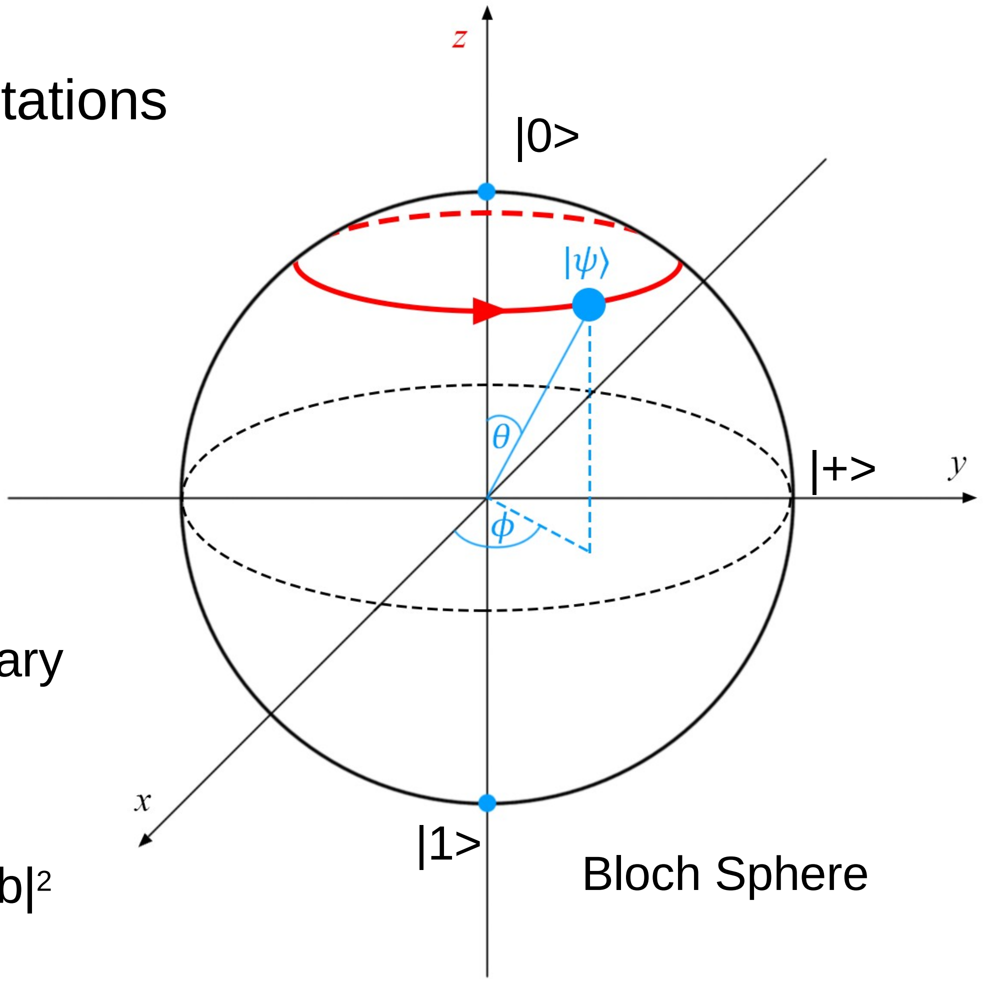
Quantum Computing @ IN2P3

F. Magniette on behalf of the QC2I Group

Quantum computing

- Using quantum object to perform computations
- Base object : quantum bit or qubit
- Qubit
  - Two pure states |q>=|0> or |q>=|1>
  - Superposition principle |q>=a|0> + b|1>
    with a and b complex numbers
  - Normalization $|a|^2+|b|^2=1$
  - Can be represented as two angles on a unitary sphere
- Measurement → Born rule
  - Measuring 0 with $|a|^2$ probability and 1 with $|b|^2$ probability
  - Projection on z axis
  - Destructive procedure → Setup multiplication

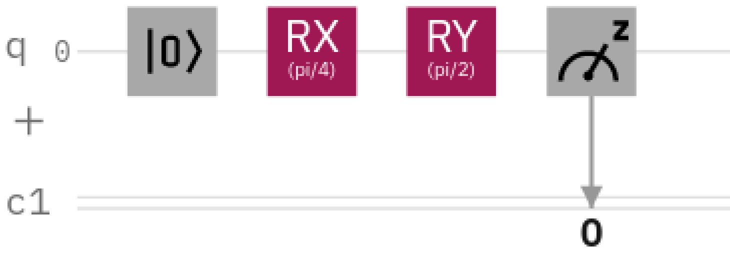


Bloch Sphere

State	Pr(0)	Pr(1)
|0>	1	0
|1>	0	1
|+>	1/2	1/2
a|0> + b|1>	$\|a\|^2$	$\|b\|^2$

Operators

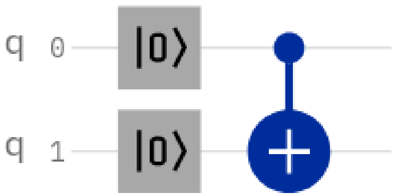
- A system of qubits can evolve but need to preserve its normalization (Hermitian operators)
- Operators are unitary $2^n x 2^n$ complex matrices
- Mono-qubit rotation
  - Can be decomposed in a series of mono-parameter rotations on an euclidian basis
- CNOT (controlled not)
  - Apply on two qubits, the control and the target
  - If control is |1>, flip the target, else do nothing :
    - |00> → |00>
    - |01> → |01>
    - |10> → |11>
    - |11> → |10>
- Rotations and CNOT are a universal operator set



$$Rx(\phi) = \begin{bmatrix} cos\phi & -isin\phi \\ -isin\phi & cos\phi \end{bmatrix}$$

$$Ry(\phi) = \begin{bmatrix} cos\phi & -sin\phi \\ sin\phi & cos\phi \end{bmatrix}$$

