Quantum Computing at IN2P3

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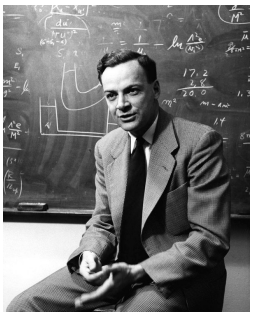
Abstract

Quantum computing is a new set of technologies implementing quantum bits (qubits) and operators on them. The first generation of quantum computers is now available but these are technically limited (low number of qubits and low decoherence time) and a lot of theoretical work is needed to fully exploit them. The QC2I project is a master project from IN2P3, created in 2021. It is composed of 22 members (researchers, engineers and students) working on quantum computing for high energy physics. The thematics covered by the project are mainly oriented on computation and algorithms. They are divided in three main themes: simulation of complex quantum systems, preparation of the quantum computing revolution and quantum machine learning.

1 Introduction

Quantum computers are new devices exploiting the laws of quantum mechanics to perform different computations. The properties of the quantum space (the Hilbert space), especially its exponential size make the quantum computers very appealing to perform calculations that are very memory-consuming in the traditional computing world. This remark has been noticed by Richard Feynman himself, in a keynote speech in 1982 [1].

> Some quantum systems are so complex, especially when the number of degrees of freedom increases, that their simulation on classical computers becomes impossible. For these complex quantum systems "Let the computer itself be built of quantum mechanical elements which obey quantum mechanical laws".
>
> Richard Feynman, 1982



This idea took plenty of time to be realised by hardware devices, but at the turn of 2020, some implementations became usable for limited problematics. These techniques can be very valuable for the high energy physics field and a master project, named QC2I, has been created at IN2P3 to design applications and algorithms for our activities.
This memoir is organized in two parts. Since the quantum technology is very recent, sections 2 to 4 describe in detail the foundations of the quantum computation and computers. These sections can be skipped without inconvenience by aware readers. In the last sections, 5 to 10, the QC2I project is presented.

2 Quantum bits

2.1 Mono-qubit algebra

The building blocks of quantum computers are qubits. They have properties that remind the bits of our traditional computers but are described by quantum mechanics. As bits, they have two states, denoted $|0\rangle$ and $|1\rangle$ in the Dirac notation. However, due to the superposition principle, they can be in any of the mixed states:

$$q = a\,|0\rangle + b\,|1\rangle \tag{1}$$

with a and b two complex coefficients obeying the normalization relation $|a|^2 + |b|^2 = 1$. This normalization constrains the values of a and b, which can be reduced to only two real parameters often represented as two angles. A very useful representation of a qubit is the Bloch sphere, represented on Figure 1.

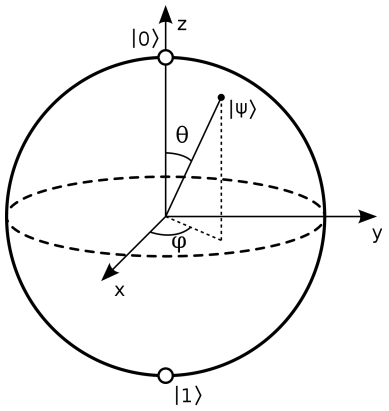


Figure 1: The Bloch sphere. Any point on the surface of the sphere is representing a possible state of a qubit. These points can be described by only two angles θ and ϕ. Any evolution of the qubit is isomorphic to a rotation on the sphere.

Any point on that sphere is a possible state for a qubit (such state is denoted $|\psi\rangle$ on the figure). It is defined by the two angles θ and ϕ. Any evolution of a qubit is isomorphic to a rotation around the x, y and z axes. Some points are remarkable on this sphere. The canonical basis $|0\rangle$ and $|1\rangle$ are the 1 and -1 points on the z axis. The equatorial points represent Hadamard states, specifically $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$, denoted $|+\rangle$, and its opposite, $\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$, denoted $|-\rangle$. These two states compose another very often used basis. Note that the Bloch sphere is just a convenient representation but is not completely intuitive. Especially $|0\rangle$ and $|1\rangle$ are orthogonal in the Hilbert space and antipodal on the Bloch sphere.
The two basic operations on a traditional bit are copying and reading. These two operations can not be realized easily on qubits due to their quantum nature. The perfect copy is completely forbidden by the "no-cloning theorem" [2]. Some approximate cloning procedures exists but they are expensive in terms of needed qubits and thus rarely used in real applications. The reading of a qubit is also complicated. The internal state of a qubit is not measurable. The only thing we can access is a statistical projection on the z axis (on the $|0\rangle$, $|1\rangle$ basis). In fact, when "reading" a qubit, we obtain a pure state, i.e. $|0\rangle$ or $|1\rangle$. To access the θ angle, it is necessary to setup multiple times the same state and to take the mean of the different measurements. The Born rule stipulates that for a qubit $q = a\,|0\rangle + b\,|1\rangle$, the probability to get $|0\rangle$ is $|a|^2$ and the probability to get $|1\rangle$ is $|b|^2$. This measurement is a destructive operation, the wave function collapses during the measurement and if another measurement is performed on the same system, it will give always the same result. An effective way of doing measurement is to perform a bunch of setups and measurements (typically 1000) and to deduce the value of $|a|^2$ from the empirical mean. The phase (the ϕ angle) can not be measured directly.

Any qubit can evolve under the application of an operator. These mono-qubit operators are 2x2 complex matrices (under canonical basis). These matrices have to be Hermitian. They can be decomposed in products of rotations around the axes. The three basic rotations around the x, y and z axis are respectively represented by the following matrices

$$Rx(2\varphi) = \begin{bmatrix} \cos(\varphi) & -i\sin(\varphi) \\ -i\sin(\varphi) & \cos(\varphi) \end{bmatrix}, \tag{2}$$

$$Ry(2\varphi) = \begin{bmatrix} \cos(\varphi) & -\sin(\varphi) \\ \sin(\varphi) & \cos(\varphi) \end{bmatrix}, \tag{3}$$

$$Rz(2\varphi) = \begin{bmatrix} e^{-i\varphi} & 0 \\ 0 & e^{i\varphi} \end{bmatrix} = \begin{bmatrix} \cos(\varphi) - i\sin(\varphi) & 0 \\ 0 & \cos(\varphi) + i\sin(\varphi) \end{bmatrix}. \tag{4}$$

A special operator, denoted H, named the Hadamard operator, allows to get a half mixed state $|+\rangle$ (resp. $|-\rangle$) if applied on $|0\rangle$ (resp. $|1\rangle$):

$$|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \tag{5}$$

and

$$|-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \tag{6}$$

The matrix of the Hadamard operator is

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}. \tag{7}$$

2.2 Multi-qubit algebra

The qubits can be associated to form a system. The notation represent all the combined states of the different qubits of the system. For example, here is a two qubit system

$$a\,|00\rangle + b\,|01\rangle + c\,|10\rangle + d\,|11\rangle \tag{8}$$

where a, b, c and d are complex coefficients. The Born rule is applied again, and the probability to measure $|00\rangle$ is $|a|^2$, and so on.
Some multi-qubit states can be obtained using the Kronecker product,

$$\begin{bmatrix} a \\ b \end{bmatrix} \otimes \begin{bmatrix} c \\ d \end{bmatrix} = \begin{bmatrix} ac & ad \\ bc & bd \end{bmatrix}. \tag{9}$$

