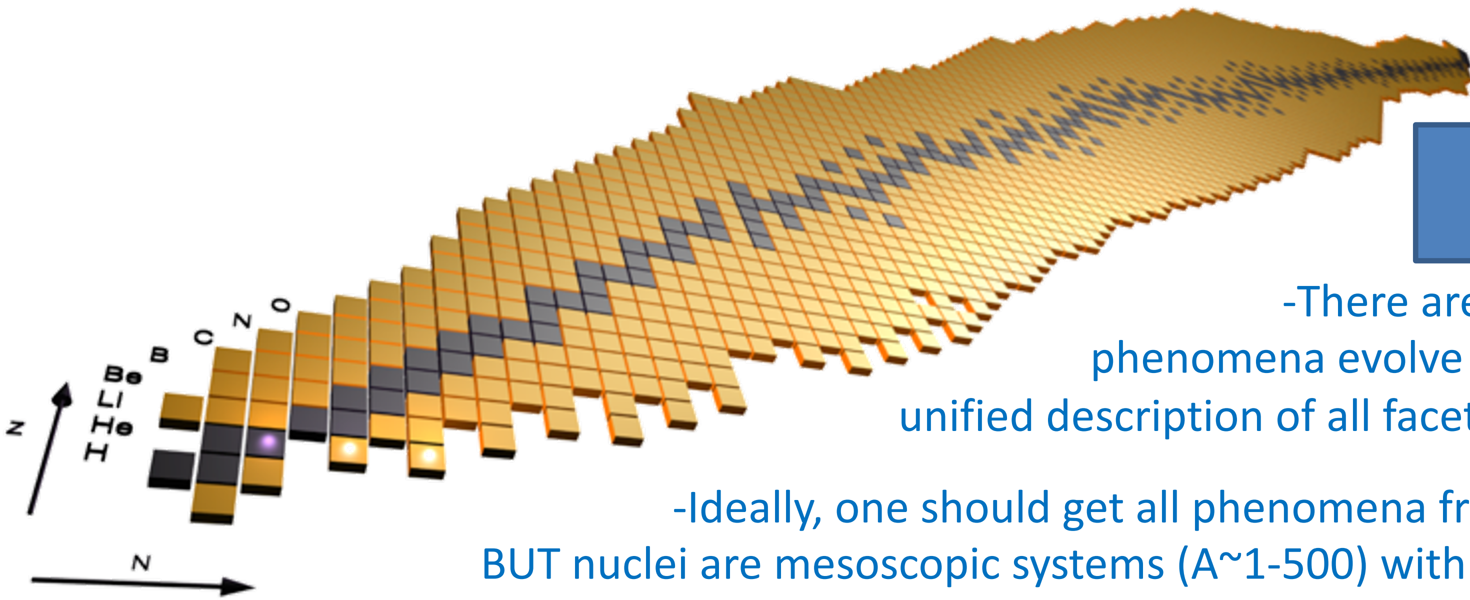
Theoretical Methods evolution: quantum computing, machine learning and A.I.

-How artificial intelligence can boost nuclear theory?
Neural network.

-Quantum computing. State of the art and applications

-**Denis LACROIX**, IJCLab
-Marcella GRASSO, IJCLab
-Guillaume HUPIN, IJCLab
-Raphaël LASSERI (CEA DRF)
-David REGNIER (CEA DAM)

Selected complex aspects of nuclear problems

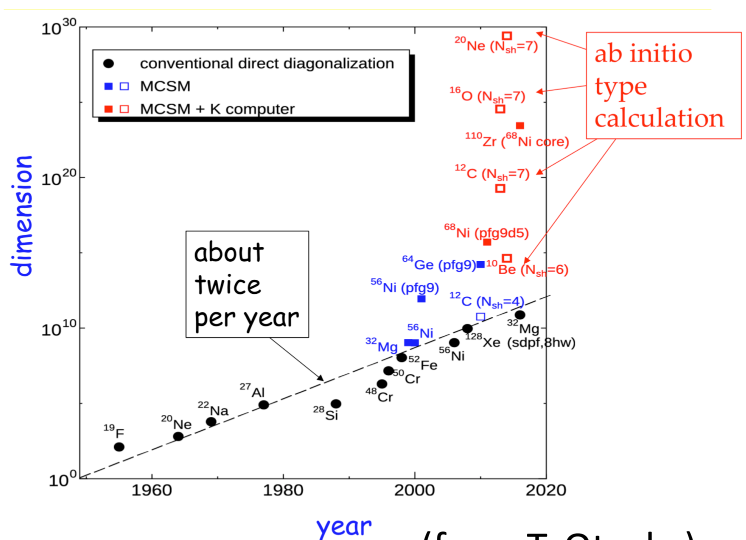


Some evident sources of complexity in nuclei

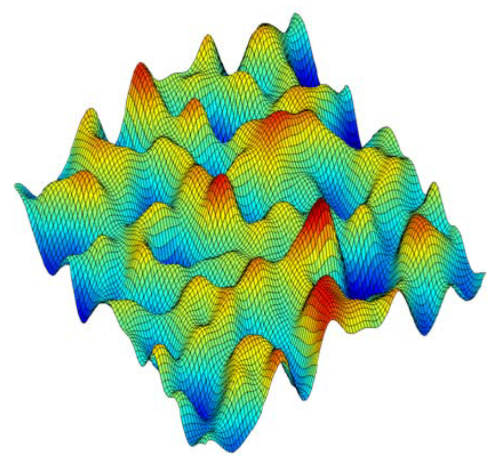
-There are many nuclei (>3000). Nuclear phenomena evolve along the nuclear chart. A unified description of all facets would be desirable.

-Ideally, one should get all phenomena from the bare interaction BUT nuclei are mesoscopic systems (A~1-500) with bad numerical scaling.

-Each nucleus is a complex problem per se.