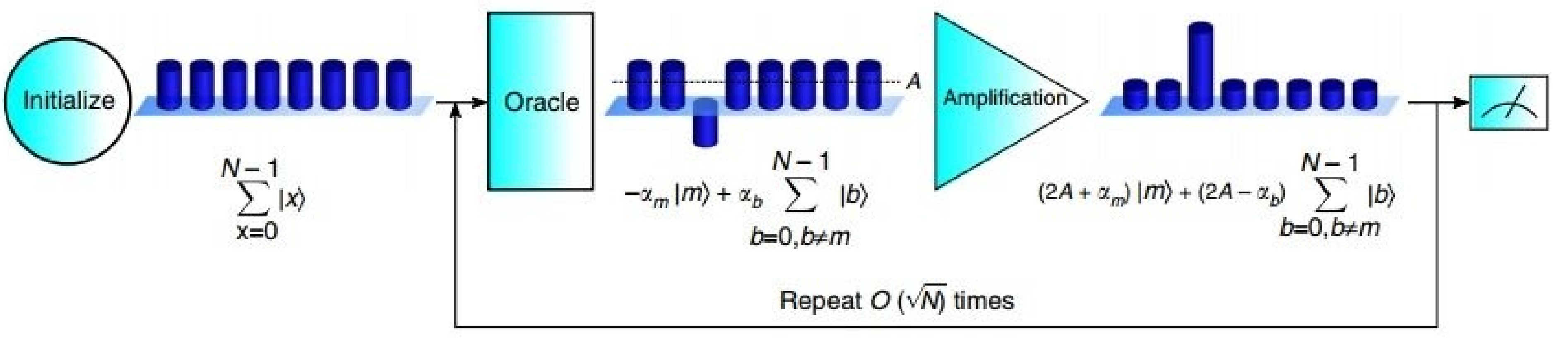
$$Rz(\phi) = \begin{bmatrix} e^{-i\phi} & 0 \\ 0 & e^{i\phi} \end{bmatrix}$$



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

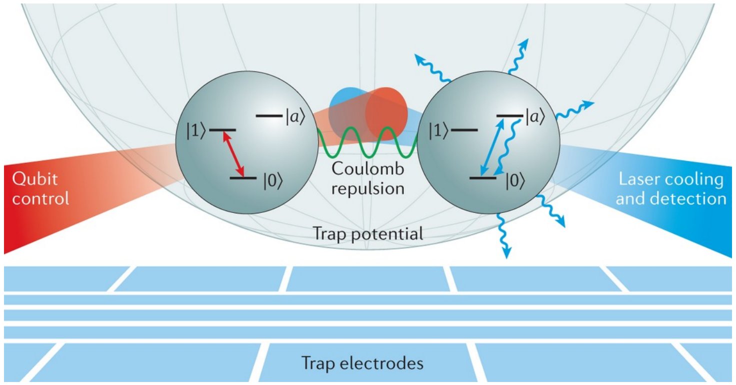
Parallelism / Grover Algorithm

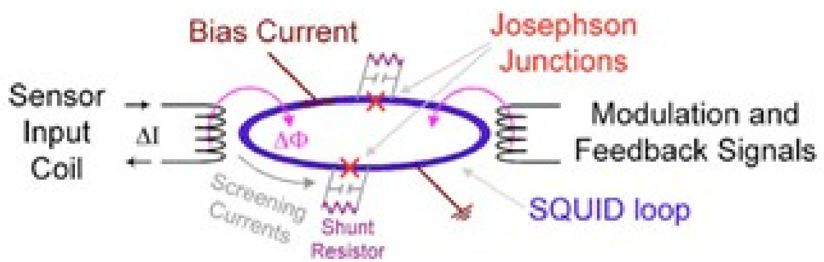
- Quantum circuits compute multiple values at the same time by superposition
- Purification / Amplification techniques
  - Alternance of oracle (specification selection) and amplification operations
  - Solve the search problem with incredible complexity O(√n)

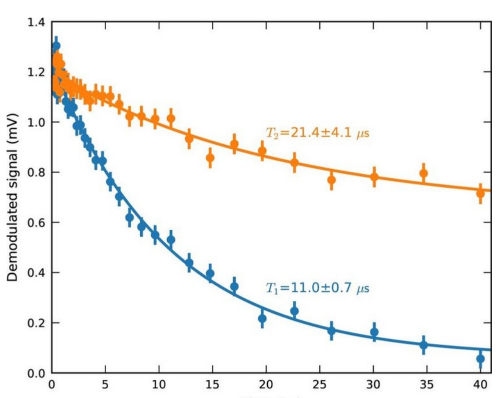


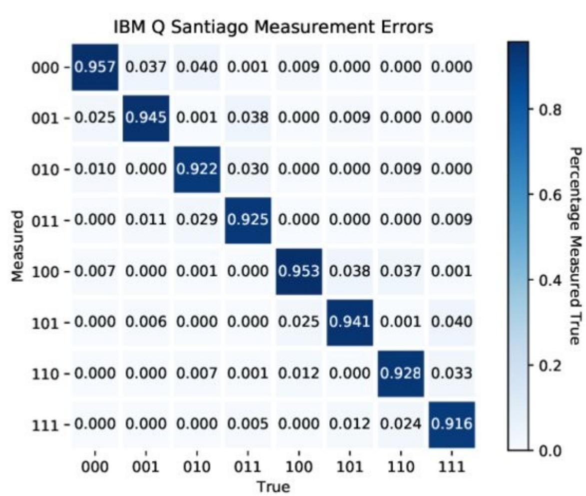
Quantum computers

- Trapped ions in synamic electromagnetic fields
  - Energy level used as qubit
  - Control and measurement by laser
- Super-conducting loops with Josephson junction
  - Phase of current used as qubit
  - Conducted microwaves for control, magnetometer measurement
- NISQ Era
  - Noisy, energy relaxation and decoherence time plus systematic operator errors
  - Intermediate Scale, few qubits and poorly connected