These are separated states, but some states called entangled states can not be obtained in this way. The operators for multi-qubit systems are also Hermitian matrices of size $2^n \times 2^n$ for a n-qubit system. They can also be obtained by the Kronecker product, if they don't contain entanglement.
A most important operator is called CNOT, which stands for "controlled not". It takes as input 2 qubits, a control one and a target one. If the control qubit is $|0\rangle$ then the target qubit is left unchanged. If it is $|1\rangle$, then the target is flipped.
Thus we obtain the following transformations

$$|00\rangle \to |00\rangle\,;\ |01\rangle \to |01\rangle\,;\ |10\rangle \to |11\rangle\,;\ |11\rangle \to |10\rangle\,; \tag{10}$$

The corresponding matrix is

$$CNOT = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}. \tag{11}$$

It has been demonstrated that CNOT and the three rotations define a complete set of operators allowing to access any state of a multiple qubit system, just as the NAND gate can reproduce any mix of traditional logic operators.
In particular, they can induce entanglement. The figure 2 shows a quantum circuit, producing a state of two entangled qubits.

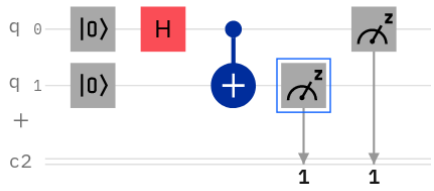


Figure 2: Entanglement circuit. The Hadamard operator H mixes the state of the first qubit. The CNOT operator creates the entanglement itself, linking the wave functions of the two qubits until decoherence. The measurement of the two qubits always gives two similar results regardless of the distance between them.

The operators are represented as boxes applied between the qubits (represented as lines):

$$|00\rangle \vec{H} \frac{1}{\sqrt{2}}(|00\rangle + |10\rangle) C\vec{N}OT \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle). \tag{12}$$

The produced state gives two entangled qubits. Even very far from one another, they will always be measured with the same outcome. This has been referred to as the EPR paradox in local space theories and has been tested extensively (up to 1200 km).
For more informations about qubits and their algebra for quantum computing, [3] is the reference book.

3 Quantum computers

There exists plenty of ways to implement qubits with physical systems: energy levels (most often fine structure) of atoms, superconducting currents... Figure 3 shows several promising implementations with pros and cons.
The two most mature technologies are now the superconducting loops and trapped ions. For both of them, real quantum computers have already been realized. In particular, the big companies Google `https://quantumai.google` and IBM `https://quantum-computing.ibm.com` have invested in superconducting loops. They have respectively implemented a 54 and a 53 qubits computer. The trapped ions are developped by some small companies like IonQ (11 qubits) `https://ionq.com` and AQT (20 qubits) `https://www.aqt.eu`. The key parameters are

- the number of available qubits,
- the connectivity of the qubits (i.e. on which pairs of qubits we can perform direct CNOTs),
- the decoherence time (d), which is the time before the quantum system is perturbed by the environment and looses its accuracy,
- the necessary time to apply a gate (g). This is a complicated notion, because any gate has to be transformed into a series of hardware specific operations and there is often a 2 to 3 factor between the number of gates in the original circuit and the one that is actually executed on the hardware,
- the error rate, i.e the percentage of “bad” measurements obtained on a dedicated setup.

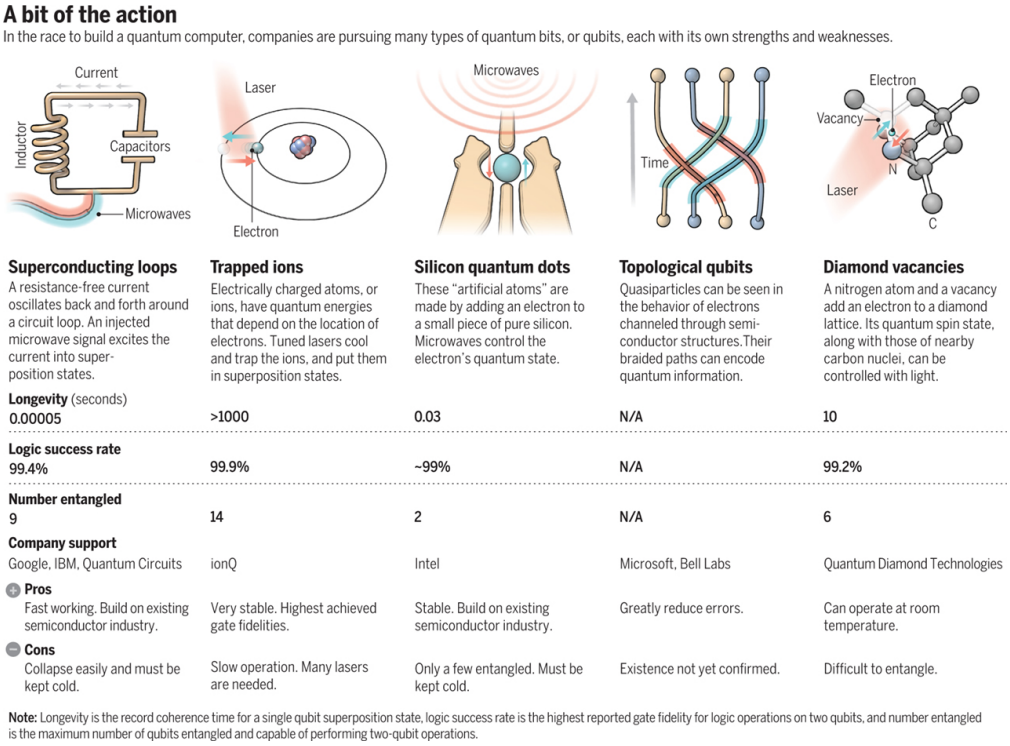


Figure 3: The different physical implementations of qubits. Credit: (GRAPHIC) C. Bickel/Science; (DATA) Gabriel Popkin.

The two parameters d and g can be shrinked in one more interesting parameter

$$G = \frac{g}{d}, \tag{13}$$

which expresses the number of gates that can be applied on the system before decoherence.
We are now experiencing what is called the NISQ era. NISQ stands for "Noisy Intermediate Scale Quantum". It means that our system has very few qubits (less than 100) which are quite noisy. On top of this, the topology of the implemented quantum computer is far from being complete and the emulation of standard gates consumes a lot of additional gates. All this means that we can only implement very simple circuits now but the field is evolving very quickly and we can hope to get better machines very soon.

