

<NE|AS|QC>

The NEASQC Benchmark Suite (TNBS)

Gonzalo Ferro (CESGA)

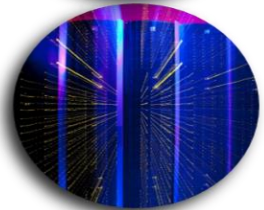
DECEMBER, 15-2023



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Galicia Supercomputing Centre (CESGA)

- > CESGA is a Public Foundation and is member of the Spanish Research Infrastructure RES (Spanish Supercomputing Network).
- > CESGA runs its own Quantum Computer (32 qubits) and participates in the major QC Spanish Initiative (Quantum Spain).



Mission

Contribute to the advancement of Science and Technical Knowledge, by means of **research and application of high-performance computing and communications**, as well as other information technologies resources, **in collaboration** with other institutions, **for the profit of society**.

Services

Adapted to technological evolution and **the needs of researchers and users of any area of knowledge** or productive sector.

NEASQC Project

NEASQC: Next ApplicationS of Quantum Computing

- > The NEASQC project brings together academic experts and industrial end-users to develop new Quantum-enabled applications that can take advantage of NISQ systems, in the near future, for solving industrial problems.

Objectives

- > Develop 9 industrial use cases where practical quantum advantage is expected in NISQ machines.
- > Develop open-source libraries from industrial uses cases.
- > Build a user community dedicated to industrial NISQ applications.
- > Develop software stacks and **benchmarks** for the Quantum Technology Flagship hardware platforms.



The NEASQC Benchmark Suite (TNBS)

The NEASQC Benchmark suite (TNBS) gathers in one suite all the developed benchmarks in the different use cases of NEASQC project.

OBJECTIVES

- > **Objective 1:** The suite must help computer architects, programmers and researchers to design future quantum computers, taking into account the variability in their performance introduced by the different components of the **stack**.
- > **Objective 2:** The suite must help to guide the **evolution** of quantum computers (more qubits, better topologies) or to **improve** the current platforms (reduction of noise, better compilers, etc.)

The NEASQC Benchmark Suite (TNBS)

OBJECTIVES

- > **Objective 3:** The suite must allow a **comparison** of the performance of different platforms. Currently, there are many different proposals for a physical implementation that use different one- and two-qubit gates. The suite must allow users and researchers to compare the performance of different platforms and find their **bottlenecks**. For users, it should allow them to find the best platforms for their applications.
- > **Objective 4:** The suite must consider **metrics** important to understand the quantum computing advantage (such as energy consumption, throughput or scalability)

The NEASQC Benchmark Suite (TNBS)

OBJECTIVES SUMMARY

- > Characterize Quantum Architectures (**QA**) using a set of **heterogeneous benchmarks** based on **applications**.
- > **Benchmarks** should be independent of the architecture.
- > Not interested in Quantum Supremacy.
- > Evaluation of all the stack: compilers, linkers, quantum technologies, etc.