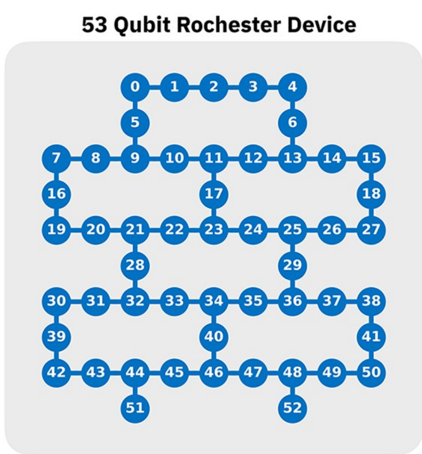




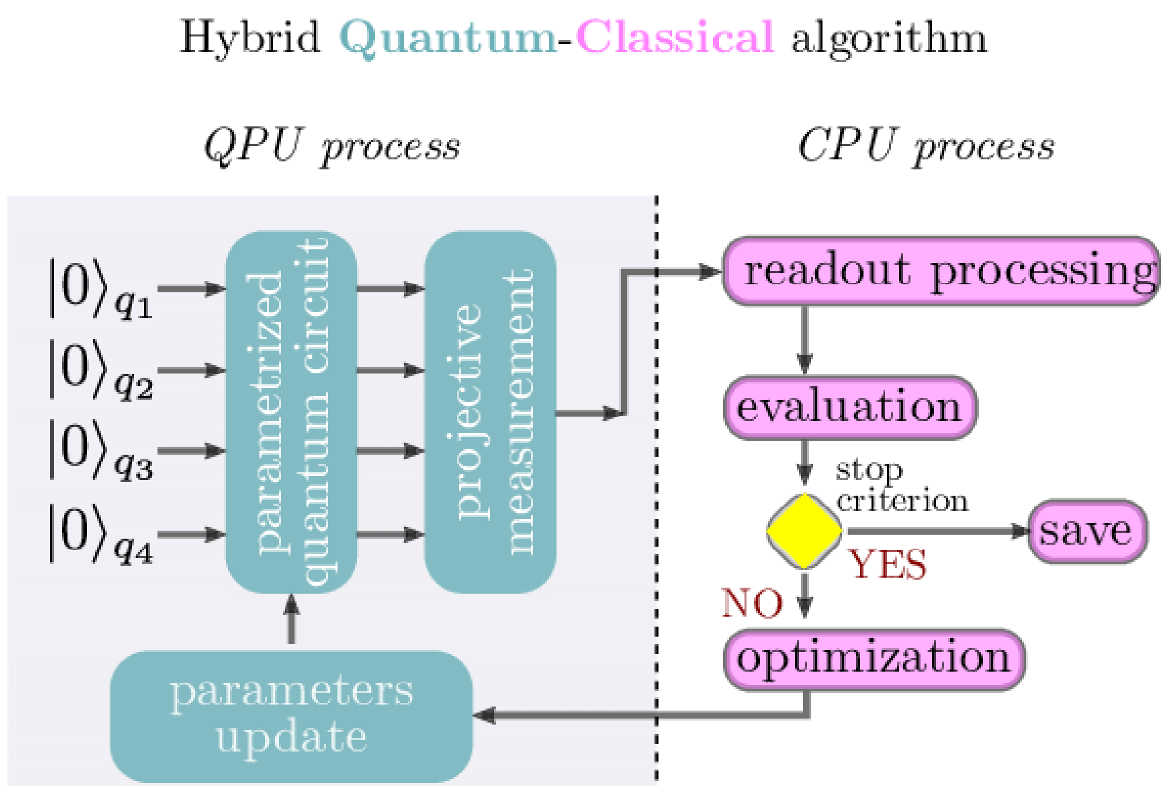




Measured \ True	000	001	010	011	100	101	110	111
000	0.957	0.037	0.040	0.001	0.009	0.000	0.000	0.000
001	0.025	0.945	0.001	0.038	0.000	0.009	0.000	0.000
010	0.010	0.000	0.922	0.030	0.000	0.000	0.009	0.000
011	0.000	0.011	0.029	0.925	0.000	0.000	0.000	0.009
100	0.007	0.000	0.001	0.000	0.953	0.038	0.037	0.001
101	0.000	0.006	0.000	0.000	0.025	0.941	0.001	0.040
110	0.000	0.000	0.007	0.001	0.012	0.000	0.928	0.033
111	0.000	0.000	0.000	0.005	0.000	0.012	0.024	0.916



Variational Hybrid Quantum-Classical Approach



Only a small part is handled by the quantum computer (adapted to NISQ)

McClean & Al, The theory of variational hybrid quantum-classical algorithms, 2015

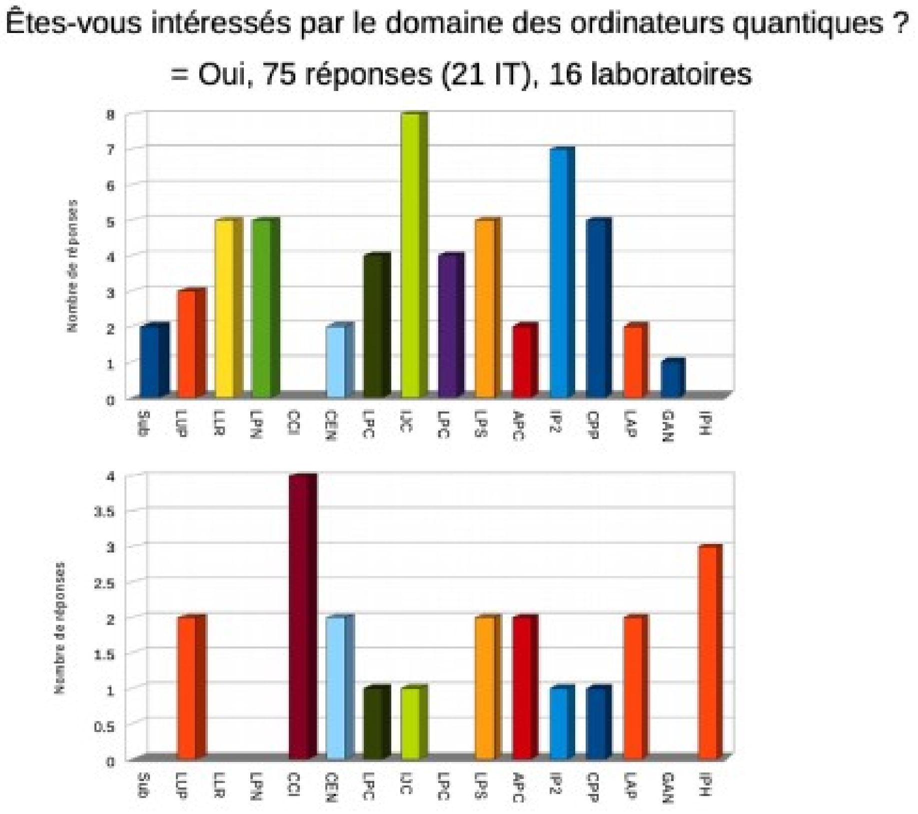
QC2I IN2P3 Master Project

- Computing project supported by IN2P3
- Goal: explore the possible applications of quantum computing for nuclear and high-energy physics
- Scientific Resp. Denis Lacroix (IJCLab)
- Technical Resp. Bogdan Vulpescu (LPC)
- 3 themes
  - Simulation of complex quantum system (Denis Lacroix)
  - Prepare the Quantum Computing Revolution (Bogdan Vulpescu)
  - Quantum Machine Learning (Frédéric Magniette)
- 22 participants – 2 levels of participation
- Website https://qc.pages.in2p3.fr/web/

