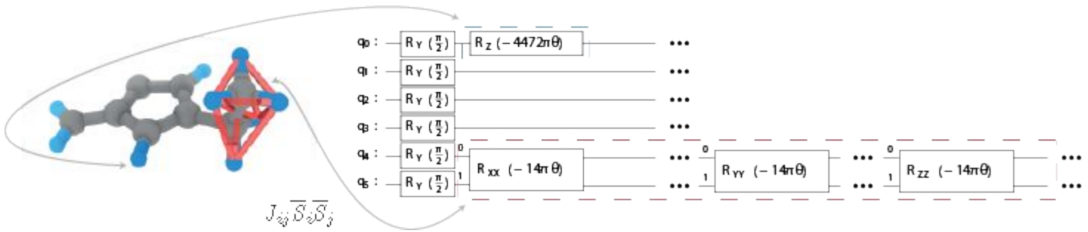
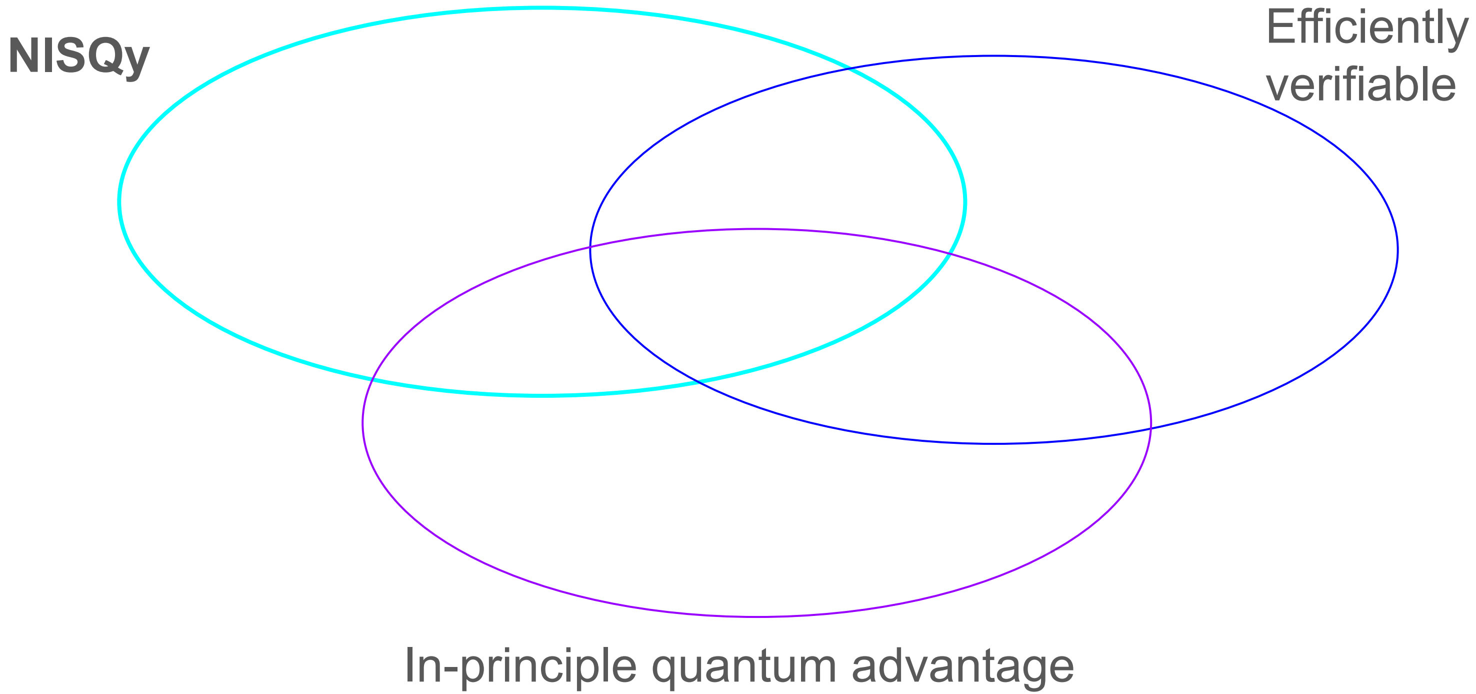
MatterDecoder: Towards quantum utility with life science use cases



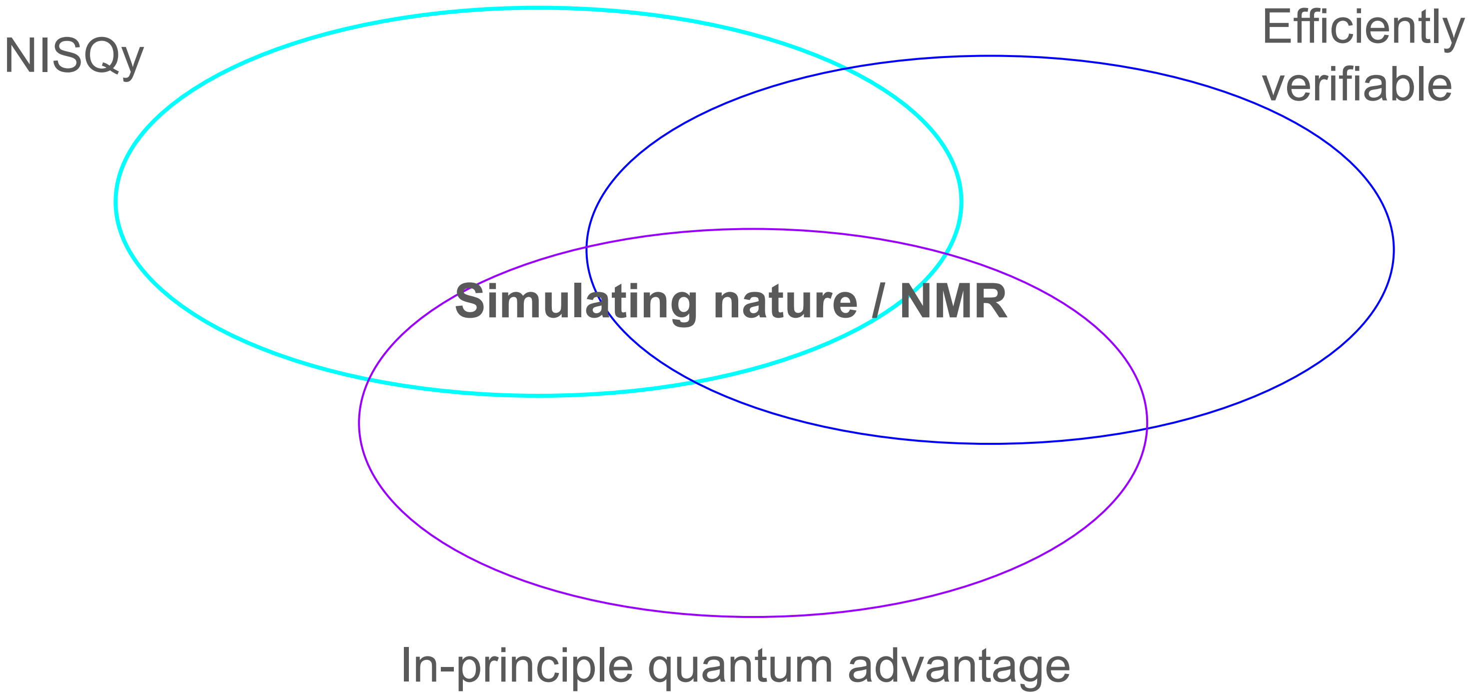
Prof. Dr. Clément Javerzac-Galy
University of Applied Sciences NW Switzerland (FHNW) // MatterDecoder
clement.javerzac@fhnw.ch

