

Quantum Computing and Simulation Platform for HEP at IHEP

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With the dramatic growth of experimental data in high-energy physics and the increasing demand for accuracy of physical analysis results, the current classical computing model and computing power can no longer meet the needs of data processing and analysis.

As a new computing device with great potential, quantum computers have become one of the possible ways to solve the bottleneck of high-energy physics data processing and computation, though quantum computers are still far away from general computing.

At such a stage that quantum computers have so many shortcomings like few physical qubits, short coherent time, and poor fidelity to solve most practical problems, it's necessary to build a development and simulation platform using classical computers to accelerate research on quantum algorithms and applications.

We've set up an interactive development platform for quantum algorithms research and quantum computing simulation, and are preparing one web portal for public education and training on quantum computing. In the future, we will pay more attention to quantum computing applications in HEP and QCD simulation.

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1. Introduction

Quantum computing has attracted increasing interest from various countries and regions due to its enormous computing potential, and many governments and organisations have developed plans for the development of quantum computing technologies. IHEP has showed its interest in applying quantum computing in High Energy Physics in the last few years as CERN showed in itss quantum computing roadmap [1]. Our work in this paper then is mainly concerned with the design and progress of quantum computing platform in IHEP, and the paper is structured as follows. We review the state of the art first and the CERN QTI from which we toke some inspiration in this section, and the following sections 2-4 describe the goals, status and outlook for the IHEP work.

1.1 Quantum Computing

A quantum computer is a computing device similar to a classical computer driven by the principles of quantum mechanics, whose computing unit is quantum bit, which can store more information than classical bits. Because of the unique quantum superposition and quantum entanglement properties of quantum systems, quantum computers can naturally "parallelize" a large number of different situations and have computing power far beyond that of classical computers. And quantum computing has therefore become one of the most promising developing directions of scientific computing.

We know that there are numerous difficult problems like the maximum cut problem, set covering problem, and graph coloring problem known as the NP problems and NP-hard problems which could not be solved via classical computers, and many scientific problems like the sign problem in Lattice quantum chromodynamics (Lattice QCD) unfortunately belong to NP problems. A quantum computer might provide a promising solution for these problems with its super computing power.

Given the super power of quantum computers, over 18 countries till mid-2021, and regions have launched their own Quantum Initiatives [2] including China, the United States and Japan, which show the significance of quantum computing.

CERN has been interested in quantum computing for a long time, especially the potential application in High Energy Physics and simulation. CERN hosted a workshop on quantum computing for high energy physics in late 2018, and then launched Quantum Technology Initiative (QTI) in Sep 2020, to explore quantum technologies. The QTI strategy and roadmap was published in late 2021, focusing on four main scientific objectives, which include quantum computing infrastructures, algorithms and applications in HEP and simulation. For quantum computing infrastructures & algorithms, CERN mainly focuses on

- a) Potential application in High Energy Physics
- b) Common libraries of algorithms, methods, tools
- c) Hybrid classic-quantum computing infrastructures

And for quantum theory & simulation, CERN is interested in developing techniques for quantum simulations like collider physics, (lattice) QCD, cosmology, etc.

Although the quantum computer may have huge potential computing power far beyond classical computers and have many exciting applications, we are still in what is called the NISQ [3] era. Quantum computers in and beyond the NISQ era have many shortages:

a) Few qubits (100 \sim 1000).

• Limits the size and complexity of problems that could be solved.

b) Short decoherence time

• Quantum circuits are limited in depth and complexity.

c) Poor qubit fidelity & quantum error

• Quantum measurements are not stable nor reliable.

d) Running at ultra-low temperatures

• Difficult to operate quantum computers.

e) Limited physical computing resources

• Difficult to access and use for developing quantum algorithms.

In short, current quantum computers have difficulty in meeting the demands of scientific research, let alone for practice purposes. There is a long way from fault-tolerant quantum computing, and we need more flexible methods to study quantum algorithms.

1.2 Quantum Simulator

The fundamental theory behind quantum computer is quantum mechanics. It's possible to simulate quantum computer on classical computers, and such a model is called quantum (digital) simulator. Quantum simulators play a vital role in developing quantum computers and quantum algorithms. One can validate the results of physical quantum computers via simulators, and develop quantum algorithms agilely especially when there are no quantum computers available.