IN2P3
INSTITUT NATIONAL DE PHYSIQUE NUCLÉAIRE ET DE PHYSIQUE DES PARTICULES

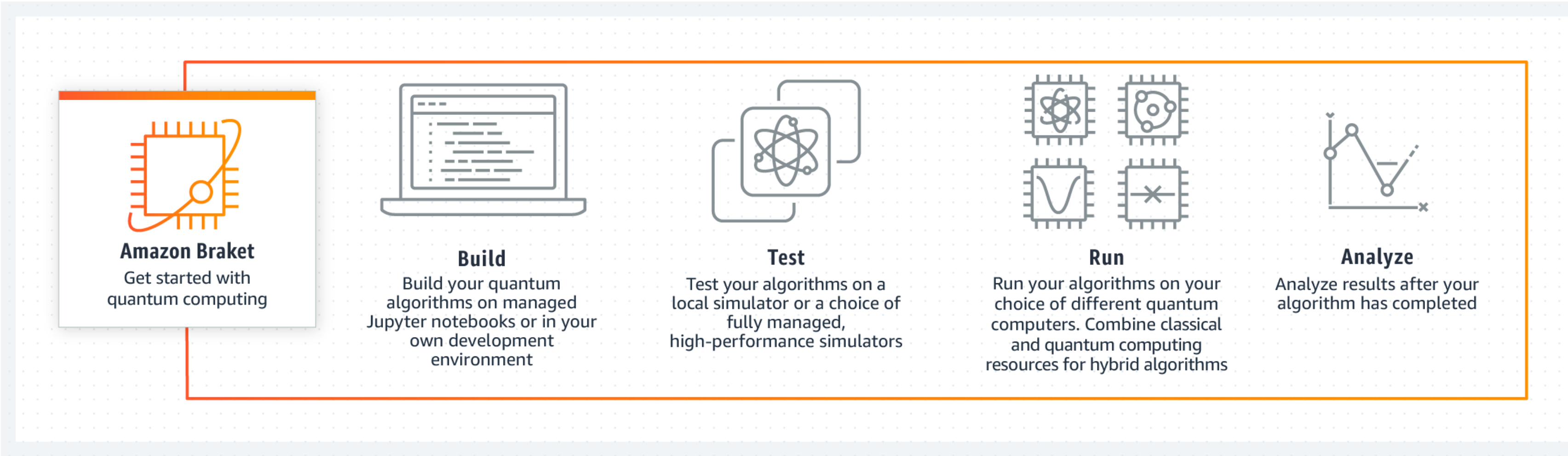
QC2I Realisations

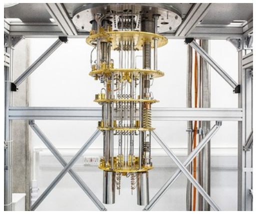
- Survey @ IN2P3
- Tools (Mailing list, newsletter, chatroom, gitlab, AWS access)
- Workshop « quantum computing, state of the art and applications », december 2019
- Seminars and journal club
- Practical sessions (IBM-Q, QML)



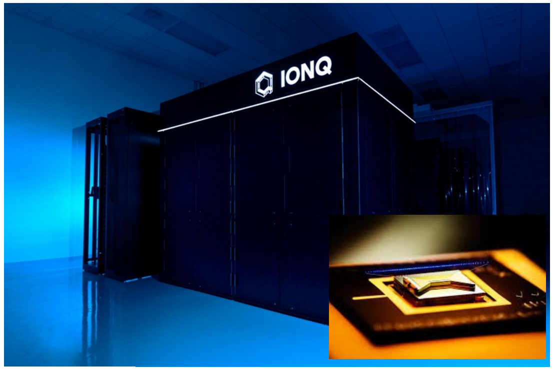
Testing quantum computers

aws

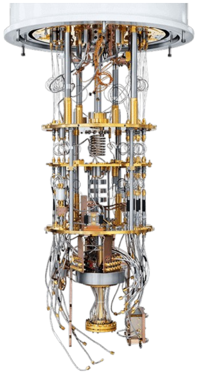




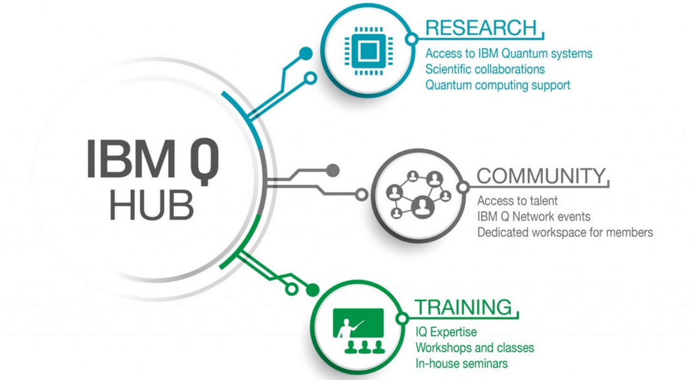
OQC



rigetti



IBM Q™

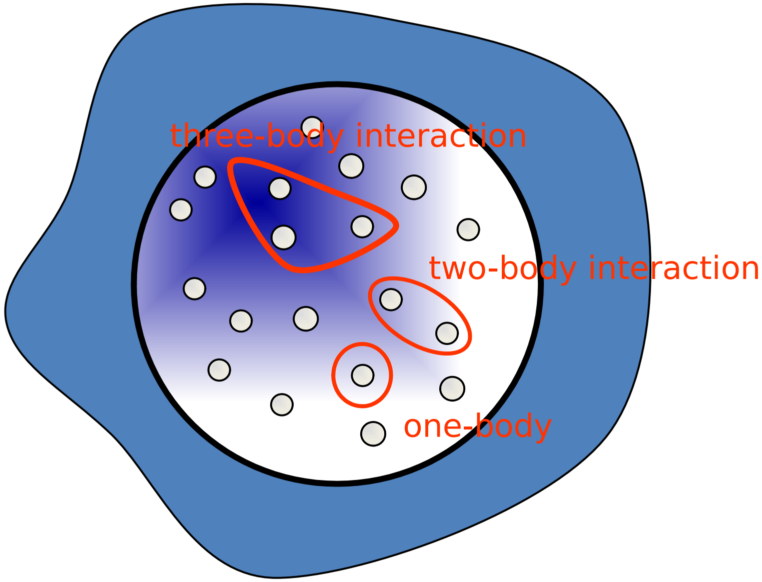


Preparing the quantum revolution

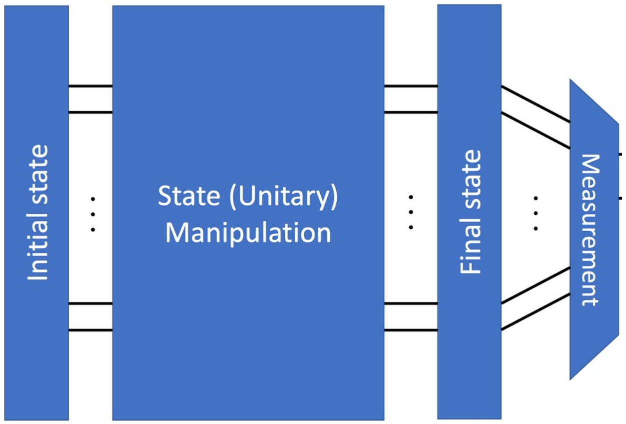
- The quantum technologies to support classical computers
- Define the new job of tomorrow’s IT, for a new information science
- Create partnership between information science and theoretical physics
- Include quantum in the IT education (mainly scientific calculation)
- Provide training materials : theoretical overviews, seminars, practical sessions (Amazon Bracket), external contributions, journal club