(from T. Otsuka)

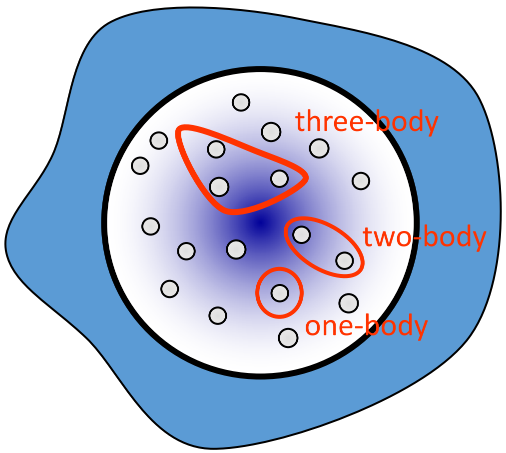


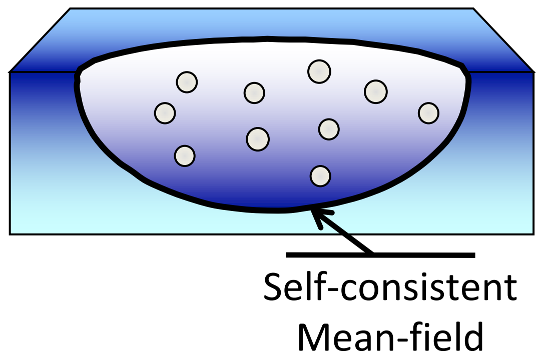
(Energy landscape of a molecule)

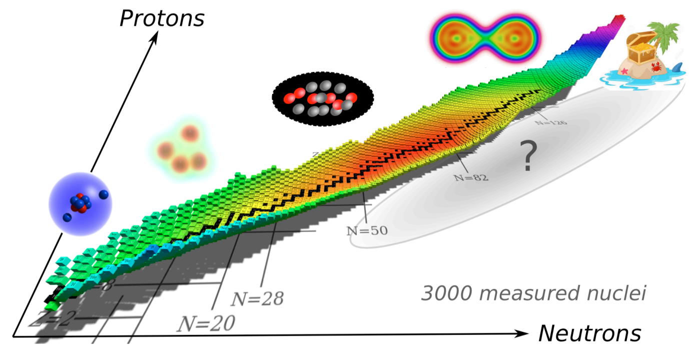
This motivates the search of disruptive techniques (high risk/high potential benefits)

An illustration with the nuclear Energy Density Functional theory

"Human guided" reduction of complexity using symmetry consideration







Machine learning: a different angle of attack

Progress of machine learning:

- Image classification:
  cancer detection, particle detection
- Generative AI:
  turbulence
- Inverse problems:
  cosmology
- Many body problem:
  spin systems, bosons

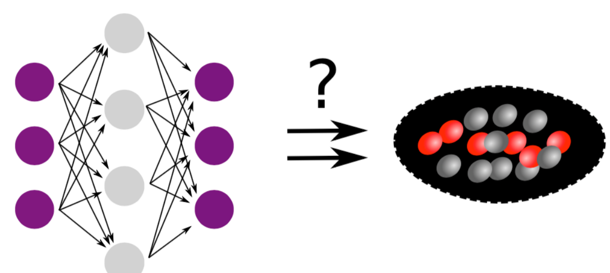
A review:

G. Carleo *et. al.*, arXiv:1903.10563 (2019)

In nuclear theory:

- Machine learning for experimental nuclear masses or radii tables
- Acceleration of EDF calculations

$\Longrightarrow$ A land of opportunities



Goals:
- Automatize the "theoretical production" process
- Reduces "significantly" the numerical cost
- Teach artificial intelligence (AI) to predict nuclear physics

Some literature...

Neural networks, Bayesian Neural Net., Gaussian Processes were used to fit:

Nuclear masses

- Athanassopoulos *et. al.* NPA 743 (2004)
  RMS = 950 keV
- Utama *et. al.* PRC 96 (2017)
- Utama *et. al.* PRC 97 (2018)
  RMS decreased by 40%
- Zhang *et. al.* J Phys. G (2017)

Drip-lines

- Neufcourt *et. al.* PRC 98 (2018)
- Neufcourt *et. al.* PRL 122 (2019)
- Niu *et. al.* PLB 778 (2018)
  Estimation of uncertainties

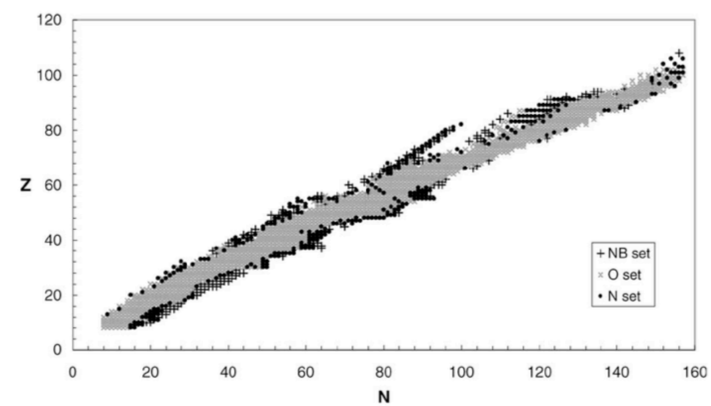
Neural networks used as a mean to IR extrapolate ($N_{oh} \to \infty$)

Nuclear radii

- Akkoyun *et. al.* J. Phys. G: NPP 40 (2013)
- Utama *et. al.* J. Phys. G: NPP 43 (2016)

Fission yields

- Lovell *et. al.* EPJ Web of Conf.(2019)
- Wang *et. al.* PRL 123 (2019)



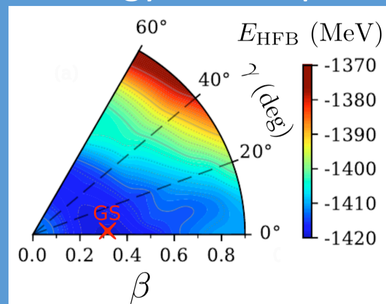
- Jiang *et. al.* PRC 100 (2019)
- Negoita *et. al.* PRC 99 (2019)