Towards quantum utility



cf. Scott Aaronson
Kim, Y., Eddins, A., Anand, S. et al. Evidence for the utility of quantum computing before fault tolerance. Nature 618, 500–505 (2023)

Towards quantum utility



cf. Scott Aaronson
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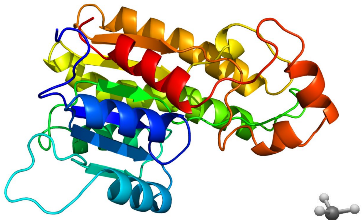
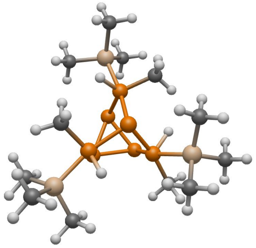
NMR* is a very powerful tool

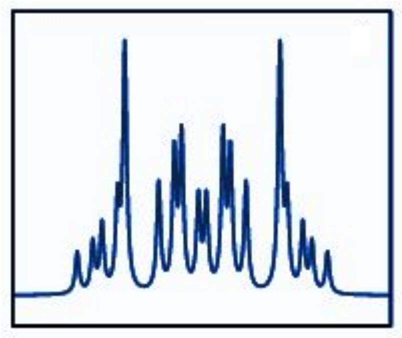
*Nuclear magnetic resonance

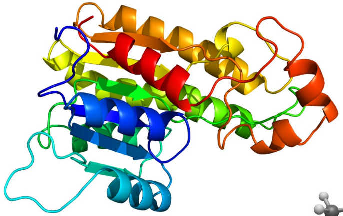


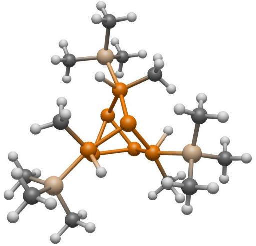


NMR is one of the most powerful methods providing atomic-level information of molecules. It can study molecules **in solution**, mimicking their native behavior in organisms, or **in solid state** form.

NMR is a very powerful tool

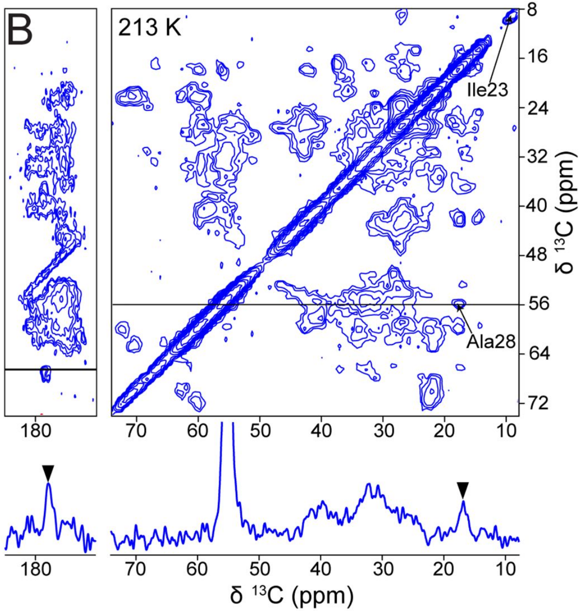




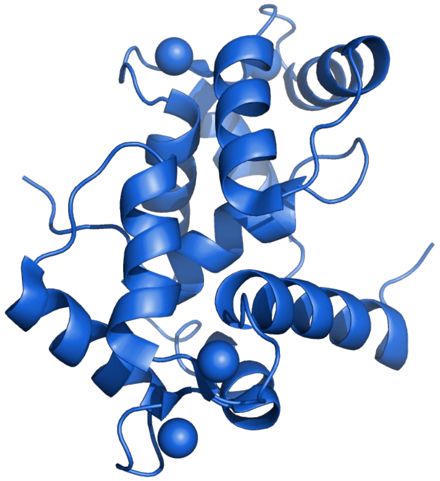


NMR is one of the most powerful methods providing atomic-level information of molecules. It can study molecules in solution, mimicking their native behavior in organisms, or in solid state form. However, spectra can be challenging to interpret, especially for large molecules & complex mixtures, with highly correlated, overlapping signals and solvent effects. It is a **labor-intensive process** that done by highly-trained personnel. There is **no fast and automated deciphering solution** that requires no human intervention, thus severely limiting the usefulness of NMR.