Complex quantum systems simulations

- Many-body systems can be simulated with quantum computers (Hilbert space increases exponentially)

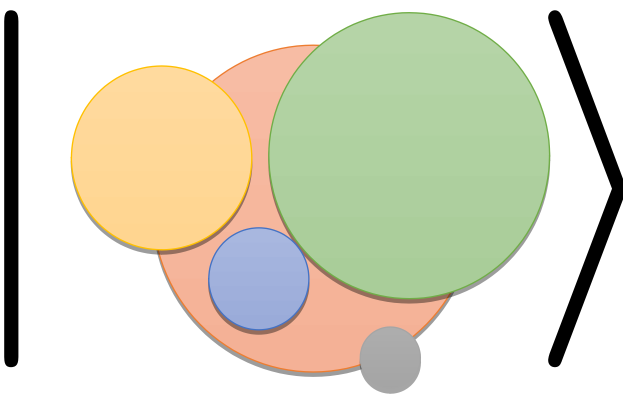


- Complex system
  - Highly non-perturbative nature of interaction
  - Importance of multi-body interactions
  - necessity of symmetry breaking / restoration



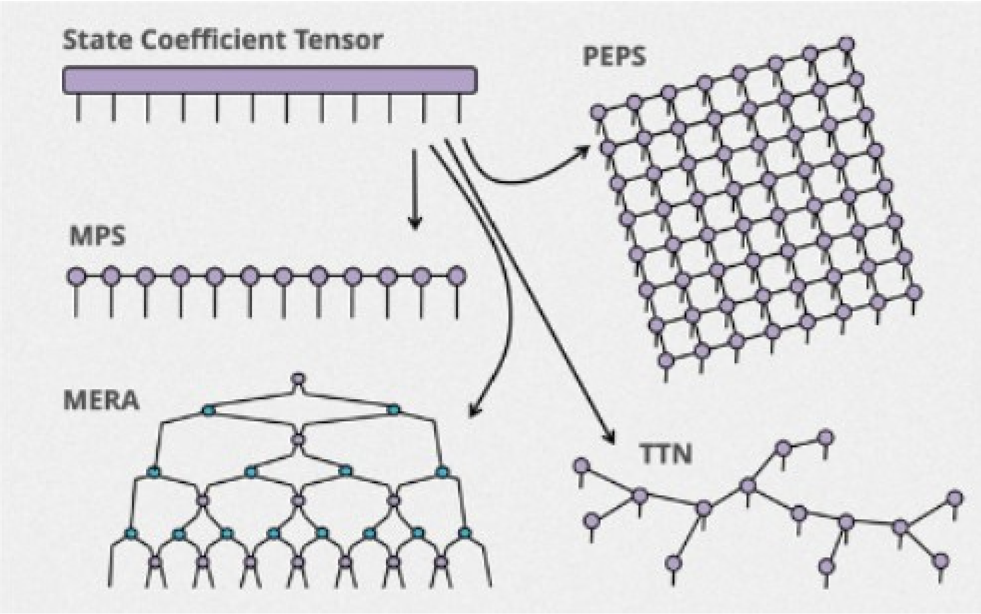
System preparation

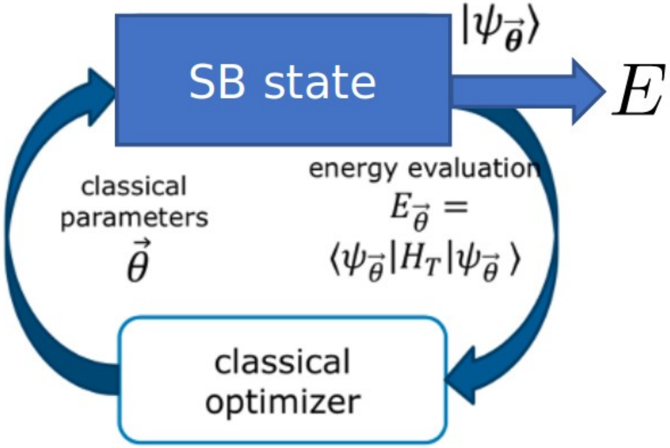
- Complex wavefunction mixing states $|\Phi_0>=\sum_i (u_i + v_i a_i^\dagger a_i)|->$
- For example, mixing 0, 2, 4, … particles
- U(1) symmetry is broken
- One qubit for each body (pair of particles)



Quantum approximation

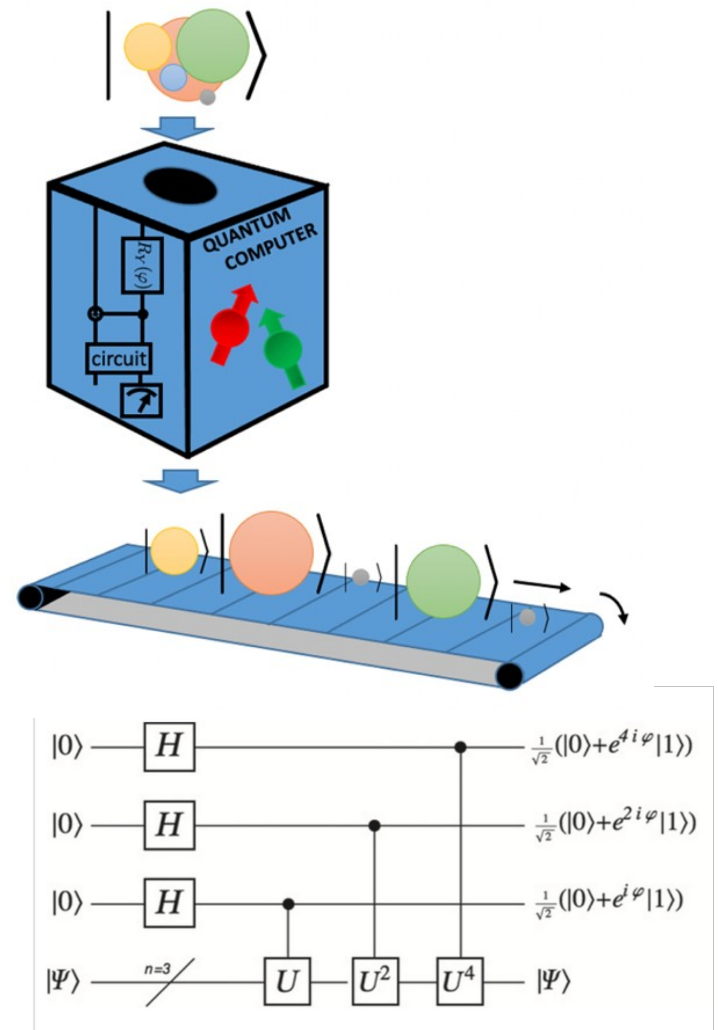
- Entangled ansatz (TTN, MERA…) approximating the Hamiltonian
- Optimization with variational hybrid technique
- Provides base energy for the system without symmetry (all states mixed)