One recent illustration: prediction of masses, deformation and spectrum by neural network

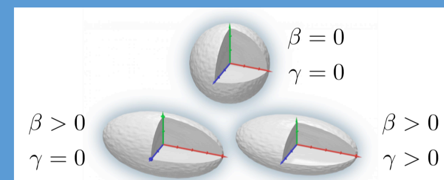
Conventional strategy

Select nucleus (N,Z)

Compute its HFB energy landscape



Map the energy Landscape onto a 5D Collective Hamiltonian

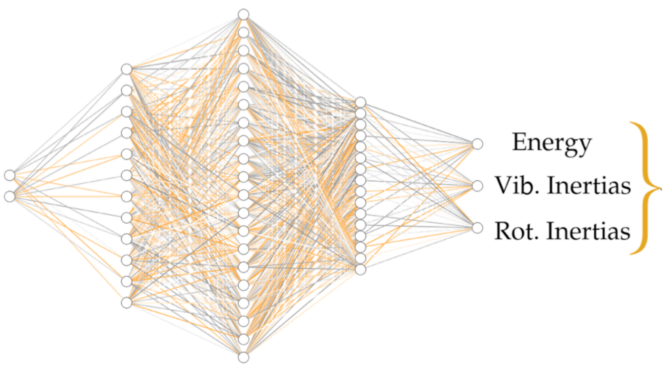


Deformations, Energy Spectrums, Transition amplitudes, …

Goal: replace the time-consuming part by a neural network

Network trained on a limited set of HFB datas

Select nucleus (N,Z)



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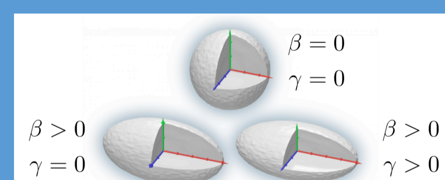

Deformations, Energy Spectrums, Transition amplitudes, …

Regnier, Lasseri, Ebran, Penon, arXiv:1910.04132

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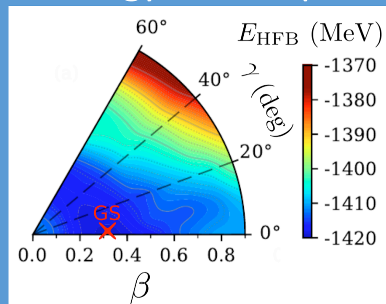

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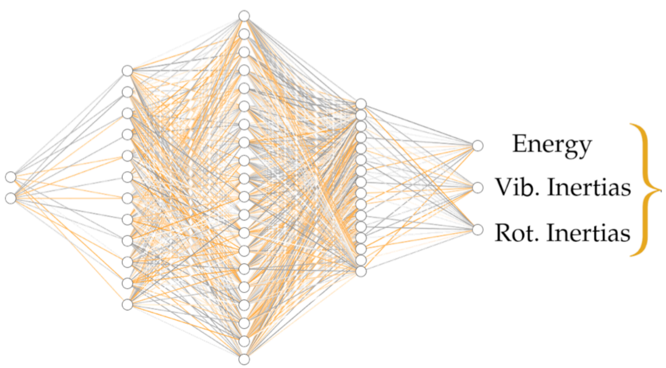

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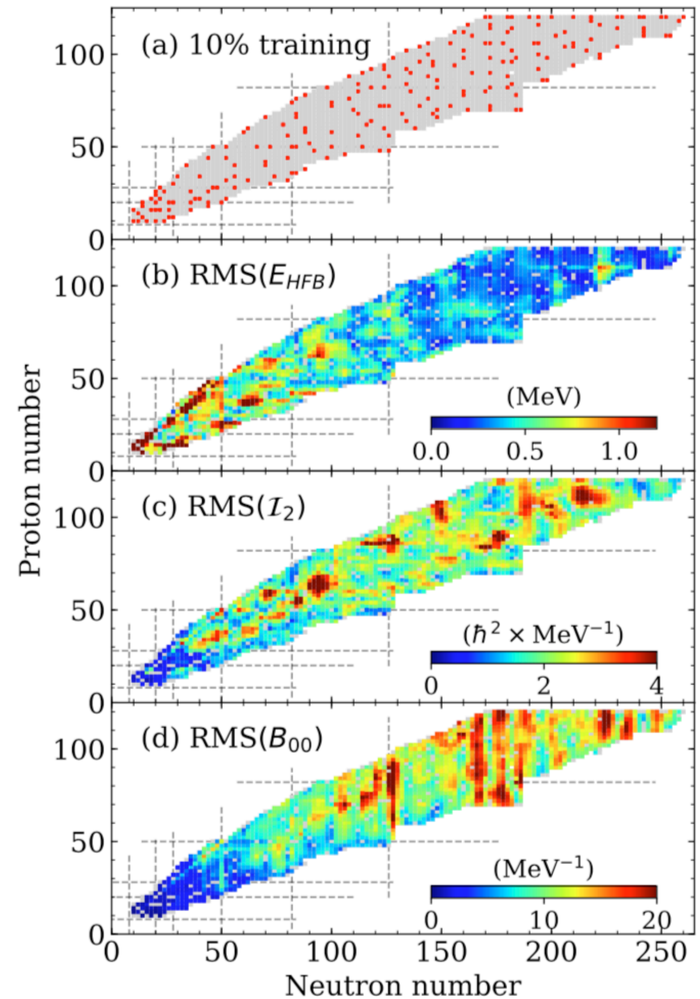
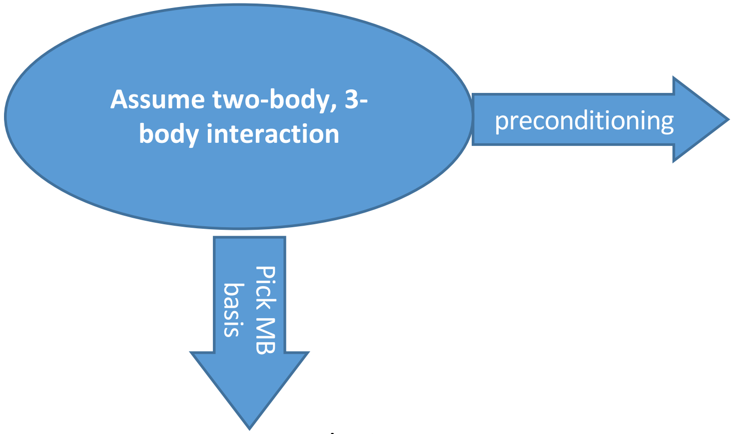
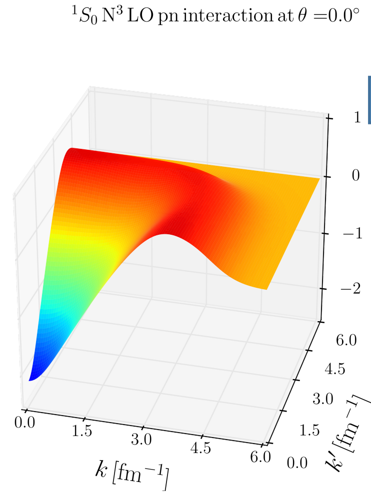