NMR spectra are hard to interpret

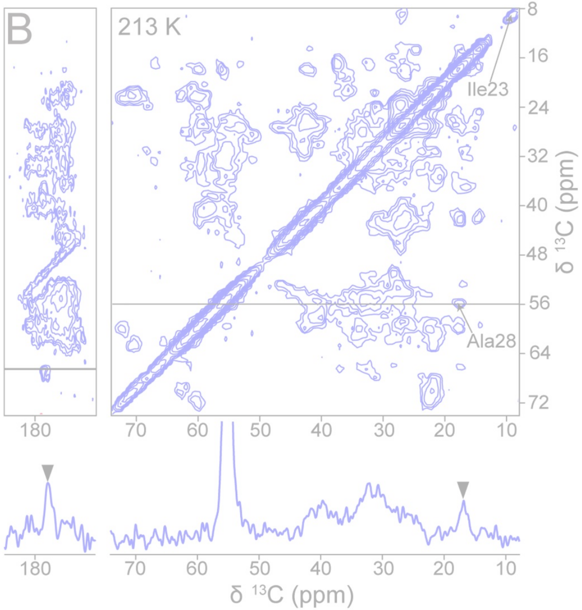


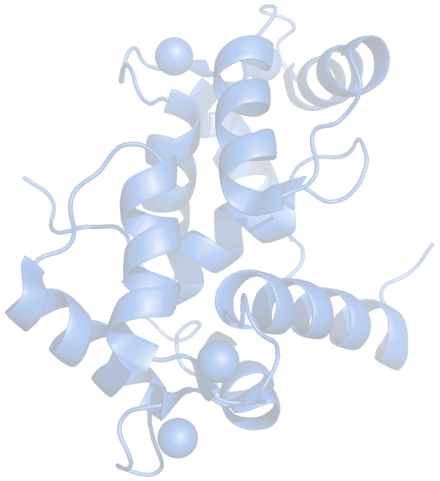
ill-posed inverse problem



From spectroscopic data to molecular structure

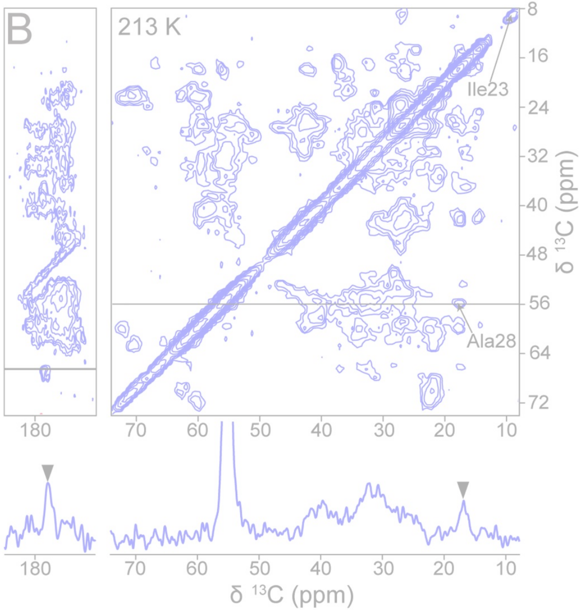
NMR spectra are hard to interpret

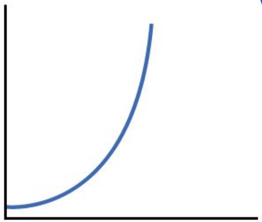


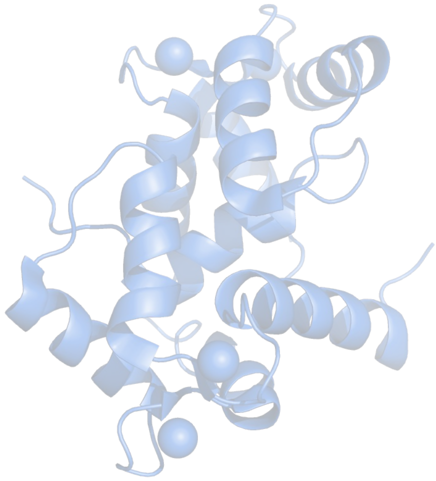


$$H_Z^r = \sum_{k=1}^{N} \omega_k I_k^Z + 2\pi \sum_{k<l} J_{kl} \bar{I}_k \bar{I}_l$$

NMR spectra are hard to interpret







$$H_Z^r = \sum_{k=1}^{N} \omega_k I_k^Z + 2\pi \sum_{k<l} J_{kl} \bar{I}_k \bar{I}_l$$

(Nuclear) spin dynamics simulation

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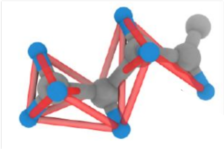
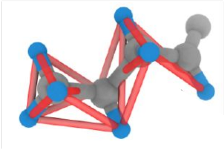
(Nuclear) spin dynamics simulation

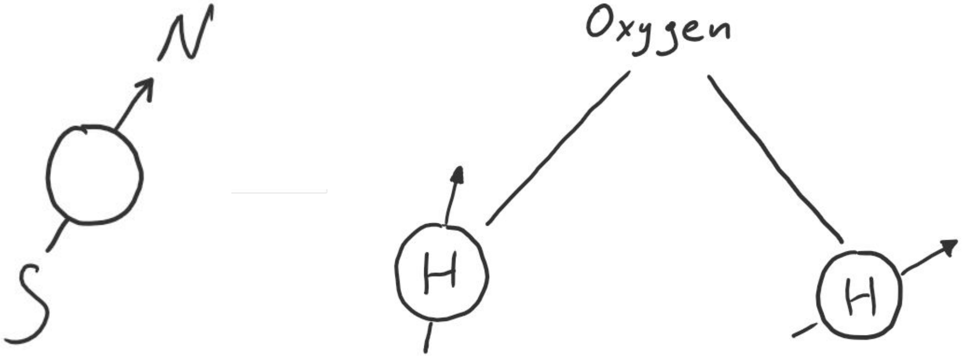
a



(Nuclear) spin dynamics simulation

a

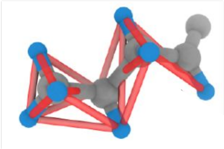


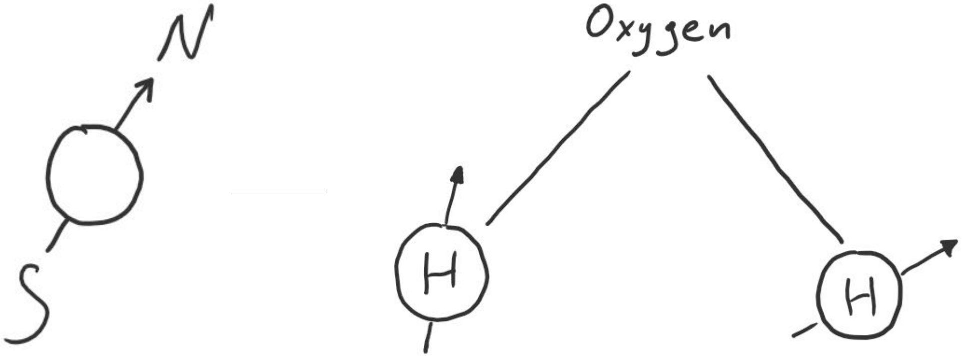


- Interact with magnetic fields
- Interact with one another

(Nuclear) spin dynamics simulation

a





- Interact with magnetic fields
- Interact with one another

$$H_Z^r = \sum_{k=1}^{N} \omega_k I_k^Z + 2\pi \sum_{k<l} J_{kl} \bar{I}_k \bar{I}_l$$