3.1 Trapped ions

The trapped ion technology is probably the easiest to implement. Positive ions are trapped in an oscillating electro-magnetic field (Paul's trap) as show on Figure 4. They stand in line, regularly distributed by Coulomb repulsion. They must be in a vacuum environment to avoid decoherence but they can remain at room temperature.
As explained by Figure 5, the first three energy levels of the ions are used to implement the qubits. The base level corresponds to the $|0\rangle$ state. The first excited level corresponds to the $|1\rangle$ state. It has to be meta-stable to guarantee the perenity of the quantum information. Mixes of the two pure states can be obtained by Rabi oscillations at resonnance, implemented by a laser (red on the figure) focused on the ions. The third level is used for reading. Another laser (blue on the figure) is applyied on the ion, giving energy to reach the third level from the base level. This third level has to immediately come back to base level by emitting photons. Thus, when illuminated, the ion emits light if it is in the $|0\rangle$ state but not if it is in the $|1\rangle$ state. Only a few

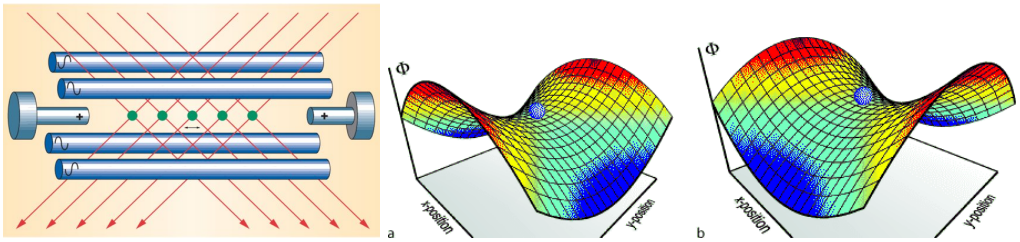


Figure 4: Left: Ions trapped in a Paul's trap. The positive electrodes constrain the ion line longitudinally and an oscillating magnetic field (represented on the right) prevents them from escaping by the sides.

atoms can meet these requirements. The most commonly used are alkaline earth atoms (Be^+, Mg^+, Ca^+, Sr^+) or ytterbium (Yb^+).

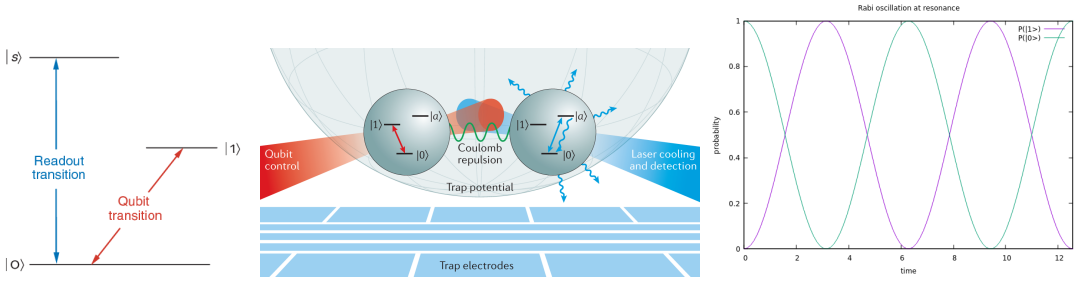


Figure 5: Energy levels of trapped ions and laser action schematics. Left and middle: The base level corresponds to $|0\rangle$ and the first excited state to $|1\rangle$ (this level should be meta-stable). The readout transition from the base level to the second excited level induces fluorescence if the qubit is in $|0\rangle$ state. Credit: `https://www.oezratty.net/wordpress/2018/comprendre-informatique-quantique-qubits/`. Right: The mix between $|0\rangle$ and $|1\rangle$ evolves like a cosine when the Rabi oscillation is at resonnance.

The multi-qubit gates are tricky to obtain. Ions can not interact directly because of the Coulombian repulsion. To implement these, we can use the motion of the whole line of ions for which there exists two collective proper modes. With a laser, it is possible to couple the quantum state of an ion to this collective mode and vice versa. Thus, by transitivity, it is possible to couple two ions.
The two main providers of trapped ions are IonQ (Maryland) and AQT (a spin-off of Innsbruck University). IonQ already sells machines, namely the Aria processor, which presently handles 11 qubits and should be extended up to 160 ions, and shares quantum computation time via the Amazon Web Services (AWS).
The linear arrangement is not very convenient if the number of ions becomes big. Thus, new architectures are designed on chips (2d Paul trap) where all ions are trapped on the surface of a chip and can migrate to different zones to be measured or to interact with other ions. The lasers are replaced by a combination of magnetic and microwave fields. A complete overview of this new technology is available in [4].
The main advantage of this technique is that it does not require a low temperature and that the decoherence time is very high (a few seconds). The cons are the focused lasers and the few number of implementable qubits. These downsides should be solved by the next generation of trapped ions composed of 2d traps where each ion can be displaced on the chip by a magnetic field, to go to specific zones with specific goals (entanglement, measurement, loading, etc.).

3.2 Superconducting loops

Using superconducting loops is another way to implement qubits. The basic idea is to build a superconducting loop interrupted by a Josephson junction. As shown in Figure 6, the Cooper pairs go through this barrier by

tunnel effect, inducing a small current. The qubit is encoded in the phase of this current. The rotations are controlled by conducted microwaves and the measurements are done by a magnetometer inside the circuit.

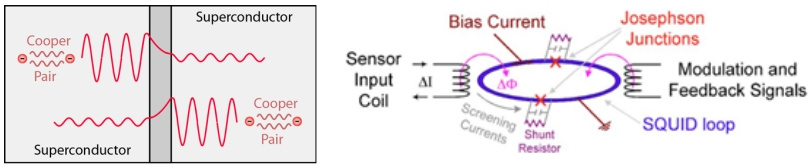


Figure 6: Superconducting loop implemented with Josephson junction. Credit `https://www.oezratty.net/wordpress/2018/comprendre-informatique-quantique-qubits/`

The multi-qubit operations are performed through dedicated qubits named "transmon" for transmission line shunted plasma oscillation qubit. They are superconducting charge qubits (to reduce their noise sensibility) and they are controlled by microwaves. The only implementable operation with the transmons is the Conditional Phase (CP), whose matrix is

$$CP(\gamma) = \begin{bmatrix} e^{i\gamma/2} & 0 & 0 & 0 \\ 0 & e^{-i\gamma/2} & 0 & 0 \\ 0 & 0 & e^{-i\gamma/2} & 0 \\ 0 & 0 & 0 & e^{i\gamma/2} \end{bmatrix}. \tag{14}$$

The CNOT can be implemented from the CP operation by combination with rotations this way:

$$CNOT_{12} = e^{i\frac{5\pi}{4}} R_{x2}(\frac{\pi}{2}) R_{z2}(\frac{\pi}{2}) R_{x2}(\frac{\pi}{2}) R_{z2}(\pi) R_{z1}(\frac{\pi}{2}) \times CP(\frac{\pi}{2}) R_{x2}(\frac{\pi}{2}) R_{z2}(\frac{3\pi}{2}) R_{x2}(\frac{\pi}{2}). \tag{15}$$

Many big actors of the traditional computing have invested in this technology, including IBM, Google and Intel. The two main constraints are the superconducting temperature and the very short decoherence time. On another hand, with this technology, it is possible to implement a big number of qubits with reasonable connectivity (53 for IBM, 54 for Google). These machines are available through the IBM-Q portal (the smaller processors are even accessible for free).

4 Quantum machine learning

The problematics of quantum machine learning (QML) is to implement neural-network-like models and gradient descent on quantum computers. Due to the limitations of the NISQ era, the full implementation of a model as complicated as a full neural network is impossible nowadays, but some basic models can be used.