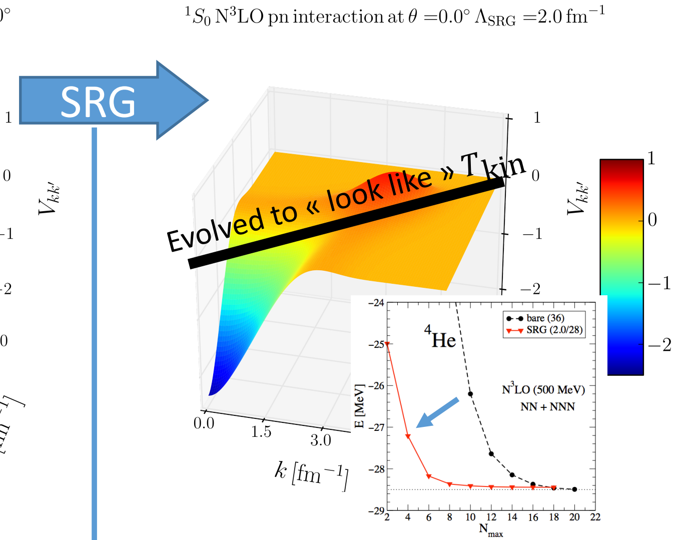
FIG. 2: (a) The AMEDEE database nuclei are plotted in grey as a function of N and Z. The red squares stand for nuclei included in the 10% training set obtained by the active learning. The panels (b),(c) and (d) display the resulting RMS per nucleus ($\mathcal{L}_t^{1/2}(N,Z)$) for the three outputs E_{HFB}, $\mathcal{I}_2$ and $\boldsymbol{B}_{00}$ respectively.

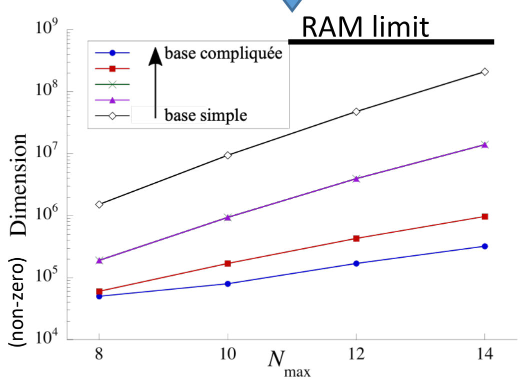
Regnier, Lasseri, Ebran, Penon, arXiv:1910.04132

Another potential use of AI: learning how to select Many-body states







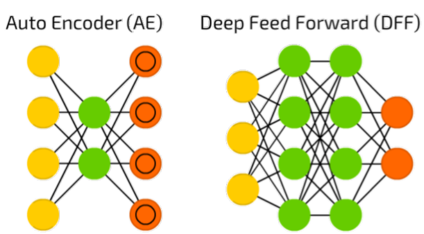


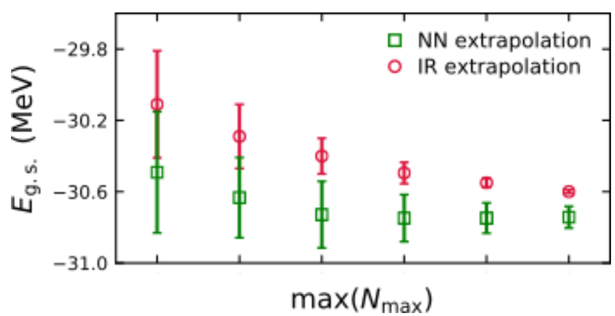
The goal is to overcome the limitation of our computing capabilities

Few ways can be followed:

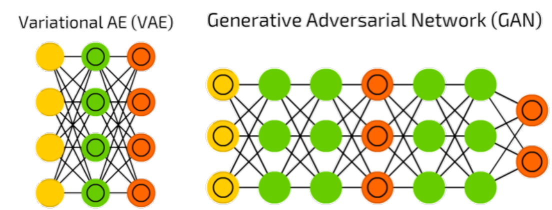
- ✓ Neural Networks used as a standard tool for extrapolation of the MB basis
- ▪ Neural Network as a classifier for un-converged computation of resonances
- ▪ Many-body ansatz based on Neural Network for fermionic species (✓bosons)

- ▪ High-dimensionality principal components analysis of Hamiltonian matrix





technology from picture manipulation to tailor SRG generator or phase-equivalent transformations