Measurement

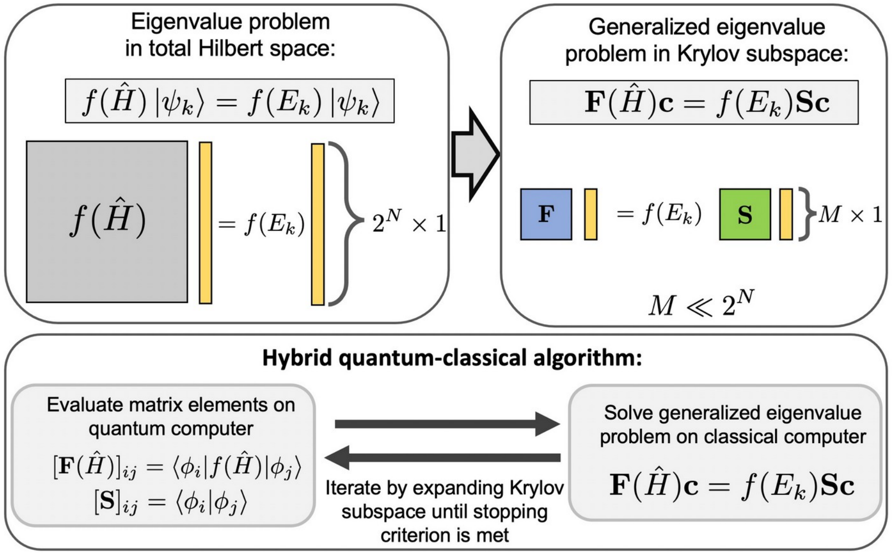
- Symmetry needs to be restored
- Ancillary qubit encode the symmetry
- Inverse QFT on register gives the energy
- Ancillary qubit restore the symmetry



- Denis Lacroix. Symmetry assisted preparation of entangled many-body states on a quantum computer. Physical Review Letters, 125, 230502, 2020.
- Pooja Siwach and Denis Lacroix. Filtering states with total spin on a quantum computer. Phys. Rev. A 104, 062435, 2021.

Post-processing

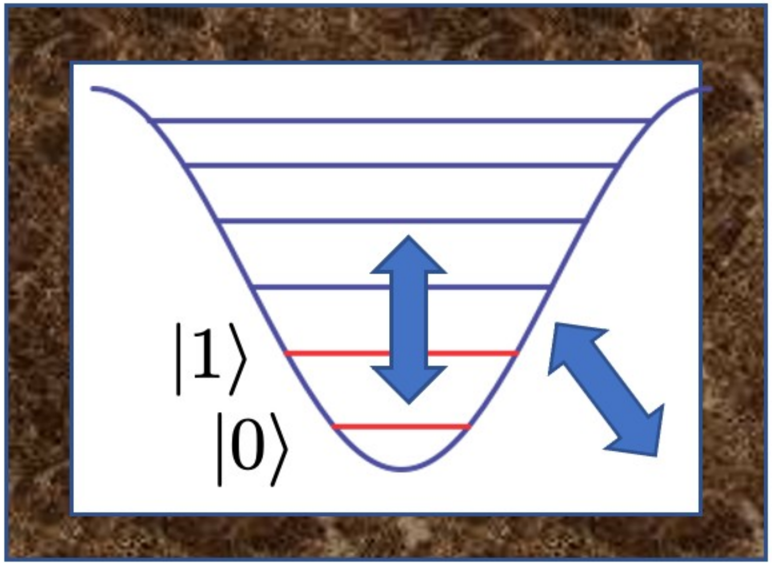
- Once the model has converged
- Generating function approach to get the moments of the Hamiltonian
- To obtain the excited states
  - Quantum Krylov algorithm
  - Quantum Equation of Motion
- Applications
  - Superfluid systems
  - Hubbard model



- E. A. Ruiz Guzman and D. Lacroix, Calculation of generating function in many-body systems with quantum computers: technical challenges and use in hybrid quantum-classical methods, arXiv:2104.08181, 2021
- E. A. Ruiz Guzman and D. Lacroix, Accessing ground state and excited states energies in many-body system after symmetry restoration using quantum computers, Phys. Rev. C 105, 024324, 2022
- M. Q. Hlatshwayo, Y. Zhang, H. Wibowo, R. LaRose, D. Lacroix, E. Litvinova, Simulating excited states of the Lipkin model on a quantum computer , arXiv:2203.01478, 2022

Noise simulation

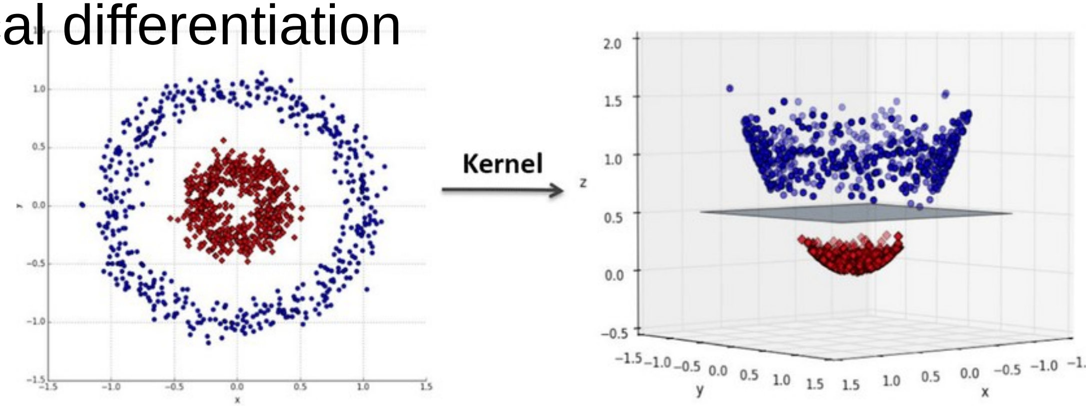
- Qubit system in interaction with heat bath
- describes exactly a qubit coupled with one or several external systems
- 3 exact methods have been proposed
- Helps to understand and describe the noise in the quantum devices

