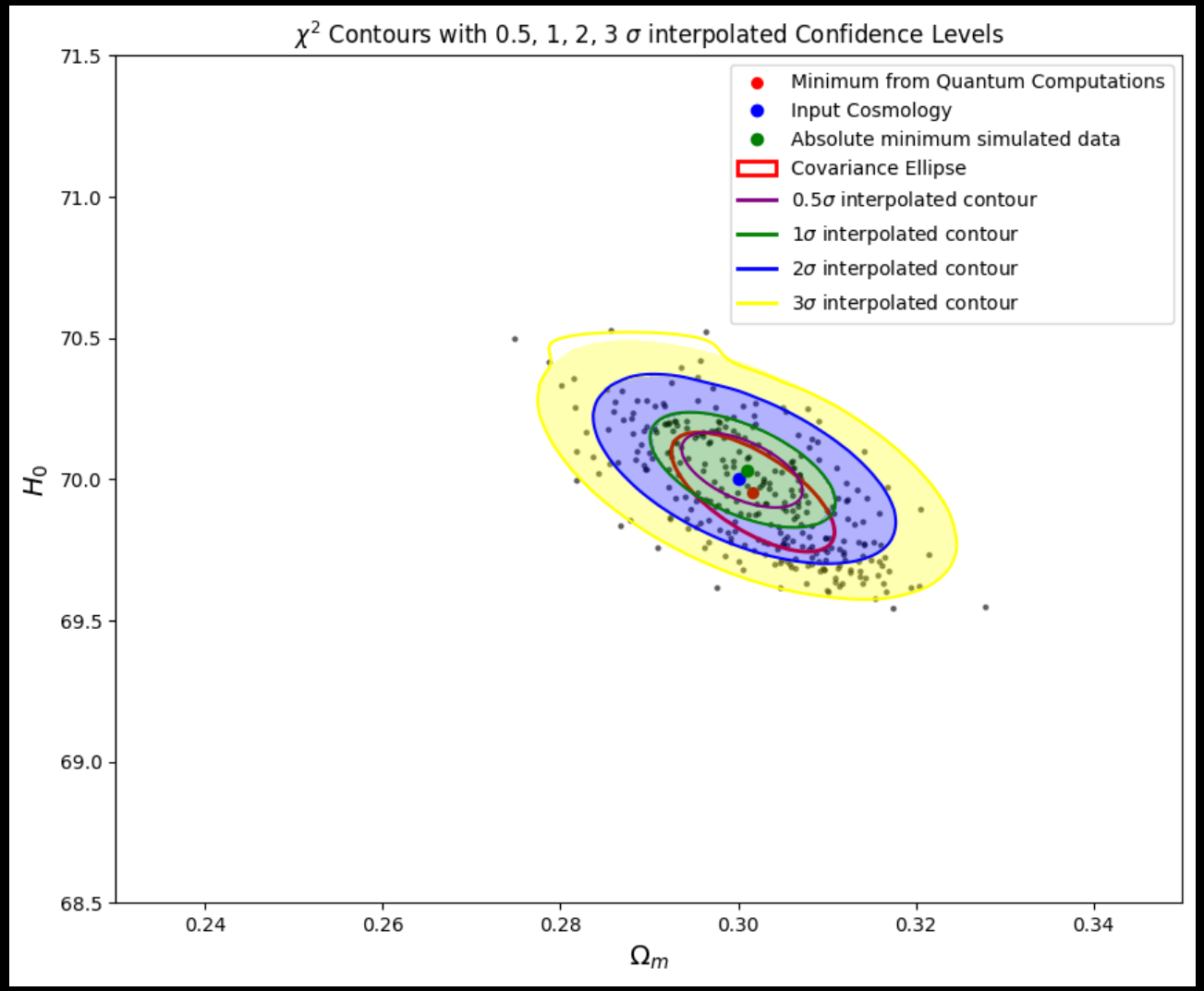


PICO and precomputed maps, BAO+CMB

Note how the PICO map is more consistent in the region around the minimum of the objective function, while loses accuracy in other zones of the parameter space, which are not represented in the PICO plot



Mock Data results



Interpolating the Chi-Squared