Compared to physical quantum computers, simulators have many advantages as follows:

- a) **"Perfect" qubits without all drawbacks of physical qubits**. Simulation results are stable and reliable.
- b) **"Unlimited" number of quantum gates** so long as there are enough computing resources. Simulating very deep and complicated quantum circuits is possible.

Nevertheless, we could only simulate as many as up to $50 \sim 60$ qubits with full states at most on the largest supercomputer, while the largest physical quantum computer till now has about 127 qubits. Large-scale simulations (>40 qubits) are time-consuming and resource intensive. Fig. 1 from Ref.[4] shows how many bytes are needed to simulate specific number of qubits using different simulation methods. For example, using the state vector method, we need about 1 TB of memory to simulate 36 qubits fully. Besides, it's not easy for simulators to simulate real quantum computers or quantum noise and error.

Many excellent quantum simulators such as Qiskit [5], Cirq and QPanda have been developed, and corresponding development ecosystems around these simulators are established. Qiskit, also as the famous developing kit, is the most popular quantum simulator among others.



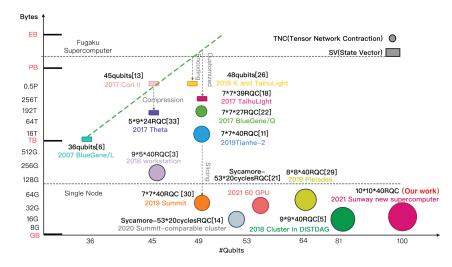


Figure 1: The relation between memory and number of qubits using different simulation methods (Ref.[4])

1.3 Quantum Computing Developing Platform

Current quantum computers are immature in terms of hardware manufacturing and software development, especially in terms of simulation platforms for high-energy physics data processing and simulation. Quantum programming has difficulties in problem abstraction, data processing, algorithm design and implementation. A large amount of infrastructures need to be implemented for the development of quantum computing.

A complete quantum computing simulation platform could be decomposed into four different level of components as show in Fig. 2. The top layer of the platform is quantum computing applications in a wide variety of subjects such as HEP, chemistry, finance etc. The framework layer consists of components needed by quantum computing development, like programming GUI, common algorithm libraries and visualization. The computing infrastructure layer then includes basic tools for quantum computing similar to those for classical computing development. The last but not least layer of the platform is hardware platform, which contains the quantum processors, quantum RAM, quantum measurement facilities as well as the classical computing resources.

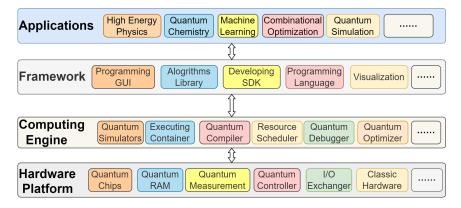


Figure 2: General structure of quantum computing simulation platform.

For quantum computing researchers like physicists, a user-friendly developing platform is cru-

cial that can help shift research mindset, reserve technology, and keep pace with the world in quantum computing. More and more quantum computing applications in many fields as well as HEP prompts us to establish **such an agile quantum computing simulation platform** to accelerate the exploration of quantum computing in HEP at IHEP. The workflow in the simulation platform we designed shows in Fig. 3.

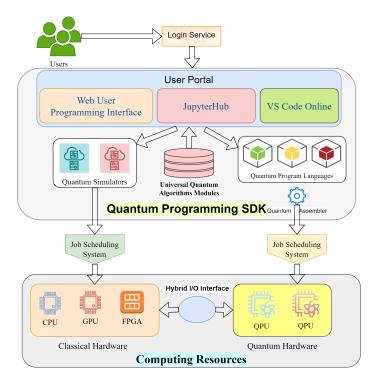


Figure 3: The workflow design of quantum computing simulation platform at IHEP

The simulation platform we are designing is

- a) A platform focusing on applications in HEP simulation and analysis
 - Explore applications in Lattice QCD and experiments at IHEP like BES, LHAASO.
- b) A "full-stack" platform including necessary components for quantum computing
 - Frameworks, interactive GUI, simulators and assemblers
- c) An integrated interactive developing platform
 - · Based on Jupyter, Kubernetes and nodejs
 - Integrates common SDKs like Qiskit, Cirq, D-Wave
- d) A distributed heterogeneous computing platform
 - Joint CPU/GPU/FPGA resources from different centers
 - · Joint classical and quantum computing resources

Based on our simulation platform, we will explore the applications of quantum computing in physical analysis and many-body simulation and other subjects together with experimental and theoretical physicists. We will develop common frameworks for HEP analysis and simulation by way of abstracting generic algorithms from specific scientific problems. Moreover, we will also conduct various quantum computing training courses, promote quantum computing to general researchers, and accelerate the research and application practice of quantum computing, which will be discussed in detail at the following sections.