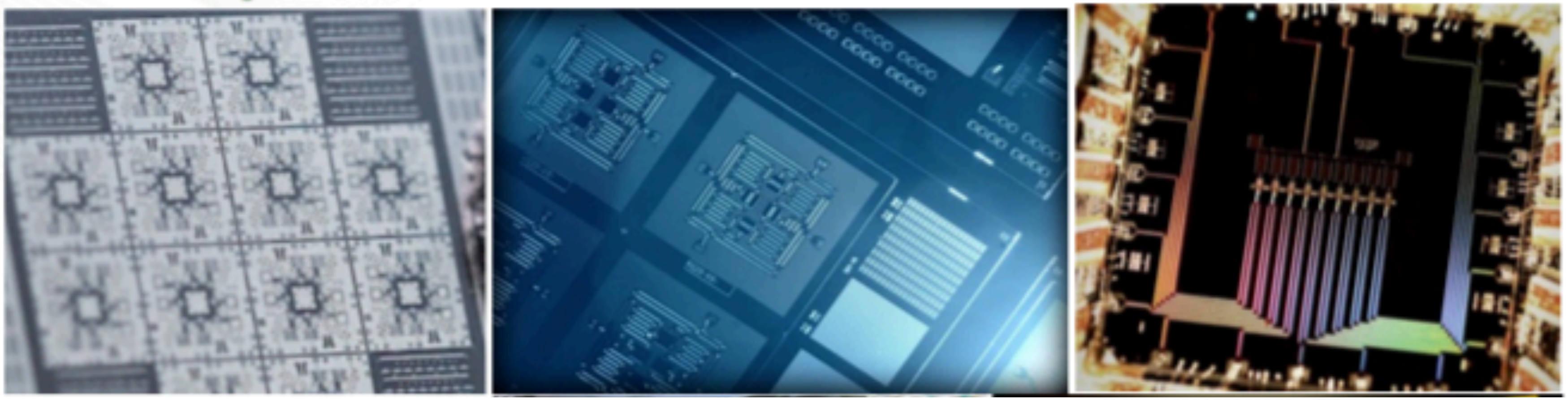


- Reduce induced interactions
- Preconditioning of MB problem

Propagate to MB (e.g. like IM-SRG) or Hamiltonian matrix generation for CI method

Entering into the Quantum Computing age

Rigetti IBM Google

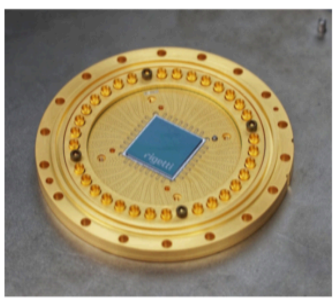


Limitations:
~ 50 qubits
~ 50 gates

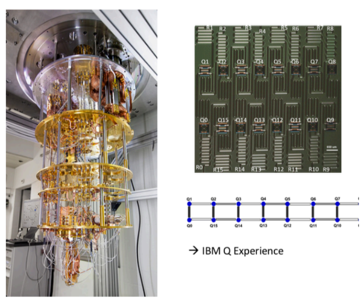
Future:
~ 500 qubits
~ 500 gates

Example

RIGETTI superconducting 19 Qubit



IBM QX5 (16 qubits)

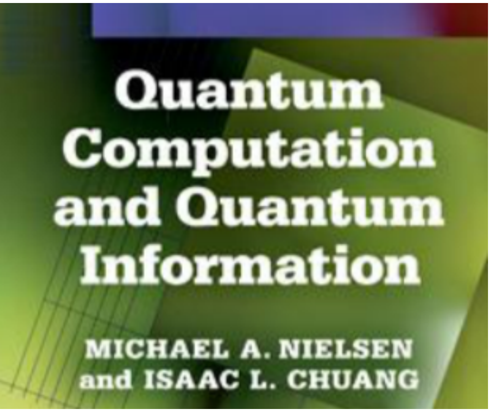


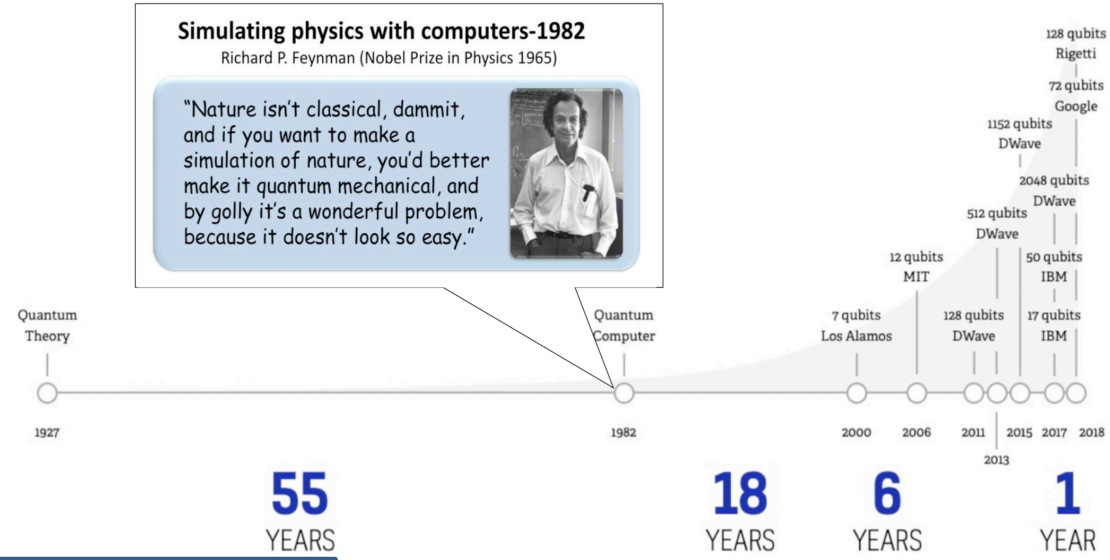
A timely period

(from G. Hagen)