4.1 Variational hybrid quantum-classical algorithms

As stated in [5], a way to optimize a quantum model is the variational hybrid technique. The principle is to encode the parametrized model in a parametrized quantum operator $U(x, \theta)$ applied on the data x. This operator is measured by the standard procedure and the error calculation is performed on a classical computer. The error is then back-propagated on the parameters on the classical computer (for example with a gradient descent) until the error is small enough. The constraint for this technique is that the quantum operator (U) must be differentiable with respect to its parameters (θ).

4.2 First generation quantum neural network

Two seminal papers describe the first implementation of quantum neural network (QNN) in 2018 [7] and [6]. They use the same kind of declination of the variational hybrid technique. Figure 7 recapitulates the four steps of the process.

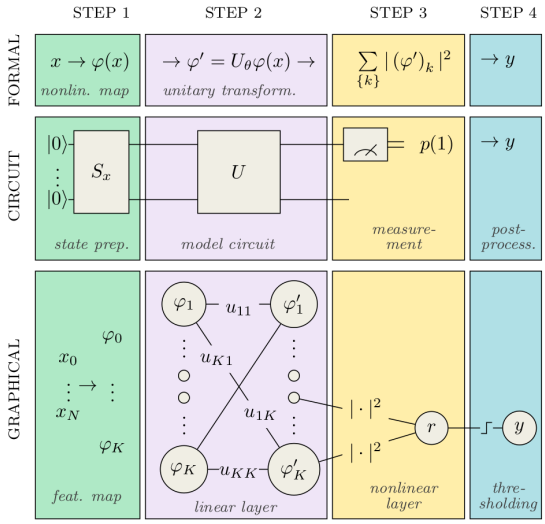
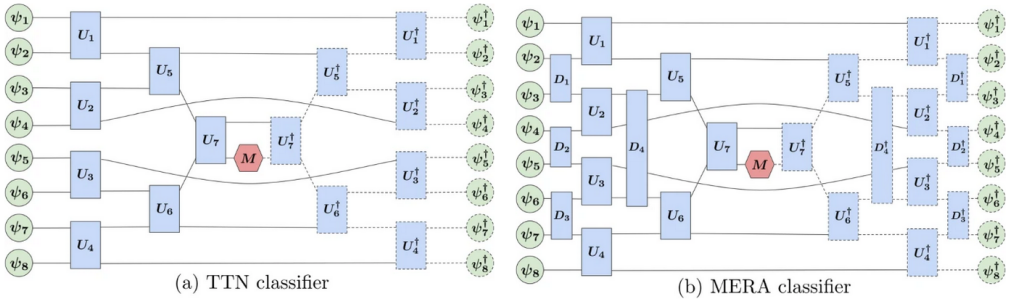


Figure 7: First generation neural network hybrid process from [6]. The system is composed of four steps running iteratively during the training. Step 1 is encoding (projection of data onto the Hilbert space). Step 2 is the model itself (linear), step 3 is the measurement and step 4 is the computation of the loss function, partial derivatives and optimization.

The first step is the encoding of the data on a set of qubits (projection in the Hilbert space). There are plenty of different techniques to encode this data. Some are minimizing the number of qubits, some other are minimizing the encoding time. The most used technique, which has become a consensus in the community, is the angle encoding. The input values must be normalized over $[0; 2\pi]$ and then the real values are encoded as an angle in the qubit with respect to z axis through a R_y rotation. This allows to encode a real number without any discretization. This technique requires one qubit per input.
The second step is to build a parametrized quantum operator that combines the data to obtain a sufficiently expressive model to allow classification or regression. Different structures can be used, often regular ones. Two main generic structures are frequently used, the so-called TTN and MERA, presented in Figure 8 from [8]. All the U_i operators are parametrized and their parameters will be the adjustable part of the model.



(a) TTN classifier (b) MERA classifier

Figure 8: TTN and MERA operators from [8]. TTN is the simplest of the mixing operators, it assembles the data by pairs, hierarchically. The MERA model comes from statistical physics and is a bit more elaborate.

The third step is the measurement of the result qubit. It can be one of the input qubits after application of the operators, or it can be a dedicated qubit (called ancillary qubit).
The last step is executed on the classical part of the system. A loss function is calculated from the measurement and a numerical derivative is calculated to update the parameters by a gradient descent with the

traditional formula

$$\frac{df}{dx}(x) = \frac{(f(x+\epsilon) - f(x-\epsilon))}{2\epsilon} + O(\epsilon^2) \tag{16}$$

Many derivations of this concept have been successfully tested for the high energy physic problematics. The survey [9] gives a nice overview of these different efforts.
Nevertheless, a bunch of drawbacks comes with this first generation of QNN. First, it is greedy in terms of qubits and thus it can be usefull only on very small data. The second drawback comes from the linear nature of the quantum operator. It is easy to demonstrate that a Hermitian operator is linear in its inputs. Thus the result can not be better than a linear classifier. As the Hilbert space is very big, the encoding can be viewed as projection of the data in a bigger space and the quantum operator as a linear classifier. This is typical of kernel methods, not a neural networks. This has been spotted by Maria Schuld in a paper [10]. Finally, the numerical differentiation is not very powerfull on noisy systems such as quantum computers. The equation (16) is accurate only if ϵ is very small. But on noisy systems, a small value of ϵ will be lost in the noise. Hopefully, new techniques will arise to solve these problems.

4.3 Second generation quantum neural network

The two problems of the linearity and of the use of qubits have been solved jointly by the elaboration of a new kind of operator, the re-uploading operator, that has been exposed for the first time by Perez-Salinas et al. in [11]. The principle, as stated in Figure 9, is to use only one qubit initialized to $|0\rangle$. Then a sequence of operators is applied to this qubit, depending not only on the parameters (θ_i) but also on the input itself (x). The quantum operators are linear in their inputs but not in their parameters. Thus, uploading x multiple time increase the complexity of the resulting expression in x. In fact, the number of re-uploading defines the degree of the polynomial expression induced by the application of the operators.

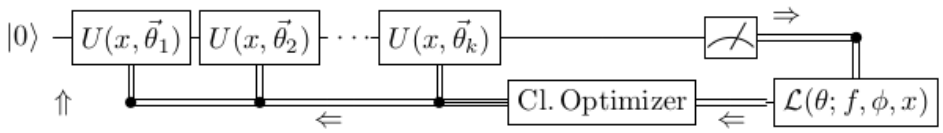


Figure 9: Re-uploading operator from [12]

The same authors have proven in [12] that this kind of sequence of operators is a universal approximator as neural networks are. This allows to integrate the non-linearity of the neural network directly inside the quantum operator and gives us hope to implement real quantum neural networks in the near future.
The second drawback, the numerical differentiation has been solved by the discovery by Mitarai et al. of a nice property of some quantum operators [13], called shift parameter rule. This can be summarized by the following equation

$$\frac{\partial G}{\partial \theta} = G(\theta + s) - G(\theta - s), \tag{17}$$

where G is the operator, θ the parameter and s is a constant that we can choose conveniently.
This means that for these operators, the derivative can be calculated by applying them two times. Note that contrary to the numerical differentiation, this is an exact value. Here is a simple example. Let us consider $G(x) = \sin(x)$. We know that

$$\sin(a+b) - \sin(a-b) = 2\cos(a)\sin(b). \tag{18}$$

Thus

$$\forall s, \quad \frac{\partial G}{\partial x} = \cos(x) = \frac{\sin(x+s) - \sin(x-s)}{2\sin(s)}. \tag{19}$$

The relation is true for any value of s, thus we choose conveniently $\pi/2$ which gives

$$\frac{\partial G}{\partial x} = \frac{\sin(x+\pi/2) - \sin(x-\pi/2)}{2}. \tag{20}$$

This comes from the trigonometric nature of this operator. It has been demonstrated by Crooks in [14], that all quantum operators can be decomposed in parts on which the shift parameter rule can be applied. This allows to differentiate any quantum operators and to use this true derivative to apply gradient descent. This technique is the base of the Pennylane software [15], which is a powerful tool, widely used by the community to implement hybrid learning systems `https://pennylane.ai`.