2. Scientific Objectives

Similar to the scientific objectives of CERN QTI, the quantum computing simulation platform we are working on now mainly focuses on four objectives summarized as following:

a) Quantum Computing Infrastructures

Includes a user-friendly interactive developing platform for quantum computing, a distributed heterogeneous computing platform for heavy simulation jobs, and quantum simulating algorithms & implementation.

b) Computing and Simulation Applications

Based on the simulation platform, explore potential quantum computing applications in High Energy Physics analysis, (Lattice) QCD simulation and computing cluster management, develop common computing frameworks for general research, and integrate quantum computing in current HEP analysis workflow.

c) Collaboration with Industries & Institutes

Collaborate with quantum computer manufacturers for compatibility. Collaborative research with industries and institutes on various scientific subjects. Establish an active quantum computing development community.

d) Quantum Computing Education & Training

Introduce and popularize quantum computing. Research introduction and progress presentation. Provide a public platform for learning and discussing quantum computing.

In the rest of this section, we will give an brief description about our objectives, and overall ideas of how to reach our objectives.

2.1 Simulation Platform

For physicists and other developers, a user-friendly developing platform can greatly improve productivity. The simulation platform we are developing is described as following

- A Unified Platform, which can be accessed via IHEP SSO service, and integrates all computing services needed like storage, scheduling system, dashboard.
- A Distributed Computing Platform, which unifies computing centers in different places via global Slurm scheduler.

- With Interactive Developing Interfaces like the Jupyter interface for lightweight tasks.
- Able to execute heavy tasks on Heterogeneous HPC Clusters like NVIDIA/AMD GPU clusters or ARM clusters.

As we know that quantum computing simulation requires huge classical computing resources depending on how many qubits, quantum gates and measurements one will simulate, therefore the efficiency of quantum simulator is critical. To increase the simulation scale or reduce the resources for simulation, it's important to optimize the quantum simulators. Fig. 1 shows how many bytes are needed to simulate specific number of qubits using different simulation methods.

Quantum simulation optimization in our programme includes two parts - **simulator execution environment** and **simulation algorithms & implementations**. Many factors affect simulator performance, such as network and computing hardware. In general, the execution environment is mainly optimized from two aspects i.e. software and hardware. For software optimization, the compiling options for simulators, the basic runtime libraries like OpenMPI, and the batch job schedulers like Slurm are worthy of further exploration. As for hardware, the most influential factor may be the accelerating chips like GPU and FPGA as well as powerful CPU. The memory on each node and the network connection between nodes also have great effects on computing performance and simulation scale.

Back to the quantum simulator, one possible way to improve simulation performance is porting heavy-computing workload from CPU to GPU or FPGA or vectorizing simulation workload via vectorization instructions of processors like AVX512 instructions from Intel/AMD, NEON, or SVE instructions from ARM. Optimizing the simulation algorithms for common quantum algorithms mentioned later could also improve simulation performance significantly. Some new simulation algorithms and techniques based on tensor network can increase the simulation performance or reduce the memory cost of simulation, which we are genuinely interested in.

As mentioned before, quantum noise and errors are the dominant factors that affect the simulation scale and accuracy of results, hence it's momentous to simulate the behavior of quantum noise and errors to compare the results from digital simulators and physical quantum computers.

2.2 Quantum Computing Applications

Our simulation platform is designed for quantum computing application exploration in HEP and other fields, and may show its advantages over classical computing. So one of our objectives is to seek good quantum computing applications in HEP in collaboration with physicists.

In the NISQ era, types and depths of practical quantum circuits are limited, due to the poor qubit quality and the limited number of qubits, and as a result, there are few practical quantum algorithms. Current quantum algorithms can be classified into two categories - Variational Quantum Algorithms (VQA) and quantum annealing Algorithms (QAA). Some specific quantum algorithms are as follows:

- Variational Quantum Eigensolver (VQE)
- Quantum Machine Learning (QML)
- Quantum Approximate Optimization Algorithm (QAOA)

• Quadratic Unconstrained Binary Optimization (QUBO)

Most of the above algorithms are hybrid classical-quantum algorithms, i.e. the quantum computer or simulator plays as computing accelerators to the classical computer.