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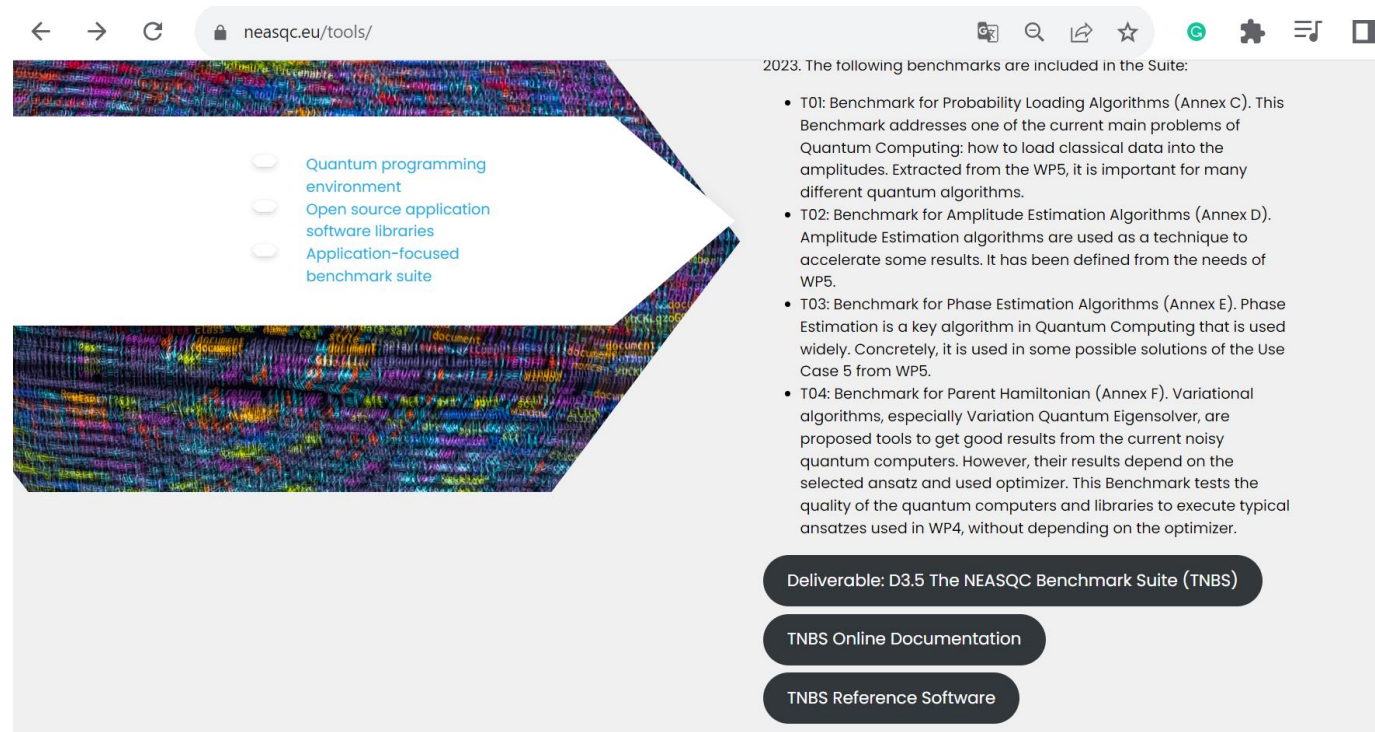
Is a Quantum Platform suitable for your problem or
your application?

TNBS Methodology

- > Each benchmark of the suite **must be** documented following the TNBS guidelines.
 - Public project deliverable: **D3.5 The NEASQC benchmark suite (TNBS)**
(<https://www.neasqc.eu/tools/>)
- > The benchmarks should be extracted from the use cases of the NEASQC project.
 - Planning release this restriction in the future.
- > Each benchmark should have a code implementation using Eviden myQLM.
 - Reference implementation: https://github.com/NEASQC/WP3_Benchmark
- > A web platform where every user of the suite can submit their own results to cross-compare different platforms.

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The screenshot shows a web browser at the URL `neasqc.eu/tools/`. The page features a navigation menu with three items: "Quantum programming environment", "Open source application software libraries", and "Application-focused benchmark suite". Below the menu, there is a section titled "2023. The following benchmarks are included in the Suite:" followed by a list of four benchmarks (T01, T02, T03, T04) with detailed descriptions. At the bottom of the page, there are three buttons: "Deliverable: D3.5 The NEASQC Benchmark Suite (TNBS)", "TNBS Online Documentation", and "TNBS Reference Software".