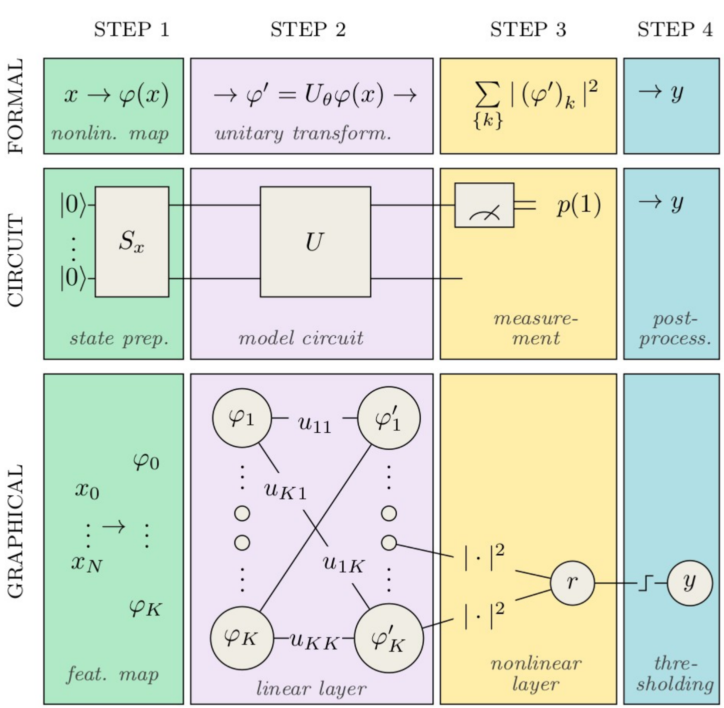


- V. V. Sargsyan, A. A. Hovhannisyan, G. G. Adamian, N. V. Antonenko, and D. Lacroix, *Applicability of the absence of equilibrium in quantum system fully coupled to several fermionic and bosonic heat baths,* Phys. Rev. E 103, 012137, 2021
- D. Lacroix , V. V. Sargsyan, G. G. Adamian, N. V. Antonenko, and A. A. Hovhannisyan, Non-Markovian modeling of Fermi-Bose systems coupled to one or several Fermi-Bose thermal baths, Phys. Rev. A 102, 022209, 2020
- and many more before….

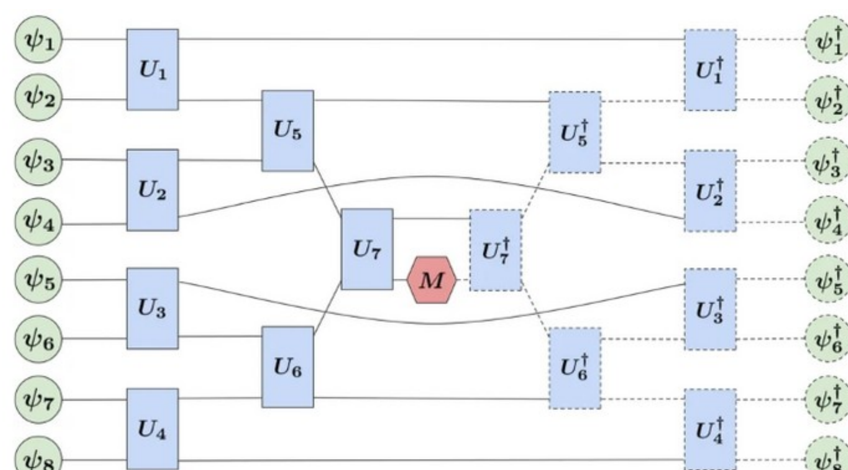
QML - First generation QNN

- 2018, two seminal papers Farhi et al, Schuld et al
- Almost same scheme
- Angle encoding (continuous rotation)
- Linear core (TTN, MERA…)
- Variational training with numerical differentiation
- Basically, kernel method





From Schuld & al 2018



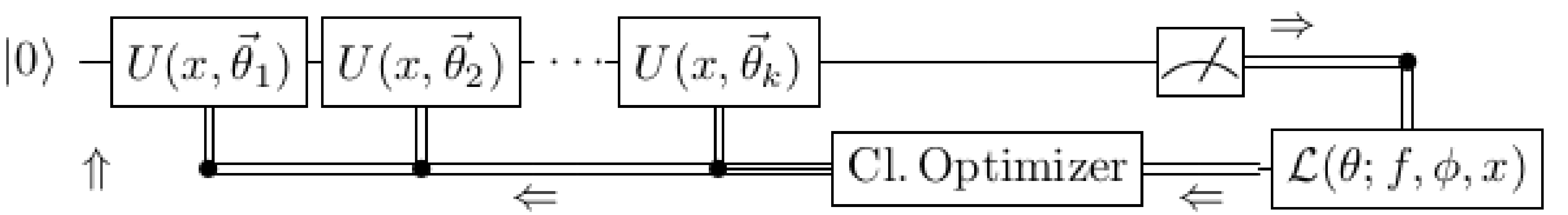
(a) TTN classifier

QNN for HEP

- Plenty of articles using this design for HEP analysis
  - Quantum Machine Learning in High Energy Physics, Guan & al, 2020, 2005.08582 (survey)
  - Performance of particle tracking using a quantum graph neural network, Tüysüz & al, 2021, 2012.01379
  - A quantum algorithm for the classification of supersymmetric top quark events, Bargassa & al, 2021, 2106.00051
  - Dual-parametrized quantum circuit GAN model in HEP, Chang & al, 2021, 2103.15470
  - ….

Second generation QNN

- Re-uploading
  - Input as parameter of every operators instead of input of a global operator
  - Non linerarity appears
  - Save a lot of qubits
  - Universal approximant (tanh, ReLu...)