There is a lot of excitement in this field due to substantial progress

1. Quantum processing units now have ten(s) of qubits
2. Businesses are driving this: Google, IBM, Microsoft, Rigetti, D-Wave, …
3. Software is publicly available (PyQuil, XACC, OpenQASM, OpenFermion)
4. First real-world problems solved: H_2 molecule on two qubits [O'Malley et al., Phys. Rev. X 6, 031007 (2016)]; BeH_2 on six qubits [Kalandar et al., Nature 549, 242 (2017)]; …





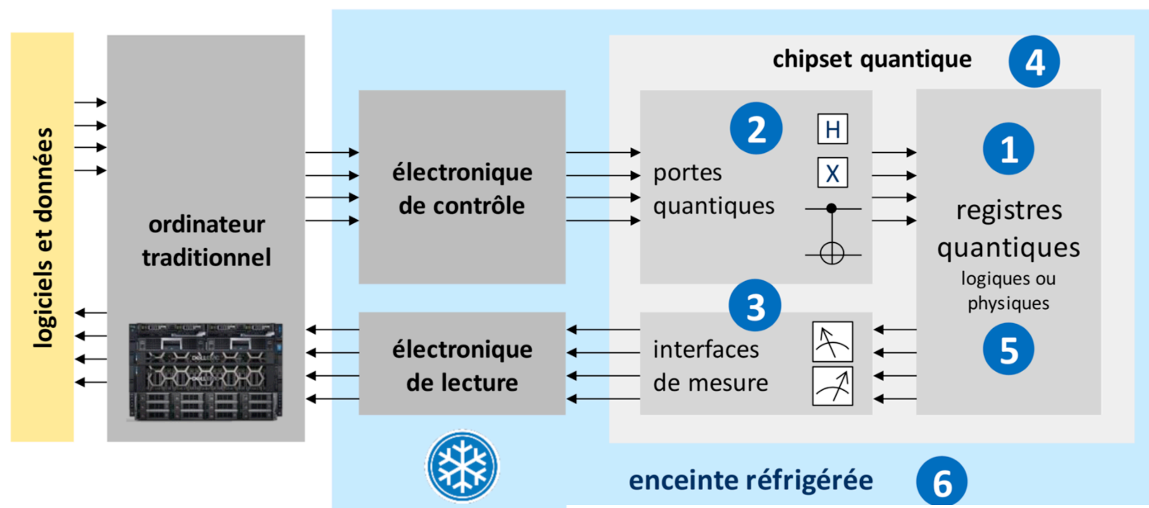
Where we are now ?

We are at the NISQ (Noisy Intermediate-Scale Quantum) era. Quantum computers can be used but they are stable for very short time (noise, decoherence, …). Only short QC circuits can be run.

When is beyond the NISQ era?