2023. The following benchmarks are included in the Suite:

- T01: Benchmark for Probability Loading Algorithms (Annex C). This Benchmark addresses one of the current main problems of Quantum Computing: how to load classical data into the amplitudes. Extracted from the WP5, it is important for many different quantum algorithms.
- T02: Benchmark for Amplitude Estimation Algorithms (Annex D). Amplitude Estimation algorithms are used as a technique to accelerate some results. It has been defined from the needs of WP5.
- T03: Benchmark for Phase Estimation Algorithms (Annex E). Phase Estimation is a key algorithm in Quantum Computing that is used widely. Concretely, it is used in some possible solutions of the Use Case 5 from WP5.
- T04: Benchmark for Parent Hamiltonian (Annex F). Variational algorithms, especially Variation Quantum Eigensolver, are proposed tools to get good results from the current noisy quantum computers. However, their results depend on the selected ansatz and used optimizer. This Benchmark tests the quality of the quantum computers and libraries to execute typical ansatzes used in WP4, without depending on the optimizer.

Deliverable: D3.5 The NEASQC Benchmark Suite (TNBS)

TNBS Online Documentation

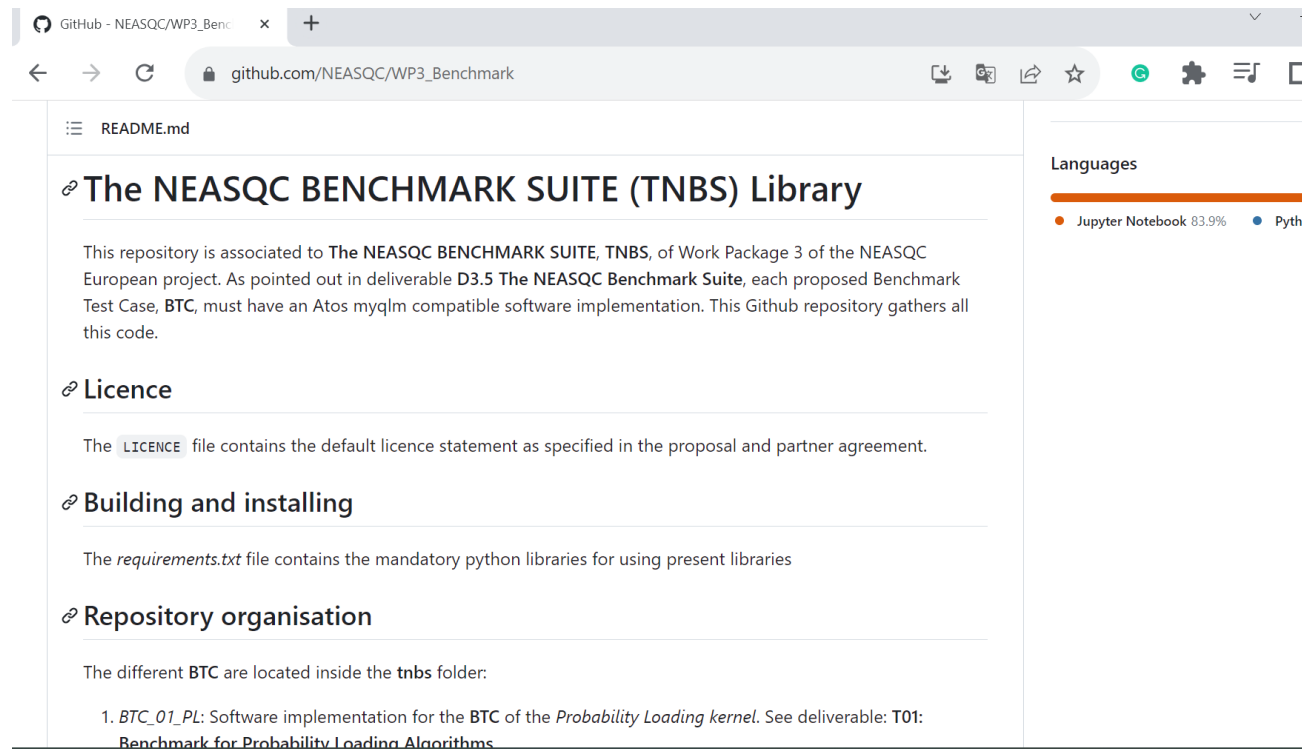
TNBS Reference Software

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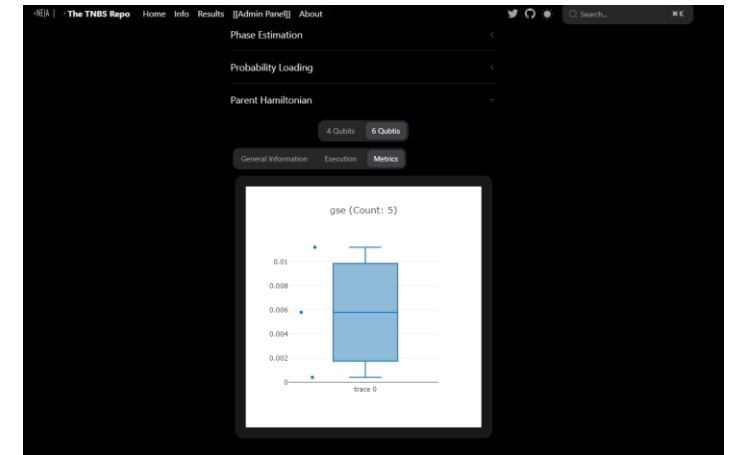
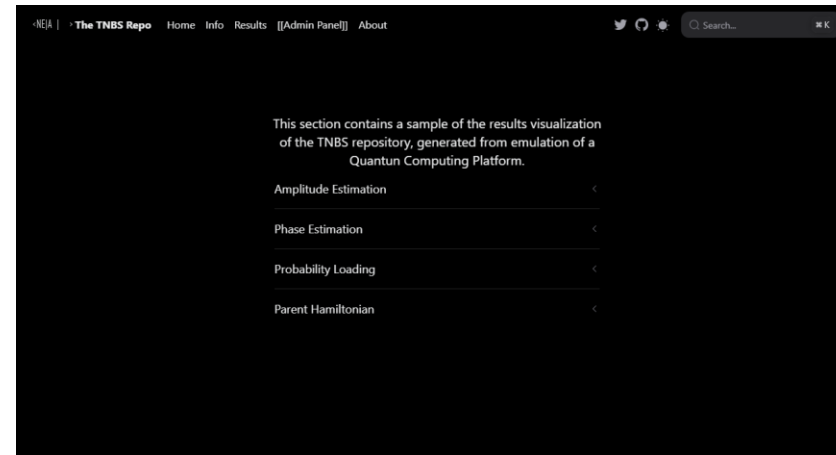
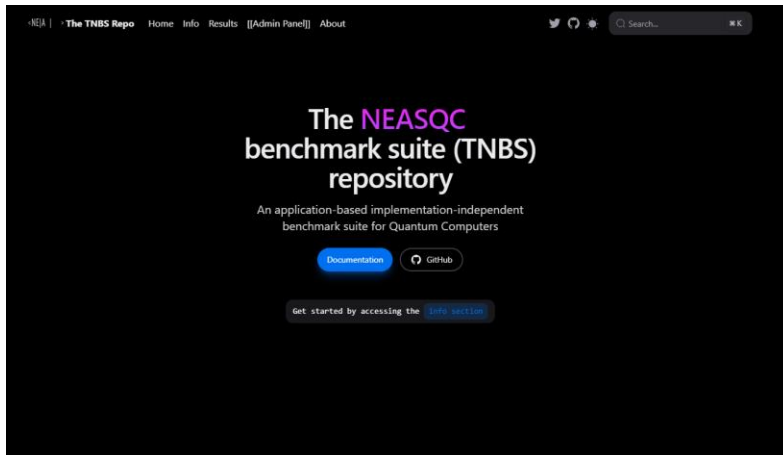


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TNBS Methodology

- > A web platform where every user of the suite can submit their own results to cross-compare results from different platforms.