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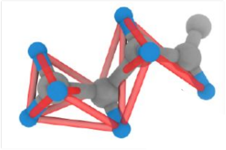
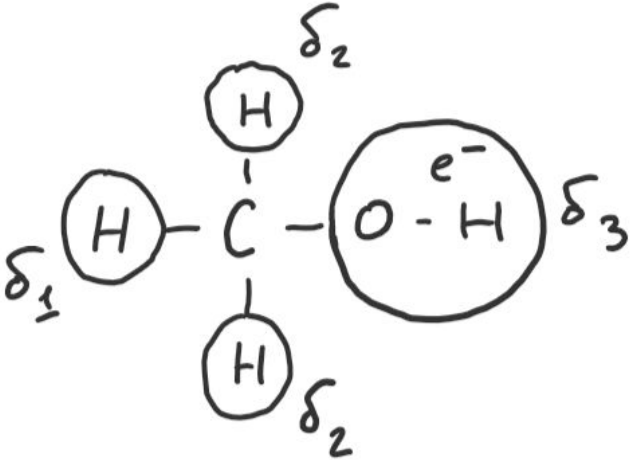
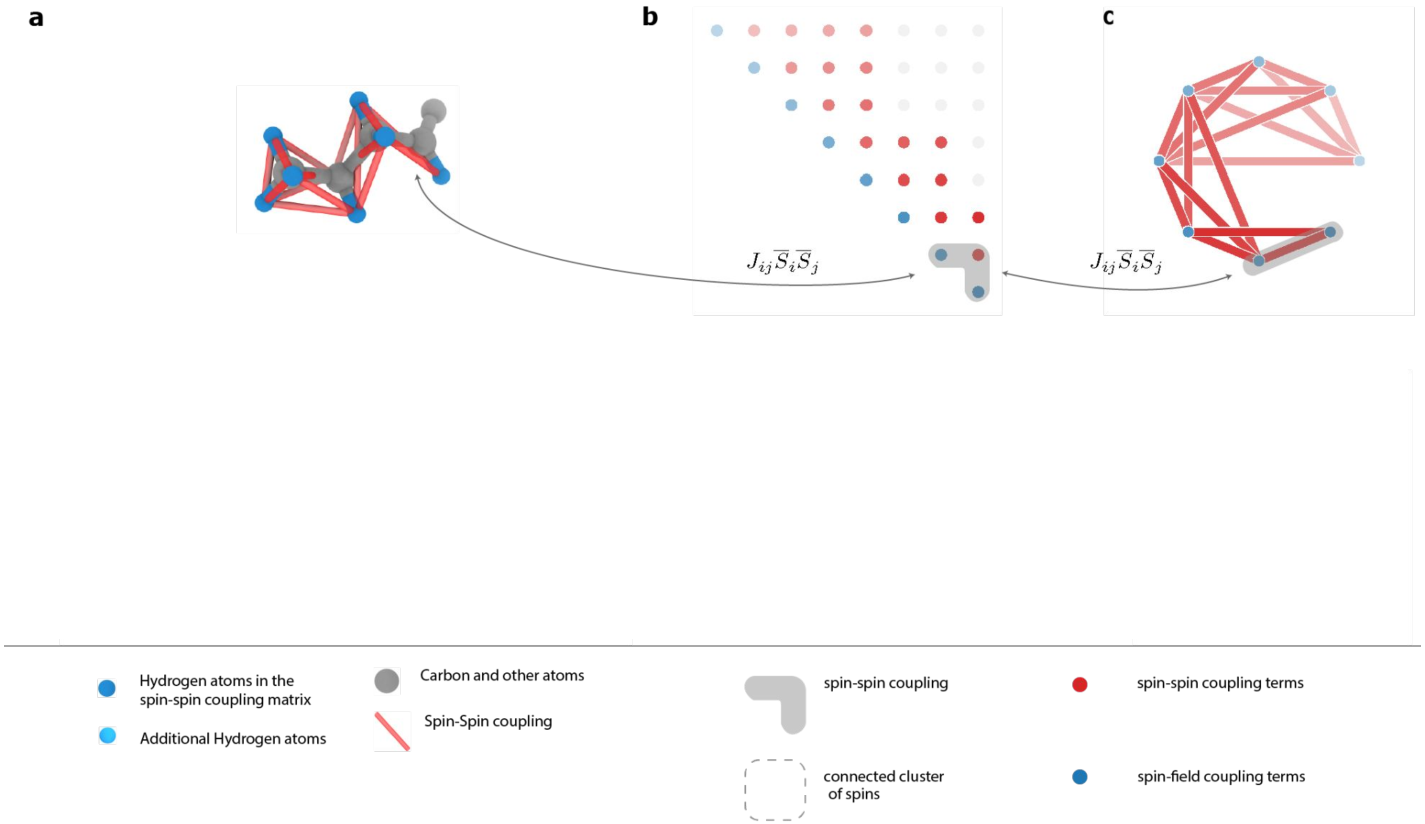