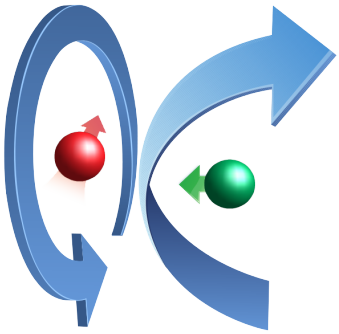
5 The QC2I Project

QC2I is a computing master project supported by IN2P3. Its goal is to explore the possible applications of the emerging quantum computing technologies to particle and nuclear physics problems as well as to astrophysics. Its main tasks are

- to identify, within IN2P3, scientists/engineers/technicians who are interested in using quantum technologies,
- to facilitate the access and training on quantum computers,
- to identify milestone applications for nuclear/particle physics and astrophysics,
- to design dedicated algorithms and proof of principle applications.

The project has three main directions: Prepare the Quantum Computing Revolution (PQCR), Quantum Machine Learning (QML) and Complex Quantum Systems Simulation (CQSS). Denis Lacroix (IJCLab) is the scientific director of the project and Bogdan Vulpescu (LPC) is the technical director.
The group is composed of 22 members from the following IN2P3 laboratories:

- IJCLab (5.5 members)
- LPC (2 members)
- LPNHE (3 members)
- LLR (6.5 members)
- CC-IN2P3 (2 members)
- LUPM (1 member)
- APC (1 member)
- LPSC (1 member)



The members have different status: researcher, director of research, engineer, postdoc and PhD student.
The project has been launched in 2021 after the success of a workshop organized by Denis Lacroix, Andrea Sartirana, Bogdan Vulpescu, Volker Beckman, Marcella Grasso, and Guillaume Hupin. The workshop title was "Journées thématiques de l'IN2P3: quantum computing, state of the art and applications". It has been held on September the 6^{th} 2019 and 70 participants have expressed their interest for the field.
The project has been funded since its creation with a budget of 5k€ in 2021 and 20k€ in 2022.

6 Complex Quantum Systems Simulation in QC2I (Resp. Denis Lacroix)

Anticipating the progress that will be made in the technological developments of future quantum computers with increasing number of qubits and with increasing fidelity of these qubits, activities have been started at IN2P3 (i) to understand these new technologies with their pros and cons, (ii) to explore how new technologies can be employed to describe complex physical systems and, (iii) to identify pilot applications where quantum processors can be used as a disruptive technology. One of the first anticipated application of quantum computers is the description of complex quantum systems themselves. Among the most challenging ones, we can mention the case of many-body systems, where the size of the Hilbert space to treat grows exponentially with the number of single-particle degrees of freedom. In IN2P3, we have started to scrutinize how quantum computers can be employed for the description of atomic nuclei. In nature, atomic nuclei are among the most challenging many-body systems and might strongly benefit from breakthroughs in quantum computing. The nuclear many-body problem has specific aspects that are hard to treat via classical calculations, like the highly non-perturbative nature of the interaction, the importance of multi-body interactions, or the necessity of using the concept of symmetry breaking/symmetry restoration. Yet, possible implementations of quantum algorithms in the nuclear context have been scarcely explored so far. Several works have been initiated to prepare the use of quantum technologies.

6.1 Description of symmetry preserving/symmetry breaking/symmetry restoration in quantum computers

Symmetries are important properties in physical problems. One might use the symmetry to reduce the complexity of a problem or, in some highly non-perturbative situation, it might be advantageous to break some symmetries in order to grasp internal correlations of a many-body problem. This is for instance the case of particle number symmetry [the U(1) symmetry] to treat superfluidity or the rotational invariance to describe the effect of deformation in atomic nuclei. The possibility to break symmetry is a crucial aspect that allows to design theories for open shell nuclei. One drawback of breaking symmetries is that these should be restored to provide observables comparable with experiments. Symmetry breaking ansatzes, and most importantly, quantum algorithms for symmetry restoration have been proposed in Ref. [16]. The method of symmetry restoration is taking advantage of the standard Quantum-Phase-Estimation method (QPE) to project the many-body wave-function onto its components that respect the symmetry under interest. The restoration of the symmetry is performed by measuring the ancillary qubits used in the QPE. A schematic illustration of the method is given in Fig. 1. In this article, applications were made on the pairing Hamiltonian. Such applications are relevant for small superfluid systems. The method has been further illustrated and improved for the case of total spin projection in Ref. [17]. In addition, in Ref. [17], we have shown how to reduce the number of operators used to project on the total spin from a quadratic to a linear number of operators together with removing the difficulty that states with good angular momentum are highly degenerated. The symmetry restoration is a crucial milestone for the description of atomic nuclei and in other physical systems where several symmetries can be spontaneously broken.

6.2 Finding eigenvalues and eigenvectors of many-body Hamiltonians

As a natural follow-up of the symmetry restoration problem, we used strongly entangled states obtained by symmetry restoration as variational trial states to be used in a Variational Quantum Eigensolver (VQE). The VQE method is a hybrid technique where, given a parametrized ansatz, the energy is computed on the quantum computer while the optimization is made on a classical device. We have shown how the projection after variation (PAV) and variation after projection (VAP) methods, that are nowadays the state of the art in quantum theory, can be transposed on quantum computers [18]. These two algorithms offer the possibility to obtained highly entangled/optimized trial states that could be used in a second step for post-processing. We extensively investigated different methods for the post-processing: the methods that have been proposed

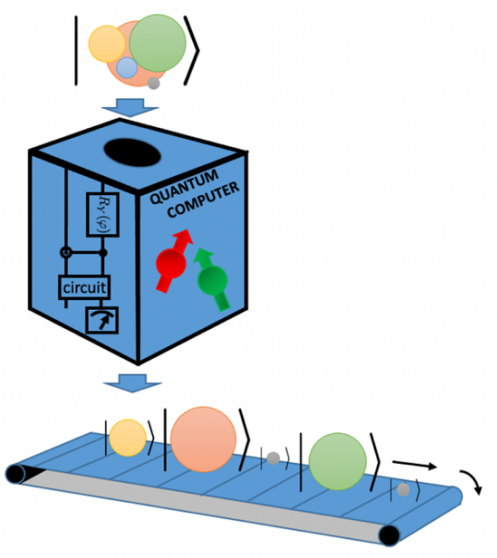


Figure 10: Schematic illustration of the symmetry restoration method for the case of the particle number symmetry. The measurement of ancillary qubits projects the system's wave-function onto a given particle number. At each event, i.e. each measurement, the system has a precise particle number that varies from one event to the other.

are the QPE, the Quantum Krylov and a new strategy based on the generating function of the propagator exp(-iHt) [19]. As an illustration of the effect of purification of the state prior to postprocessing, we show in Fig. 11 the result of the QPE approach after preparing an optimized state in the HF, Quantum-PAV and Quantum-VAP with a varying number of ancillary qubits that determines the precision on the eigenvalues of the Hamiltonian. We see for instance in this figure that the Quantum-PAV techniques leads to a highly purified state with strong overlap with the exact ground state on Figure 11-i.