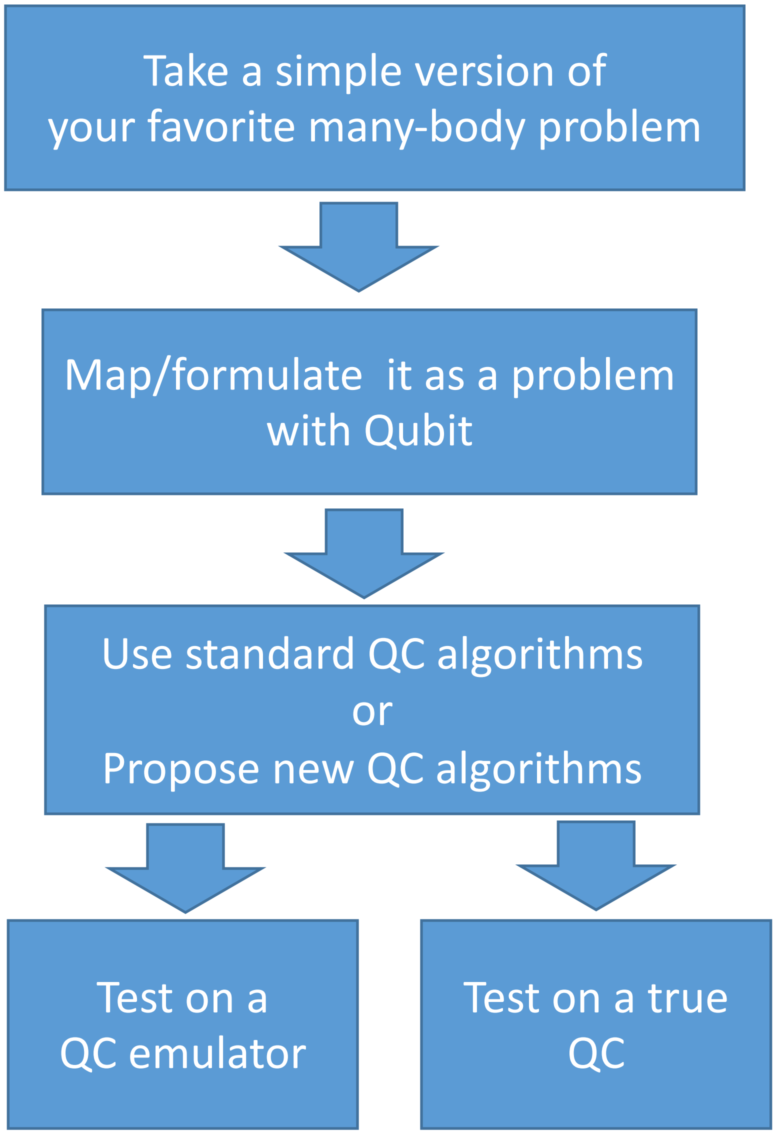
International context

The QC/QIS scientific community

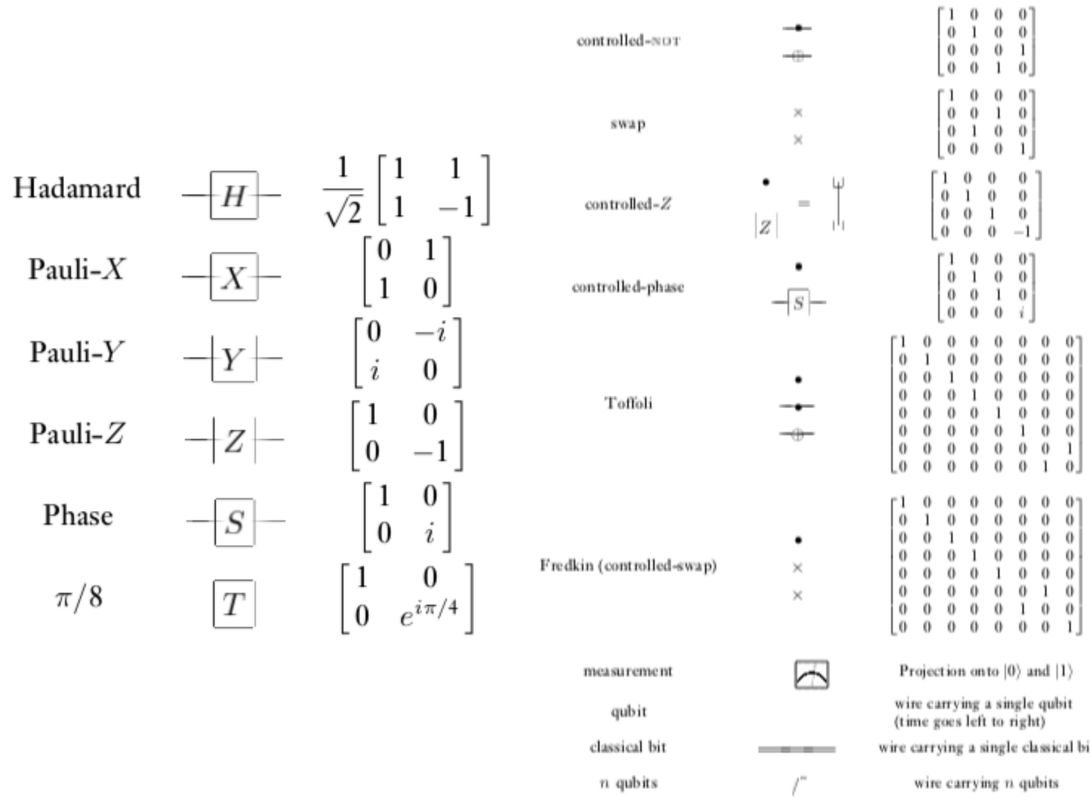


Comprendre Informatique Quantique Olivier Ezratty.pdf

Strategy



Constraint: -Work with a restricted number of operation



-Design new algorithms adapted to the many-body problem

-Control the inherent quantum noise

Illustration I

Strategy

Take a simple version of your favorite many-body problem

↓

Map/formulate it as a problem with Qubit

↓

Use standard QC algorithms
or
Propose new QC algorithms

↓ ↓

Test on a QC emulator | Test on a true QC

PHYSICAL REVIEW LETTERS **120**, 210501 (2018)

Editors' Suggestion Featured in Physics

Cloud Quantum Computing of an Atomic Nucleus

E. F. Dumitrescu,[1] A. J. McCaskey,[2] G. Hagen,[3,4] G. R. Jansen,[5,3] T. D. Morris,[4,3] T. Papenbrock,[4,3,*] R. C. Pooser,[1,4] D. J. Dean,[3] and P. Lougovski[1,†]

Schematic deuteron Hamiltonian in Harmonic basis

$$H_N = \sum_{n,n'=0}^{N-1} \langle n'|(T+V)|n\rangle a_{n'}^\dagger a_n.$$

$$n, n' = 0, 1, \ldots N-1$$

$a_n^\dagger (a_n)$ create (annih.) 1 deuteron in $|n\rangle$

Use Pauli matrices+Jordan-Wigner transformation

$$a_n^\dagger \rightarrow \frac{1}{2}\left[\prod_{j=0}^{n-1} -Z_j\right](X_n - iY_n)$$

0 (1) particles in $|n\rangle \rightarrow |\uparrow\rangle (|\downarrow\rangle)$

→ This automatically map the Hamiltonian as a function of Pauli Matrix

→ Use the VQE quantum-classical algorithm with 10000 measurements on QX5 (19Q)

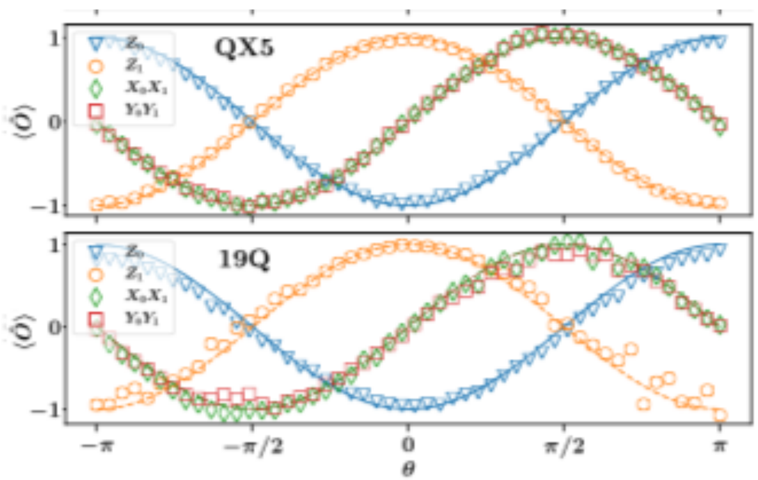


Illustration II

PHYSICAL REVIEW LETTERS 123, 090501 (2019)

Strategy

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↓

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σ Models on Quantum Computers

Andrei Alexandru,[1,2,*] Paulo F. Bedaque,[2,†] Henry Lamm,[2,‡] and Scott Lawrence[2,§]

(NuQS Collaboration)

Start with the discretized σ model

$$\mathcal{H} = \sum_r \left(\frac{g^2}{2} \boldsymbol{\pi}(r)^2 + \frac{1}{2g^2 \Delta x^2} [\mathbf{n}(r+1) - \mathbf{n}(r)]^2 \right)$$