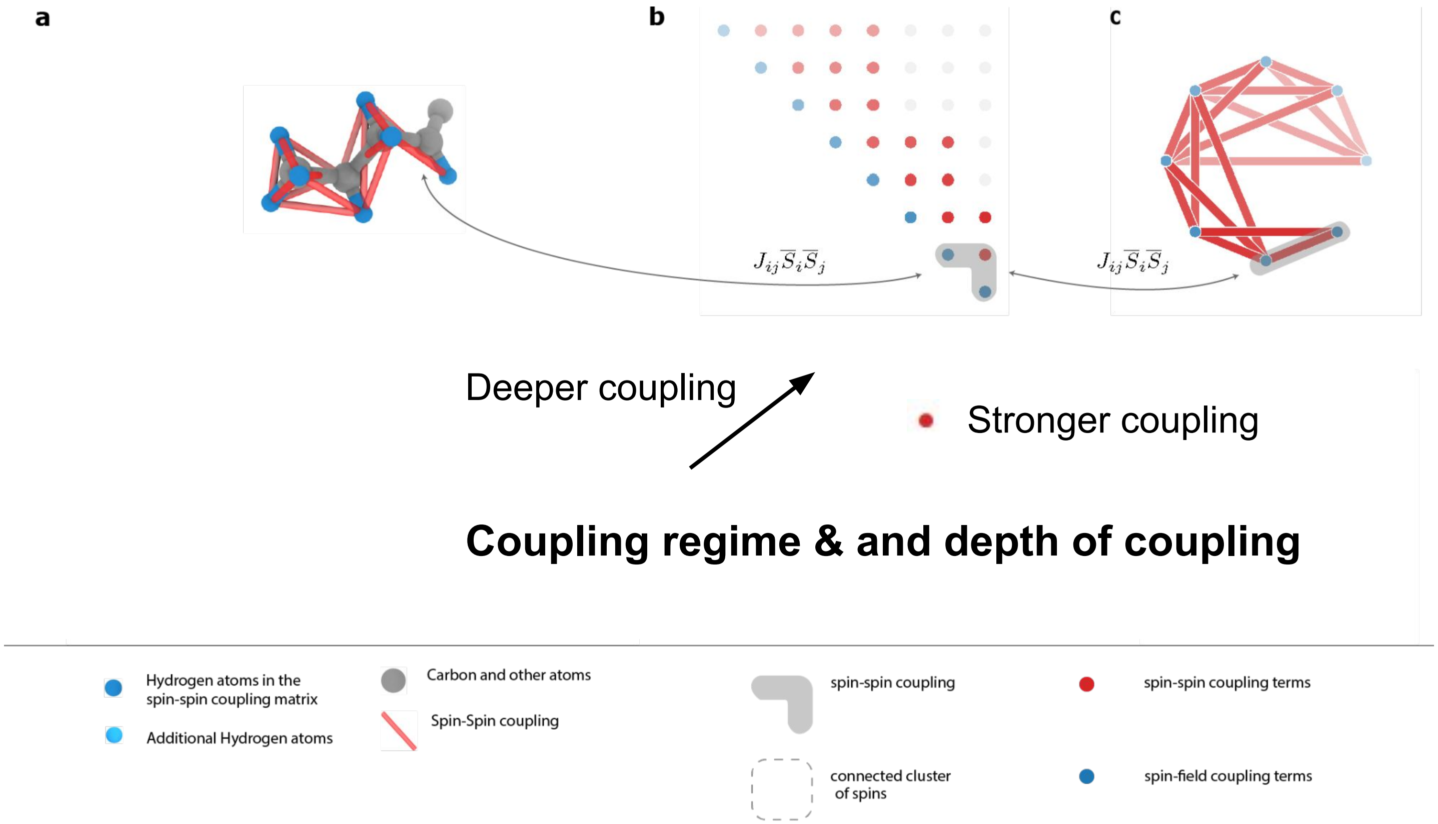


- Nuclear spins are shielded from B
- Unique electronic structures serve as "fingerprints" of molecules

(Nuclear) spin dynamics simulation

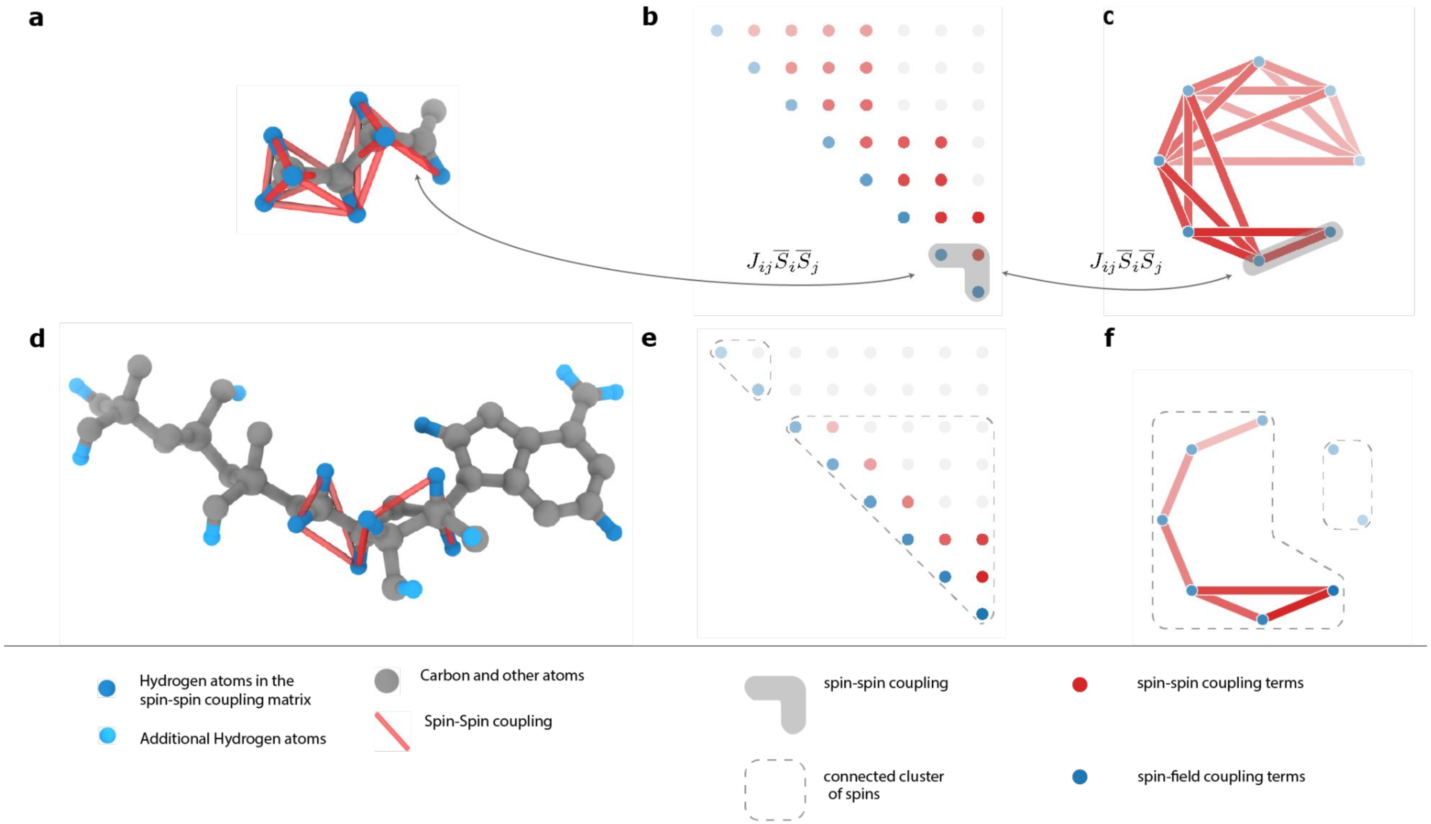


(Nuclear) spin dynamics simulation



Coupling regime & and depth of coupling

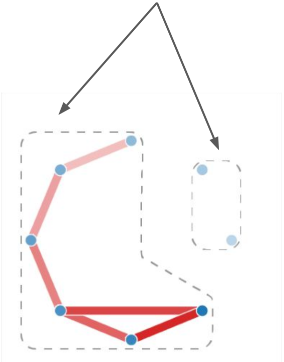
(Nuclear) spin dynamics simulation



(Nuclear) spin dynamics simulation

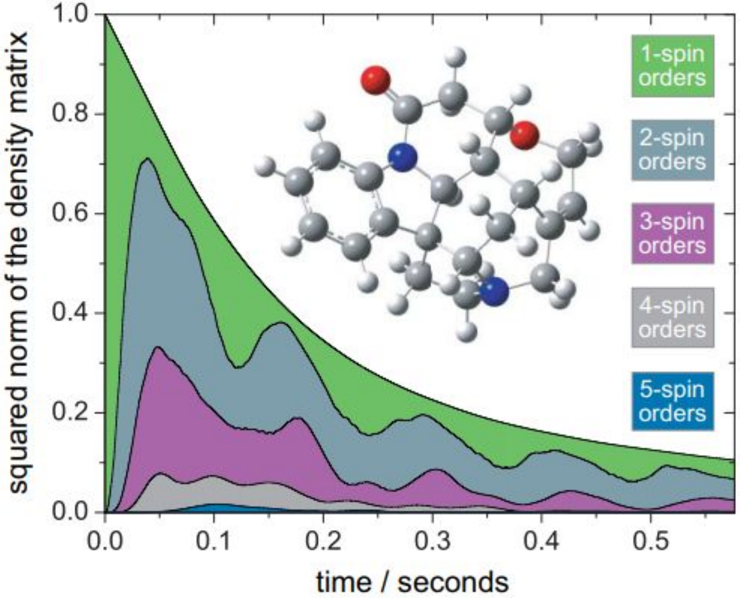
Clusters

Small weakly coupled systems



(Nuclear) spin dynamics simulation

Reducing complexity to polynomial scaling (**for liquid state NMR**).