6.3 Solving quantum equation of motion on a quantum computer

More recently, we also investigated how collective excitations can be obtained using the quantum equation of motion (qEOM) method. The method is general and can lead to a set of approximations of the collective problem with increasing complexity. At lowest order, it leads to the so-called RPA method that is standardly used in nuclear physics using classical computers. The next order leads to the so-called second RPA that is at the limit of what can be done currently on most powerful classical computers. The qEOM has been applied for a schematic model (the Lipkin model that corresponds to the problem of a set of degenerated two-level systems) that is relevant for the nuclear many-body problem. Using a combination of the qEOM together with Gray code encoding on qubits and symmetry-preserving trial state, we have obtained very encouraging results using real computers provided in the IBM Cloud [20].

6.4 Treatment of non-Markovian effects on qubits

Although it is slightly different from the previous works, we mention that there are currently intensive works on the theoretical description of qubits coupled to one or several environments. These activities are relevant in the context of computing in NISQ devices. We mention the recent works [21] and [22].

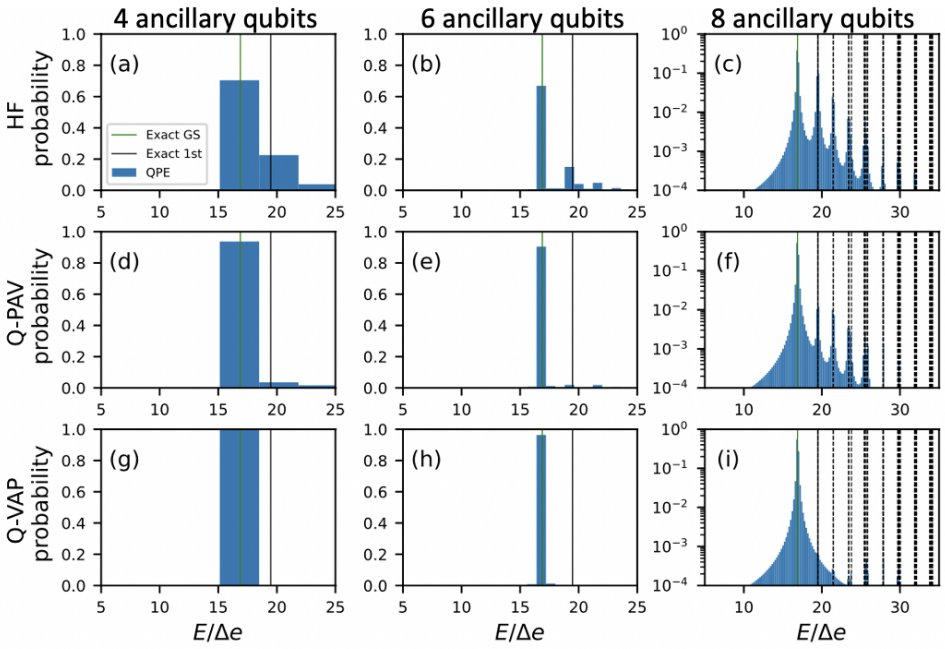


Figure 11: Illustration of the QPE method applied on the operator exp(-iHt) after having prepared an optimized state with different levels of sophistication: HF state (top), Quantum-PAV (middle) and Quantum VAP (bottom). From left to right, different numbers of ancillary qubits are used, leading to different precisions in the extracted eigenvalues. The height of the peaks correspond to the amplitudes of the initial state decomposed on the eigenstates of the Hamiltonian. On the left side, the exact eigenenergies are indicated. We see that the Quantum VAP is highly purified and is mainly composed of the ground state at variance with other states. Figure taken from Ref. [18].

6.5 Collaborations

The number of permanent scientists in IN2P3, mainly theoreticians, working on the description of complex quantum systems in quantum computers is still rather limited (mainly IJCLab and LPSC). Currently, there are two PhD students and one postdoc being trained on this topic and contributing to this subject. In addition, in recent years, several new collaborations are emerging. This is the case with a starting strong collaboration with the scientists in CEA-Saclay working on many-body systems. We also initiated regular discussions, with Atos especially, for future use of quantum devices. At the international level, two ongoing collaborations with the US have been initiated, one for the description of collective excitations (Western Michigan University) and one of quantum information in neutrino oscillations (Univ. of Wisconsin). Discussions on future collaborations have been initiated also with the Quantum Initiative in CERN and scientists in Trento, Italy. The IN2P3 teams working on many-body systems will also take part of the "National QC infrastructure research program" and will take the lead of the WP4.1 on "Quantum simulation of nuclear many-body systems". Regarding the access to real quantum devices, up to now, tests on real machines have been made mainly through the quantum IBM cloud. With the national project, a new machine provided by Pasqal and based on Rydberg atoms technology will be also accessible. Other accesses are or will also be explored (CERN Hub, Amazon, ...).

7 Prepare the Quantum Computing Revolution (Resp. Bogdan Vulpescu)

The goal of this thematics is, on one side, to aggregate talents from IN2P3 to create a group of enthusiasts and give them some insights on the quantum computing, but also to work on the differents possibilities to give them access to resources to be able to test these new techniques and eventually to concretize in in different domains covered by IN2P3. The different goals can be summarized in five points:

- identifying current and future quantum ressources that could be used for our projects,
- facilitating the transition of technicians/engineers/physicists to this new technology through the organization of meetings/schools/workshops,
- identifying pilote applications where the quantum supremacy can be decisive to solve problems relevant for the IN2P3 fields,
- developing quantum algorithms specifically dedicated to our science domain,
- contributing to the quantum revolution.

For the first part of the task, a survey has been performed to identify all the forces inside the IN2P3. The results of this survey show different typologies of profiles and interest of the members of the group, as shown in Figure 12.