TNBS Terminology

Each **benchmark** of the suite should be composed of:

- > **Kernel:** core quantum subroutine high-level defined (mathematically or procedurally). Common to several algorithms. It could be implemented using different procedures.
- > **Benchmark Test Case (BTC):** problem whose solution involves the execution of the **Kernel**. Output verifiable analytically or through a classical simulation. Used for evaluating the performance of a Quantum Architecture.
- > **Metric:** Parameter for evaluating the performance of a **QA** for solving the **BTC** (so it depends on it).
 - **Verification:** *Is the provided result by the QA correct?*
 - **Performance:** *How fast is the execution of the BTC in the QA?*

TNBS Current microbenchmarks

- > T01: Probability Loading microbenchmark.
- > T02: Amplitude Estimation microbenchmark.
- > T03: Quantum Phase Estimation microbenchmark.
- > T04: Parent Hamiltonian microbenchmark.

T01: Probability Loading microbenchmark

Kernel: Probability Loading. Build a unitary operator for loading a discrete probability distribution P into the amplitude of a quantum state.

$$\mathbf{P} = \{p_0, p_1, \dots, p_{2^n-1}\}, p_i \in [0, 1] \quad \sum_{i=0}^{2^n-1} |p_i|^2 = 1$$
$$\mathbf{U}|0\rangle_n = \sum_{i=0}^{2^n-1} \sqrt{p_i} |i\rangle_n$$

BTC: Load a known Gaussian probability distribution function

$$p(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

Metrics (verification): compare the measured (Q) and the theoretical distribution (P) using:

Kolgorov-Smirnov:

$$KS = \max \left(\left| \sum_{j=0}^i P(x_j) - \sum_{j=0}^i Q_j \right|, \forall i = 0, 1, \dots, 2^n - 1 \right)$$

Kullback-Leibler divergence :

$$KL(\mathbf{Q}/\mathbf{P}) = P(x_j) \ln \frac{P(x_j)}{\max(\epsilon, Q_k)}$$

Applications: QPCA, HHL, Quantum Amplitude Estimation...

T02: Amplitude Estimation microbenchmark

Kernel: Amplitude Estimation. Estimate a given a unitary operator \hat{A}

$$|\Psi\rangle = \hat{A}|0\rangle_n = \sqrt{a}|\Psi_0\rangle + \sqrt{1-a}|\Psi_1\rangle$$

BTC: Estimating the integral of a sine function encoded in a

$$F = \int_a^b \sin(x)dx = \cos(a) - \cos(b)$$

Applications: Finance, Chemistry, numeric integration.

Metrics (verification): Absolute error between Riemann sum of the integral and the estimation

$$\epsilon = \left| S_{[a,b]}^I - S_{[a,b]} \right| \quad S_{[a,b]}^I = \frac{b-a}{2^n} \sum_{i=0}^{2^n-1} \sin(x_i) \sim F$$

Several algorithms for AE can be used:

- Quantum Phase Estimation
- Maximum Likelihood AE
- Iterative Quantum AE
- Real Quantum AE

T03: Quantum Phase Estimation microbenchmark

Kernel: Quantum Phase Estimation. Given a unitary operator U estimate their eigenvalues

$$U|\psi_j\rangle = e^{2i\pi\lambda_j}|\psi_j\rangle$$

BTC: Estimate the eigenvalues of a $R_z^{\otimes n}(\theta)$

$$R_z(\theta) = \begin{pmatrix} e^{-i\frac{\theta}{2}} & 0 \\ 0 & e^{i\frac{\theta}{2}} \end{pmatrix} = e^{-i\frac{\theta}{2}}|0\rangle\langle 0| + e^{i\frac{\theta}{2}}|1\rangle\langle 1|$$

2 different angle selection:

- Random
- Exact: $\theta_{i+1} = \theta_i + a\delta\theta$. $a = \{-1, 1\}$. $\delta\theta = \frac{4\pi}{2^m}$