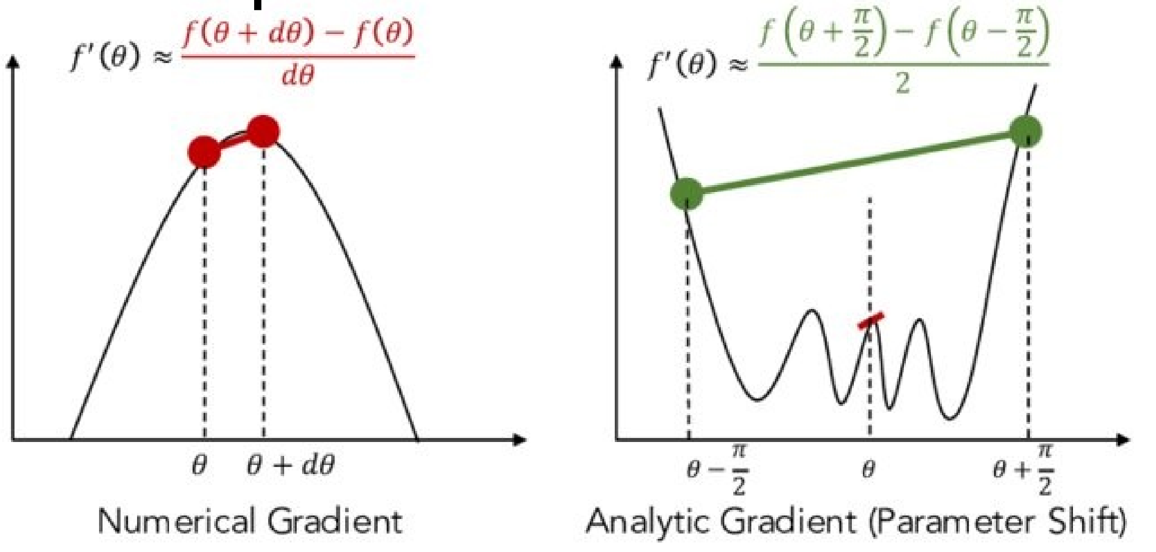


- Perez-Salinas & al, Data re-uploading for a universal quantum classifier, 2019
- Perez-Salinas & al, One qubit as a universal approximant, 2021

Parameter Shift Rule

- Property of some quantum operator

$$\frac{\partial f}{\partial \theta} = f(\theta + s) - f(\theta - s)$$

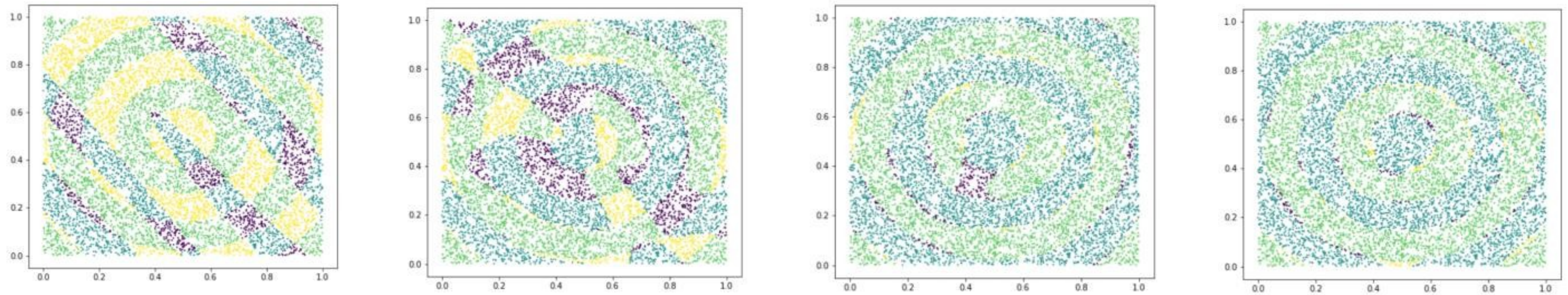


- Exact differentiation (s is fixed and not small)
- Can be extended to any unitary operator
- Implemented in Pennylane

- Mitarai & al, Quantum circuit learning, 2018
- Schuld & al, Evaluating analytic gradients on quantum hardware, 2018
- G.E. Crooks, Gradients of parameterized quantum gates using the parameter-shift rule and gate decomposition, 2019

Re-uploading QNN Tests

- Definition of benchmarks 1D,2D, 3D → binary classification (F. Magniette)
- Definition of physical benchmark (variables of interest from calorimeter showers)
- Work of Andrea Sartirana, Frédéric Magniette and Yann Beaujeault-Taudière (Postdoc 21-23 LLR/IJCLab)
  - Simulation of re-uploading learning circuits on benchmarks → very performant models
  - Implementation of a complete methodological framework to compare the expressiveness of the different models

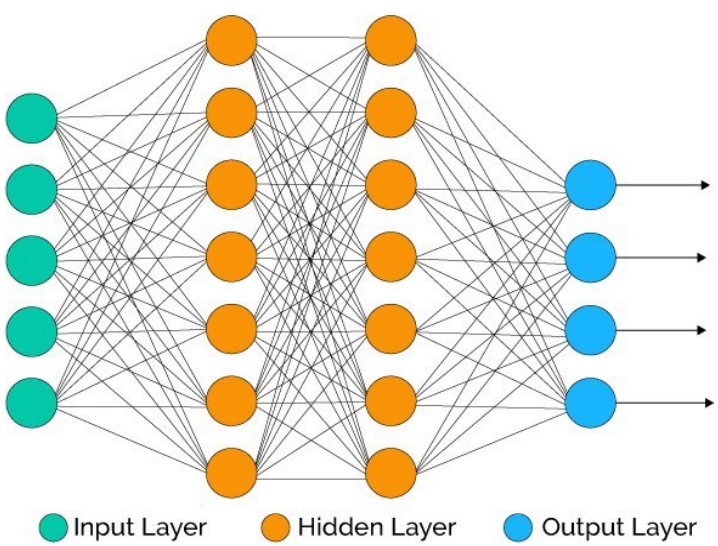


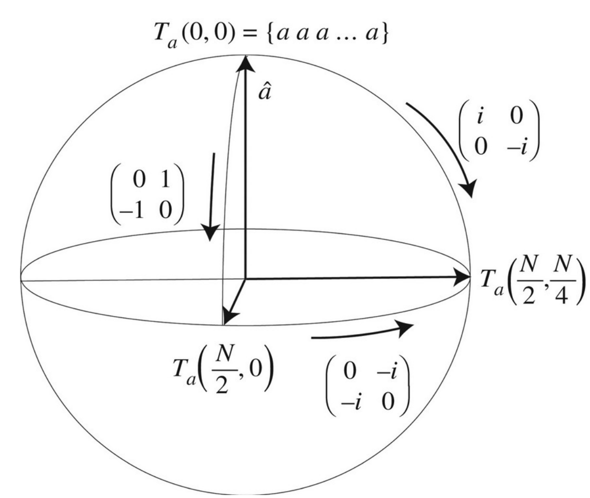
Quantum NN approximation

- Multi-layer perceptron formalism

$$Y = \sigma(W_1\sigma(W_2\sigma(...\sigma(W_dX + B_d) + B_{d-1}) + ... + B_2) + B_1)$$

- Approximation of σ by decomposition (Fourier, polynom…)
- Implementation on re-uploading circuit
- Implementation on Hadamard test circuit
- To be published soon





Perspectives

- Continuation of QC2I action to prepare scientists and engineers to the quantum revolution.
- Developement and applications of efficient algorithm for complex quantum systems.
- Applications to many-body problems: atomic nuclei, neutrinos, quantum systems on lattices.
- Test of Quantum Neural network and developement of efficient algorithms for data mining
- Test of re-uploading method for classification problems and application to HEP data
- Access to quantum computers