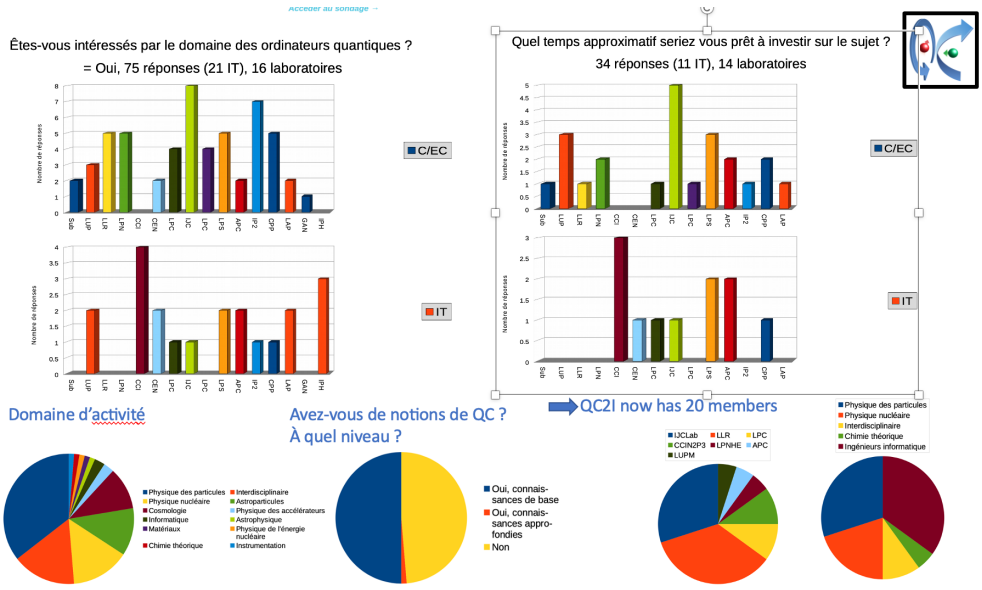


Figure 12: Different results from the survey

This preparatory work allowed to constitute a group of 22 persons motivated by the quantum computing, with very different profiles.
Different meetings have been organized:

- two general assemblies have been organized to share informations and structure the group,
- multiple sessions have been organized to share theoretical informations between participants, mainly under the form of a journal club,

- two tutorials have also been organized to give an overview of some technology aspects, one on the implementation of circuits on IBM quantum computers (B. Vulpescu) and one on the quantum machine learning (F. Magniette).

Several tools have been deployed to help participants to communicate and share informations and codes:

- a QC2I website with many ressources listed `https://qc.pages.in2p3.fr/web/`,
- a "newsletter" to broadcast the news,
- a GitLab group of projects, hosted by the IN2P3 computation center, allowing the members of the group to share their codes and the tutorials,
- a chat is online for casual discussion,
- a mailing list is also available on which all the announces of quantum computing related events are forwarded.

Recently, a section of the QC2I budget for this year was dedicated to be spent on the quantum resources available on the Amazon Web Services (IonQ, DWave, Oxford Quantum Circuits). Several accounts have been created, allowing the members of the group to perform simulations and to execute their codes on real quantum devices.

8 Quantum Machine Learning (Resp. Frédéric Magniette)

Developments around the QML have been essentially done by LLR and IJCLab. In a common effort, we obtained a grant from the P2IO Labex, funding a two year postdoctoral position. Yann Beaujeault-Taudière has been recruited on this grant, and is dedicated to this subject. He has integrated the team on the first of December 2021.
The works on QML have followed two opposite directions, that should combine eventually. One direction is purely theoretical and consists in searching for mathematical correspondance between quantum re-uploading operators and traditional perceptrons. The other direction is driven by engineering goals, mainly to understand and implement QML models to study their expressivity and classifying power on a set of adapted benchmarks.

8.1 Theoretical approach

A lot of well-working models have been developed on the artificial neural network paradigm. It would be very interesting to use them in the quantum context. To be able to perform this, we need to find an easy way to implement this model on a quantum computer. The effort has been concentrated recently on hybrid systems and architectures that do not relate directly with the neural network formalism (kernel methods). Unfortunately, the two models have a lot of mathematical differences, namely, the difficulty to implement non-linearity with the quantum operators. But on the other side, there are really interesting properties of the quantum system that can be used. For example, the amplitude amplification technique used in the Grover algorithm could replace the traditional training to find the optimal parameters of a model.
In the first part, we will describe how the multi-layer perceptron can be integrated in a quantum system.
The mathematical model of a multi-layer perceptron is very simple as long as we can implement a non linearity. A single layer has the form

$$\hat{Y} = \sigma(W^T X + B), \tag{21}$$

and its composition in multiple layers is simply the composed form

$$\hat{Y} = \sigma(W_1^T \sigma(W_2^T \dots \sigma(W_n^T X + B_n) + \dots + B_2) + B_1). \tag{22}$$

On the quantum side, the apparition of non-linearity can only be implemented through the re-uploading technique with a caracteristic equation which is radically different:

$$Z_n = \langle 0|U_n^\dagger Z U_n|0\rangle\,, \tag{23}$$

where U_n is a composition of Hermitian operators which have the same matrix representation but with different parameters. Some recurrences can be established to obtain the general form of these operators.
To obtain the mathematical match between these two very different forms, it is necessary to decompose the non-linearity of the perceptron to integrate parts of it inside the operator recurrence. The Fourier decomposition is a good candidate for this and it gives enough constraint on the nature of the usable operators.
Once the mono-layer perceptron is modeled with the re-uploading operator, it can be composed linearly to provide multi-layer perceptron as shown in Figure 13. This work has given interesting results that will be published soon.

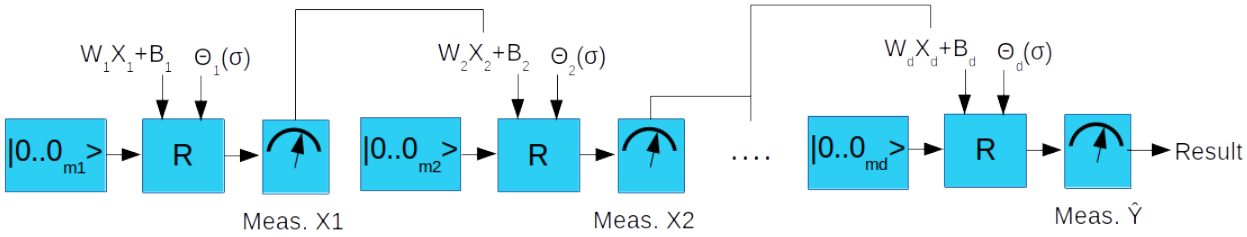


Figure 13: The mono-layer perceptron quantum model is composed to obtain a multi-layer perceptron. The geometry of the hidden layers is reproduced by the size of the qubit vectors at each step (m_i). Due to the sequential nature of the operation, the qubits can be reused from one layer to another.

In this second part, we focus on a very recent work, trying to get rid of the hybrid method by adapting the Grover algorithm to find the optimal parameters of a quantum model. The Grover algorithm, published in 1996 in [23], solves the problem of searching in an unstructured database. By a smart mechanism of amplitude amplification, it exploits the quantum parallelism to extract information from a list of n entries, without reading the entries one by one (one nice example is to find a name in an address book by knowing only the phone number). The complexity of implementation is only $O(\sqrt{n})$, while the traditional implementations need $O(n)$. Such a technique has been used to optimize the parameters of a QML problem in [24]. The main drawback is that the parameters need to be discretized into a sum of decreasing angles (π, $\pi/2$, $\pi/4$...) multiplied by binary inputs. This induces a loss of precision but also the need for a lot of qubits (to inject the binary factors).
We are working on the exact evaluation of the induced loss of precision but also on a possibility to keep the parameters real all along the computation. This work is in a preliminary stage.