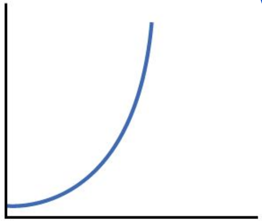
Classically tractable

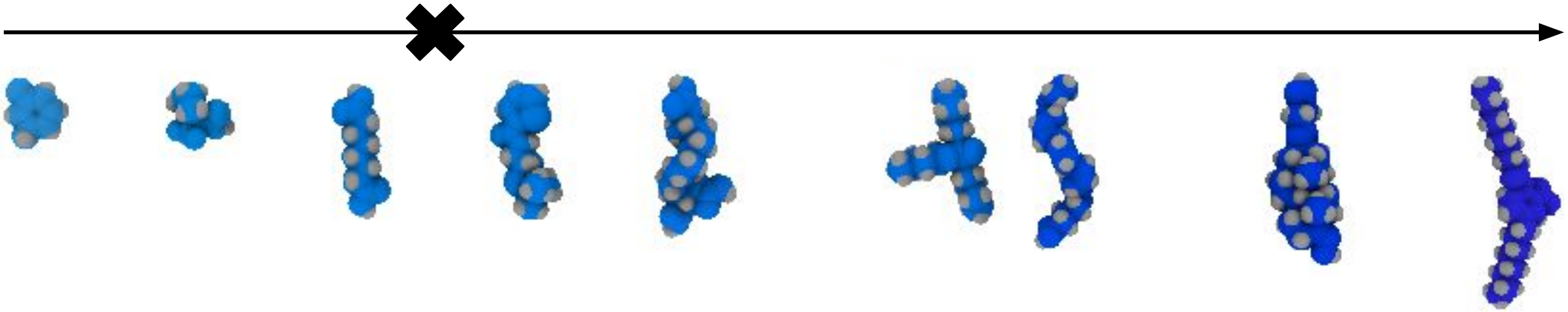
Polynomially scaling spin dynamics simulation algorithm based on adaptive state-space restriction (2007, Kuprov)

Hard (Nuclear) spin dynamics simulation

Hard / classically intractable simulations:

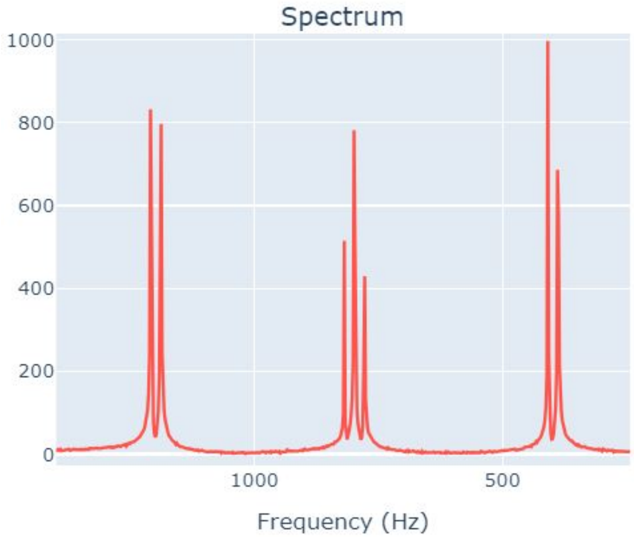
- For large clusters
- Strong coupling
- Weak field
- etc



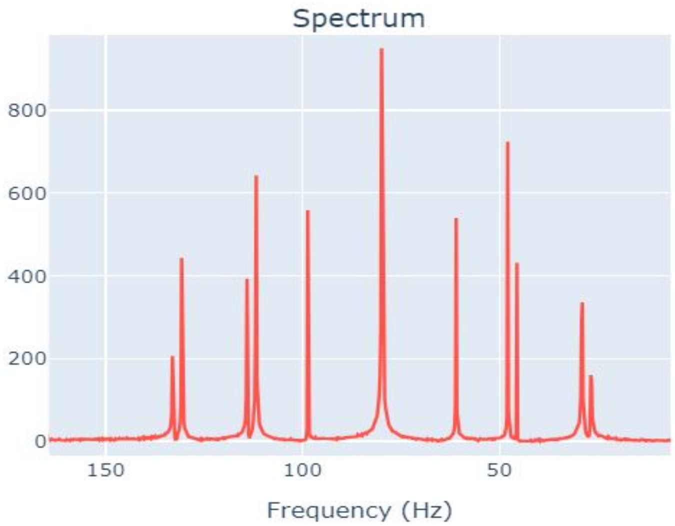


Hard (Nuclear) spin dynamics simulation

e.g. low field NMR



Field B = 400MHz

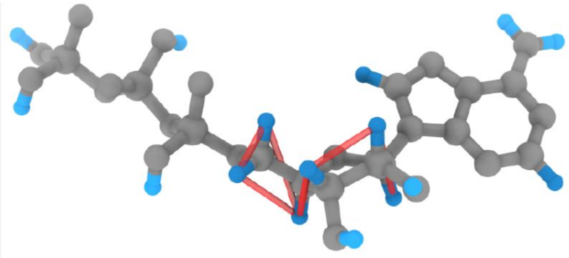


Field B = 40MHz

Hard (Nuclear) spin dynamics simulation

From semi-classical to **quantum mechanical treatment**

A native quantum problem



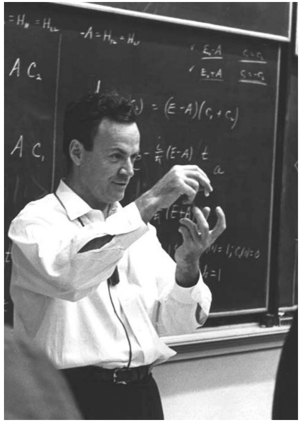
Simulating Physics with Computers

Richard P. Feynman

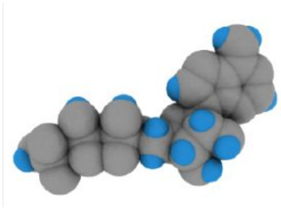
Department of Physics, California Institute of Technology, Pasadena, California 91107

Received May 7, 1981

needed. I don't know, maybe physics is absolutely OK the way it is. The program that Fredkin is always pushing, about trying to find a computer simulation of physics, seem to me to be an excellent program to follow out. He and I have had wonderful, intense, and interminable arguments, and my argument is always that the real use of it would be with quantum mechanics, and therefore full attention and acceptance of the quantum mechanical phenomena—the challenge of explaining quantum mechanical phenomena —has to be put into the argument, and therefore these phenomena have to be understood very well in analyzing the situation. And I'm not happy with all the analyses that go with just the classical theory, because nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy. Thank you.