Till now there are already many quantum computing applications in HEP analysis, as well as chemistry, materials, biology, etc., such as particle identification and classification, track pattern recognition and reconstruction. Alex Mott et al. used quantum annealing methods to study the Higgs optimization problem for the first time on quantum simulators and physical machines [6], and Vasilis Belis et al. then used quantum classifiers to identify Higgs from other particles [7]. In Ref.[8], Koji Terashi et al. discussed the applications of quantum machine learning in the case of event classification in HEP. It turns out that quantum machine learning algorithms might play an important role in the HEP analysis, as widely probed in Ref.[9–12], and most algorithms are based on quantum kernel methods, variational algorithms and annealing algorithms.

The QCD theory, especially **Lattice QCD** is another important area that quantum computing may bring significant innovation. Some wondrous and inspiring attempts of implementing fermion field and gluon field on quantum computer have been proposed [12–16], though not practical on current machines. The International Symposium on Lattice Field Theory which is the largest Lattice QCD symposium has set up a parallel session for quantum computing algorithms years ago, and more and more quantum algorithms and simulation schemes are being proposed. Our simulation platform then could provide the testing ground for physicists to examine their ideas.

2.3 Quantum Computing Education & Training

For most of us, **quantum computing is quite different from conventional computing**, due to its counter-intuitive properties like superposition and entanglement. There are some thresholds for researching and developing quantum computing, and therefore, **training and education about quantum computing are imperative** to developing quantum techniques and algorithms, which decreases the difficulty of researching and developing and cultivates young generations for quantum computing technology.

Certainly, there are already many excellent tutorials, training courses, and popular articles about quantum computing, but it's still very meaningful for us to make efforts in these areas. And here are some possible approaches:

- Web portal to introduce quantum computing.
- Detailed tutorials based on our developing platform.
- Open video courses, academic reports and conferences.

And these are exactly what we are working on now.

3. Current Progress

In the early stages of our project, we are primarily concerned with the development and deployment of quantum computing simulation platform to provide a convenient developing platform for designing and verifying quantum algorithms efficiently. At present, the simulation platform mainly focuses on the performance optimization of interactive development platforms and quantum simulators on different computing hardware.

3.1 Simulation Platform

Our simulator platform mainly provides two interactive developing environments to meet different usage requirements. One is the Jupyter development environment, mainly used for interactive development and debugging of quantum algorithms, and the other is a drag-and-drop interactive interface similar to IBM Quantum Composer [17], mainly used to visualize quantum circuit and measurement results, by which users can have an intuitive understanding of quantum computing and bring down the threshold of quantum computing to a certain extent. Both two environments are integrated into our user dashboard interface, from where users can choose the appropriate development interface based on their needs.

Our Jupyter development environment runs inside a customized Docker image, integrating commonly used quantum development frameworks and simulators, such as Qiskit, Cirq, etc. At present, once the user logs into the Jupyter Development environment through IHEP SSO service and selects a type of containers such as CPU-based or GPU-based container at the container selection interface, our small Kubernetes cluster will automatically spawn a container and user will be led to the Jupyter homepage. Our computing containers are integrated with our distributed shared storage system so that users' projects can be persisted.

Due to the limited computing resources of the interactive cluster, user can only simulate limited qubits (e.g. ≤ 20). And for larger quantum circuits, user can submit the simulation tasks to the HPC cluster equipped with NVIDIA Tesla V100. Fig. 4 illustrates the spawn progress. In the future, we will integrate the Slurm task system with the Jupyter interface, which allows users to view the computing task queue and results in real-time.

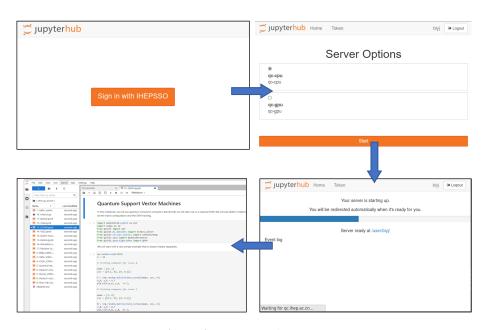


Figure 4: Jupyter environment.