8.2 Engineeral approach

The second part of our work is oriented on a pragmatic approach. Returning to the fundamentals of machine learning, we test different models on different data to measure their performance and their flexibility. The main difficulty to test the quantum models is that only a very few qubits are available (on real quantum computers but also in simulations that become intractable due to the computational complexity).
The first work has been to select different benchmarks to test the models. The constraint to select such dataset is the small number of inputs associated with complex functions to approximate. We have selected different functions known for their complexity in terms of machine learning and their non-linearity. The first benchmark is a set of 1d functions often used in machine learning: cosine, sigmoid, hyperbolic tangent, ReLu... For the 2d tests, we have chosen different shapes traditionally hard to solve in statistics systems like horizontal and vertical lines, recurrent shapes... Figure 14 shows some of the selected challenges. Finally,

we have taken well-known particle physics problems, namely particle identification based on variables of interest. These variables are form factors extracted from particle showers in a sampling calorimeter. We made an analysis of these variables with BDT and sorted them in order to take the most significant ones depending on the number of inputs of our model.

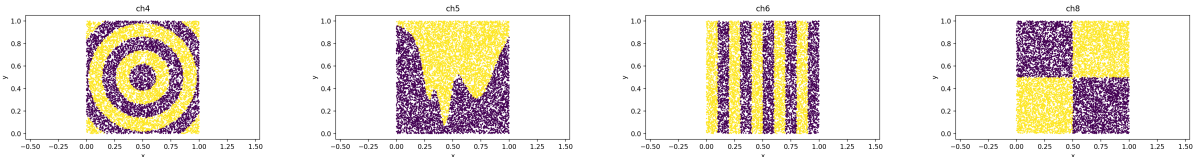


Figure 14: 2D Challenges adapted to quantum machine learning. Each input is just composed of the coordinates of the points and the label is the color (binary). The different challenges correspond to different complex problems for neural networks.

We have tested extensively these data on different models, QNN first and second generation, traditional multi-layer perceptrons and so on. The results are interesting. It seems that the form of the models reduce the number of needed parameters to fit these data.
To comfort these intuitions, a simulation framework is developped, to give some objective measurements and perform a systematic study. We aim to perform a methological comparison of the different models and to estimate the expressivity of all of them with respect to the nature of the input data. This work should be published in the middle term and should help the HEP community to evaluate if the quantum machine learning can be helpful for further physics analysis.

9 Perspectives

The countries investing in the future of the quantum technologies have started their education programs in the disciplines connected to this field. In France, many high level courses exist already on several sites, preparing the next generation of researchers and IT engineers, with a Quantum Computing profile. In the meantime, there will be a transition phase necessary to prepare the ground in the research laboratories (of IN2P3) and the activities of the QC2I project have such a goal.

9.1 Future strategy for the description of complex quantum systems

The development of quantum algorithms to treat the specificities of the nuclear many-body problems is still at its infancy. With the recent work, we have initiated different directions that can be seen as starting building blocks for the description of atomic nuclei. In the coming years, the goal will be to apply quantum technology in the context of the nuclear many-body problem, with three main objectives: (i) Test the pertinence of state-of-art quantum algorithms and methods, mainly developed in other fields, in nuclear physics applications; (ii) Design new quantum algorithms tailored to nuclear systems; (iii) Investigate the possible feedback of nuclear-physics approaches to quantum simulations of other interacting many-body systems. Applications will be systematically tested on simple models relevant for quantum many-body problem in the non-perturbative regime. Ultimately, our targeted goal is to make applications of ab-initio methods that starts from bare interaction based on modern techniques like the Effective Field Theory. These methods are particularly challenging on classical computer and still restricted to a small fraction of the nuclear chart. We anticipate the following roadmap:

- Development of a set of realistic model Hamiltonians encoded on quantum computers for light nuclei (with a nucleon number $A < 12$) to be used as test-bed for the algorithms. The development of a Hamiltonian on qubits is strongly impacted by the encoding method. The different encoding method (Jordan-Wigner, Standard Binary, Gray code,...) will be systematically investigated.

- Application to nuclear systems of existing many-body ansatzes used in quantum simulations and development of new quantum algorithms based on symmetry breaking/symmetry restoration.
- Application of these ansatzes using two different techniques (a) we wish to test different implementations of the Variational Quantum Eigensolver (VQE) and, (b) we would like also to explore the possibility to develop Green's functions on quantum computers that are among the most powerful approaches used nowadays on classical computers for many-body nuclear structure calculations.
- Another direction that will be explored is the possibility to directly formulate the nuclear many-body problem on a lattice using pionless effective field theory.
- In all these developments, it will be necessary to increase the expertise of the working team for the use of noisy devices.

9.2 Future strategy for the quantum machine learning

Our strategy for quantum machine learning is divided in different parts, depending on the evolution of the quantum computers maturity.
For the short term, we plan to make an implementation of the converting system between multi-layer perceptrons and their quantum counterparts. As these techniques are approximations, we need to evaluate the degree of degradation induced by the approximations and draw some kind of Pareto front to choose the implementation with respect to the desired precision. Presently, the multi-layer perceptron is implemented as a piling of mono-layer perceptrons separated by a measurement operation. This kind of implementation is not very efficient, due to the number of setups necessary to perform a measurement. We plan to try to integrate multiple layers directly into the re-uploading operator. We have seen that some composed functions appear (like $\sin(\sin(x))$) and they can be approximated directly by Fourier decomposition. This would provide a very efficient implementation of the multi-layer perceptron and ease its training. We plan also to use our implemented framework to perform a big methodological study to gain intuition on what kind of operators can be useful depending on the nature of the input data. New benchmark data will be specifically designed and tested.
For the middle term, we plan to implement a real application on physics data. This could be linked to some already existing machine learning project at IN2P3 to find a real application and compare the performance obtained on quantum systems with the traditional implementations. As a lot of different implementations have already been tried with first-generation QNNs, it should be easy to compare them with the second generation of QNNs.
For the long term, we anticipate the development of better quantum computers that should appear on the market in the near future. If the number of qubits increases and the error rate decreases, we can consider full quantum systems. To prepare this important step, we plan to develop and implement systems based on Grover algorithm, allowing to perform the parameters optimization directly in the quantum circuit. This should provide a considerable gain in the training time due to the quantum parallelism. The quantum search has a complexity in $O(\sqrt{n})$ while the traditional optimization has a $O(n)$ complexity. There already exist articles on this subject like [24] but they use an approximation based on a decomposition of the parameters in decreasing power of Π, consuming a lot of qubits. We plan to work on a fully continuous solution, reducing jointly the decomposition error and the consumption of qubits.
This way, we could imagine two kind of applications. First should be to transfer the traditional model to quantum system and perform very quickly the optimization, reducing the training time for the models. The second objective is more ambitious, it consists of developping quantum systems that can be integrated directly in our detector systems (off-detector electronics), to perform very quickly complicated neural network tasks online (for example in the trigger of big experiment like LHC detectors).

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