Metrics (verification): Compare the theoretical ($P_{\lambda,m}^{th}$) and the obtained ($P_{\lambda,m}^{QPE}$) probability density of eigenvalues:

$$\text{Random case: } KS = \max \left(\left| \sum_{k=0}^i P_{\lambda,m}^{th} \left(\frac{k}{2^m} \right) - \sum_{k=0}^i P_{\lambda,m}^{QPE} \left(\frac{k}{2^m} \right) \right| \right)$$

$$\text{Exact case: } fidelity = \frac{\sum_{k=0}^{n-1} P_{\lambda,m}^{th} \left(\frac{k}{2^m} \right) * P_{\lambda,m}^{QPE} \left(\frac{k}{2^m} \right)}{|P_{\lambda}^{th}| * |P_{\lambda}^{QPE}|}$$

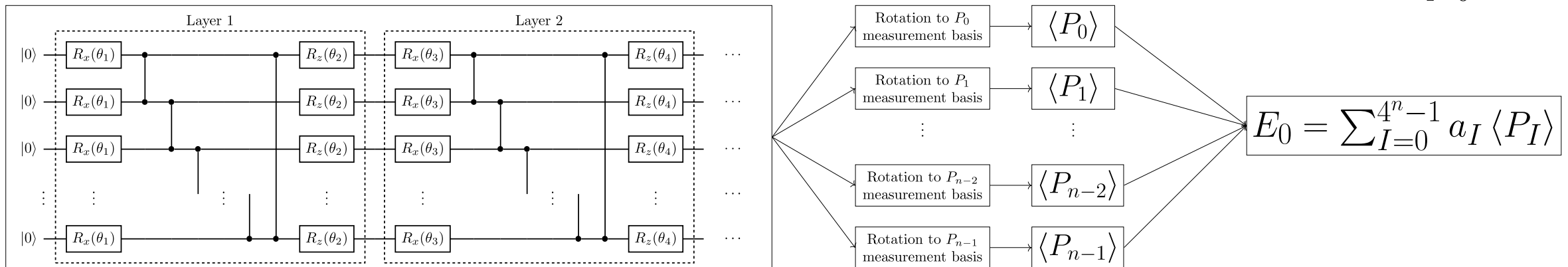
Applications: Shor's algorithm, quantum linear equation solver, VQE...

T04: Parent Hamiltonian microbenchmark

Kernel: Parent Hamiltonian. Given an ansatz with state $|\Psi(\theta)\rangle$ its parent Hamiltonian, H^{PH} , is such that:

$$H^{PH} |\Psi(\theta)\rangle = E_0 |\Psi(\theta)\rangle \quad E_0 = 0$$

BTC: following Ansatz for different number of layers: $|\Psi(n, d, \theta_i)\rangle \rightarrow H^{PH} \rightarrow H^{PH} = \sum_{I=0}^{4^n-1} a_I P_I$



$$\theta_i = (i + 1)\delta\theta \quad i = 0, 1, \dots, 2n_l - 1 \quad \text{where } \delta\theta = \frac{\pi}{4 * (n_l + 1)}$$

T04: Parent Hamiltonian microbenchmark

Metrics (verification): The computed ground state energy E_0 should be compared with theoretical one: 0. So the metric is E_0 .

Applications: Variational Quantum Algorithm (particularly VQE).

- > The GitHub provided the Pauli decomposition from 3 to 30 qubits and from 1 to 4 layers (for each qubit) ansatzes.
- > Additionally, a code for building the parent Hamiltonian and its Pauli decomposition for any ansatz is provided (using myQLM library).
- > Implementation of BTC Parent Hamiltonian using MPS.

Conclusions

- > Developed a benchmark suite for assessing quantum devices based on use cases of the NEASQC project.
- > TNBS should help to improve the complete stack of a quantum hardware device.
- > Microbenchmarks are composed of **Kernel** and a **Benchmark Test Case**.
- > Four microbenchmarks have been developed:
 - Probability Loading
 - Amplitude Estimation
 - Quantum Phase Estimation
 - Parent Hamiltonian

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Thank you for your attention!

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CESGA. SPAIN.



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