The drag-and-drop development interface and the user dashboard interface are currently under design and development. The main purpose of the drag-and-drop interface is for user training, so the scale of quantum circuits it can simulate is relatively small. When the user uses the drag-and-drop interface to design quantum circuits, the code area will generate the appropriate Qiskit code automatically, and user then can download the generated code to a local file system or save it into the shared storage for subsequent use.

3.2 Simulation on Various Architectural Hardware

At present, the ARM processor has become an important player in HPC. Japan's Fugaku supercomputer, ranked No. 1 on the TOP500 list in June 2021, uses a customized A64FX chip with a performance of 442PFlops. China's Tianhe-2a partly uses Matrix 2000 chip with a performance of 61PFlops, and Tianhe-3 is also equipped with a large number of ARM chips. IHEP has also deployed a large ARM cluster of about 10,000 cores using Kunpeng920 at China Spallation Neutron Source at Dongguan, Guangdong Province.

Although the application's performance on a single ARM core is usually weaker than x86 Chips in most cases, the overall computing performance of Kunpeng 920 is not much worse than Intel/AMD x86 chips thanks to its many-core design. Qiskit can use SSE, AVX, AVX512 and other vectorization instructions to improve computing power on x86 chips, though it could not make full use of SIMD instructions of ARM chips at present, which makes the simulation efficiency not satisfied. We're currently working on vectorization of Qiskit on ARM chip, and will provide NEON support accordingly. According to our experience, vectorization can increase computational performance greatly.

Qiskit currently runs on NVIDIA GPUs, using the CUDA-based Thrust library for accelerated computing on GPUs, but does not work on AMD GPUs. Over the past decade, AMD has been gradually catching up to NVIDIA in the HPC field with its open-sourced ROCm [18] development architecture. The supercomputers with performance over 1 Exaflop under construction - Frontier & EI Capitan will be equipped with AMD GPUs/CPUs. Therefore, it is necessary to explore AMD CPU/GPU support for simulators such as Qiskit. We are currently making effort to port Qiskit from CUDA to ROCm. The code portion has been finished, including CUDA and assembly codes, but the compiling of Qiskit is held up due to the compatibility of the ROCm library and driver.

3.3 Quantum Computing Education & Training

A tentative web portal for quantum computing education and research communication has been deployed and will be publicly accessible soon. The web portal will provide a platform to follow the latest development in quantum computing, and to share and learn about quantum computing. Besides, the web portal is also the entrypoint to our interactive developing platform.

4. Outlook

The simulation platform is still under development and construction, and we are primarily focusing on the computing infrastructures and interactive platform in the early stage. Quantum computing and simulation algorithms, applications, collaborations and training will be our major objectives besides the platform development. Specifically, we will pay more attention to:

- a) Quantum Computing Infrastructure.
 - Optimizing run-time environment for simulators
 - Expanding computing resources for simulation
 - Developing global job scheduling system for large simulation
- b) Quantum Computing Simulation Techniques
 - · Simulator optimization and development
 - Quantum noise simulation
 - New simulation approaches like tensor network
- c) Quantum Computing Education & Training
 - Systematic workshop, school, lectures
 - Conferences for communicating and learning
 - Detailed tutorials for different levels
- d) Potential Quantum Computing Application Exploration

For the potential quantum computing applications, we will focus on HEP, quantum simulation in QCD and computing cluster health monitoring. For HEP, the following topics are what we are concerned about:

- Noise Filtering from real signal in LHAASO [19].
- Event Classifications in collider experiments like BESIII & CEPC.
- Track Pattern Recognition in Colliders.
- Energy Spectrum for hadron physics.
- Quantum Algorithm Optimization for general purpose.

As for QCD simulation, the following subjects are attracting us:

- Lattice QCD simulation on quantum machines
- Process simulation in colliders experiments

And for computing cluster monitor, we will explore the possibility of anomaly detection for cluster running status and network traffic analysis to filter attacks.

Yujiang Bi

5. Summary

Quantum computing has shown its potential to solve such problems virtually impossible under classic computing architecture and is one of the most promising directions for scientific computing. We are establishing an agile development platform to accelerate the exploration of quantum computing and simulation in HEP at IHEP.

The distributed heterogeneous and interactive computing simulation platform focuses on computing infrastructures, quantum & simulation algorithms, potential applications, collaborations, education & training. A preliminary interactive simulation platform is available and is in preparation for public access.

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