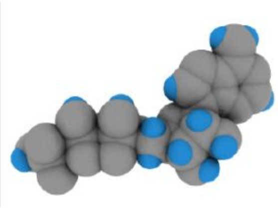


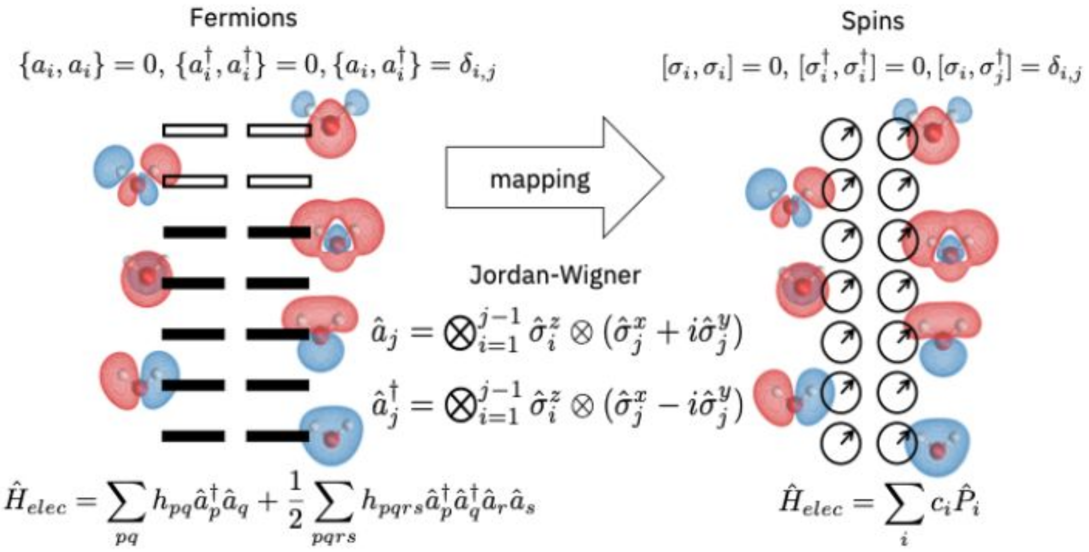
A native quantum problem



A native quantum problem

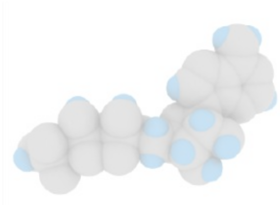
Like electronic structures?

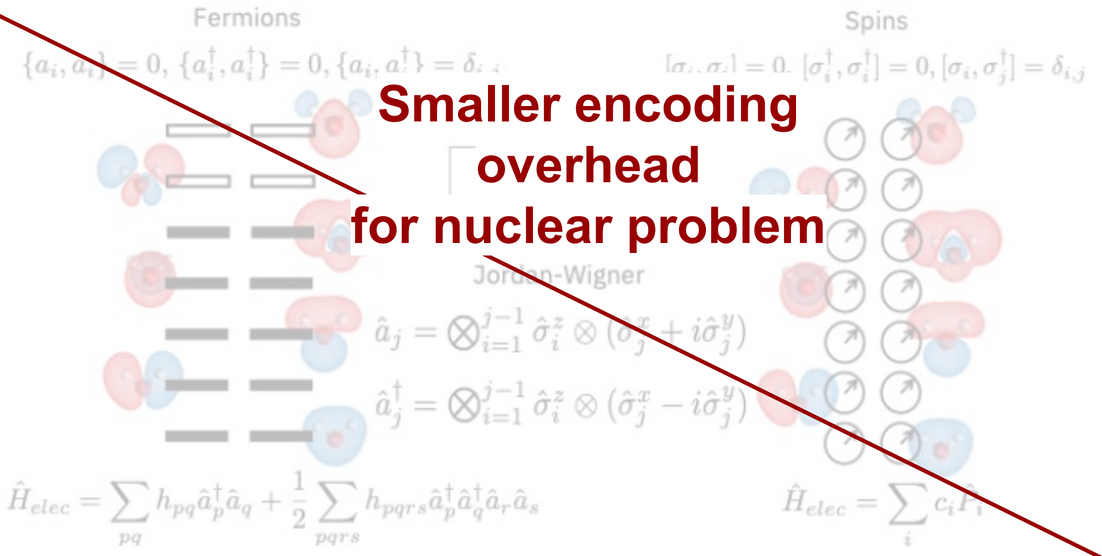




A native quantum problem

Like electronic structures?





Smaller encoding overhead for nuclear problem

A native quantum problem - Hamiltonian Simulation.

The nuclear problem:

$$H_Z^r = \sum_{k=1}^{N} \omega_k I_k^Z + 2\pi \sum_{k<l} J_{kl} \overline{I}_k \overline{I}_l$$

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar} H t} |\psi(0)\rangle$$

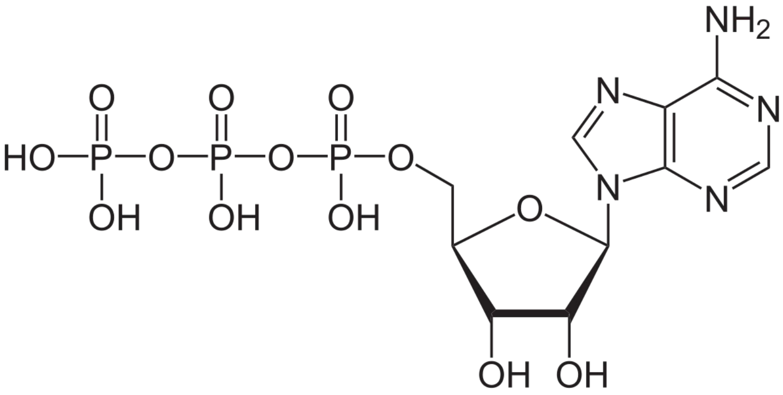
$$H_n = \underbrace{\begin{pmatrix} H_{11} & H_{12} & \cdots & H_{1,2^n} \\ H_{21} & H_{22} & \cdots & H_{2,2^n} \\ \vdots & \vdots & \ddots & \vdots \\ H_{2^n,1} & H_{2^n,2} & \cdots & H_{2^n,2^n} \end{pmatrix}}_{\substack{\text{rows: } 2^n \\ \text{columns: } 2^n}}$$