Map it to a Spin algebra (fuzzy sphere)

$$-\frac{g^2}{2} \nabla^2 \psi \to H^0 \Psi = \kappa \frac{g^2}{2} \sum_{k=1}^{3} [\mathbb{J}_k, [\mathbb{J}_k, \Psi]],$$

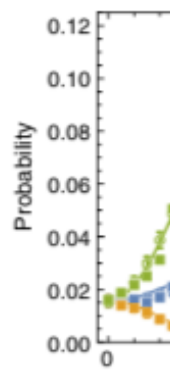
J_k are generators of the SU(2) algebra

"only" j=1/2 was considered

$$j_1 = \mathbb{1} \otimes \sigma_2 / \sqrt{3}, \quad j_2 = \sigma_2 \otimes \sigma_3 / \sqrt{3}, \quad j_3 = \sigma_2 \otimes \sigma_1 / \sqrt{3},$$

This gives the link with Pauli matrices

→ Use the Suzuk
+ specific QC



GAUGE THEORIES FOR QUANTUM COMPUTING

Very limited studies exist, e.g.:

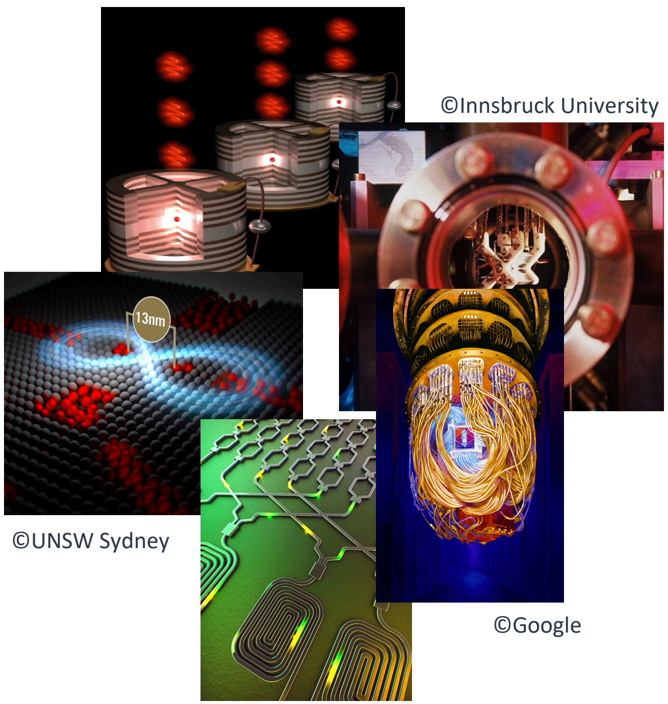
- 1+1 D QED (Schwinger model) on a few-qubit trapped-ion quantum computer [E. A. Martinez et al., Nature 534 (2016) 516, arXiv: 1605.04570]
- Quantum-Classical calculation of Schwinger Model [N. Klco et al., Phys. Rev. A 98 (2018) 032331, arXiv:1803.03326]
- U(1) lattice gauge theory without matter in 2 & 3 spatial dimensions [D. Kaplan, J. Stryker, arXiv:1806.08797]
- Zeta-regularized vacuum expectation values [T. Hartung, K. Jansen, arXiv:1808.06784]
- O(3) nonlinear sigma model in 1+1 dimensions [F. Bruckmann, K. Jansen, S. Kuhn, arXiv:1812.00944]

Extending the studies to 2+1 dimensions is extremely hard and has not been established yet on quantum devices

(from M. constantinou, Santa Fe)

Summary

- A.I. is an existing widely used technology
- Can potentially boost the nuclear theory field.
- Possible impact: guiding exp. on where are the relevant information



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- Quantum computing is a high risk/high benefit interdisciplinary field
- It might lead to unprecedented boost in theory (see emerging US program)
- It leads to natural link between public research and private companies (IBM, Google, …)
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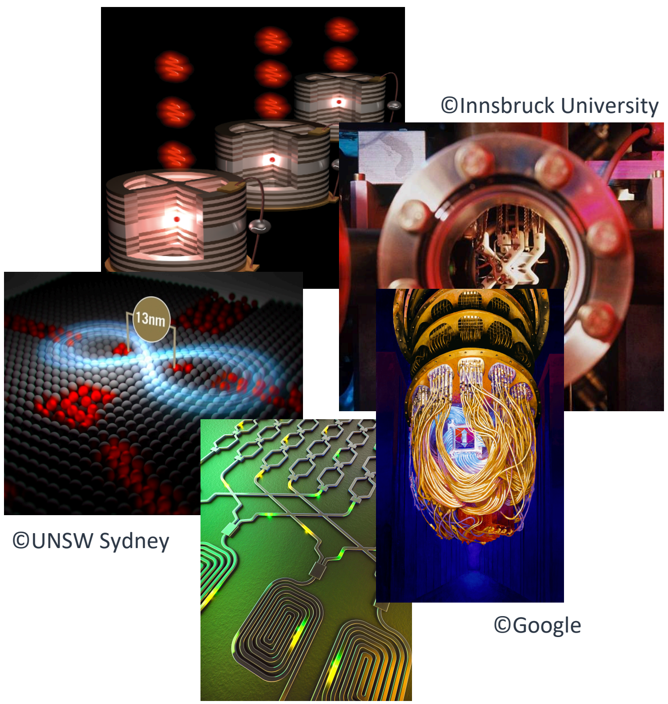
- Emerging QC programs in France

- A.I. is an existing widely used technology
- Can potentially boost the nuclear theory field.
- Possible impact: guiding exp. on where are the relevant information

Synergy between CNRS, CEA, CEA-DAM



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Synergy:

Impulse [Phynet team in IJCLab Orsay]

In IN2P3 – First workshop in Orsay (~70 participants, physicists, engineers and computer scientists)