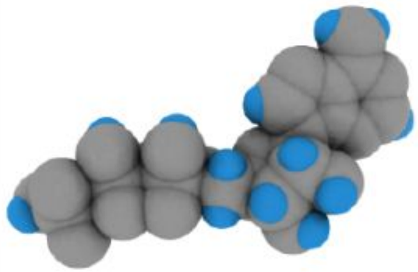
Complexity:
cannot be stored, but
the circuits can

e.g. Adenosine triphosphate (ATP)

A *8 active spins* system (1H NMR, *liquid state*)

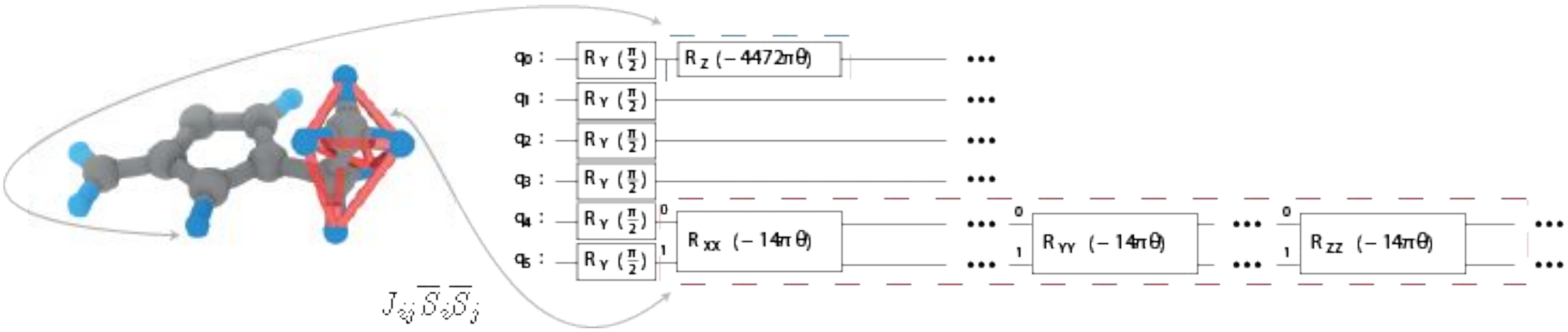
Found in all known forms of life, it is often referred to as the "molecular unit of currency" of intracellular energy transfer.





e.g. Adenosine triphosphate (ATP)

Ex. of transpiled circuit:



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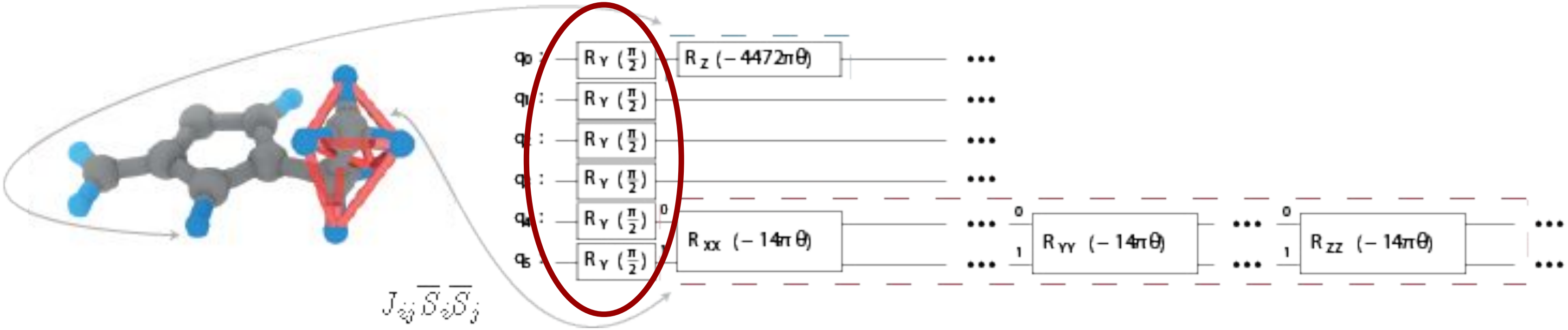
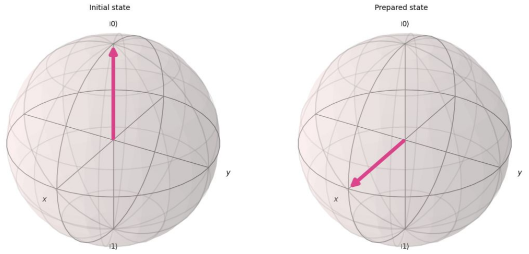


Simple state preparation (*no density matrix here*)



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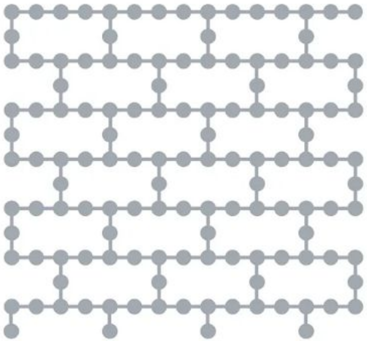


A major milestone in system performance:

Eagle R3

Mean T1 = 269 us
Mean ECR gate time = **537 ns**

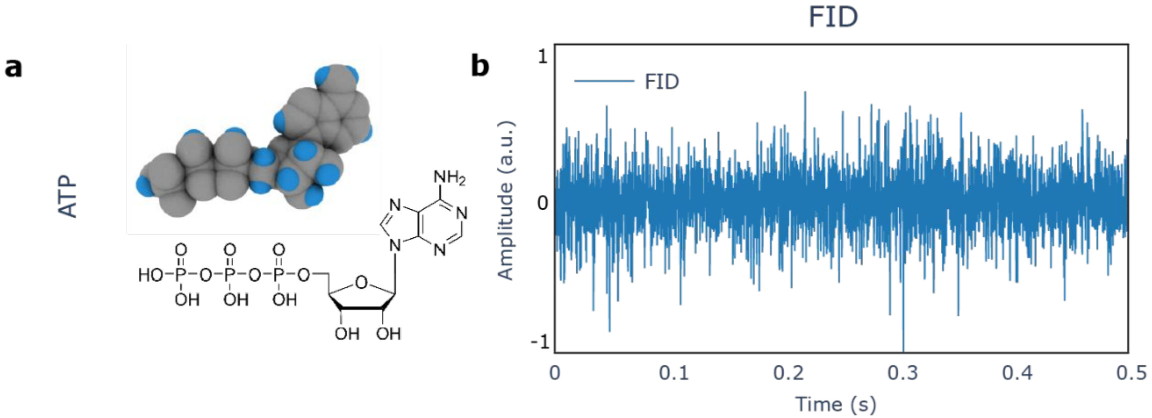
~ 500 gates in T1 time

127-qubits chip IBM

QuantumBasel
Center of Competence for Quantum and Artificial Intelligence

e.g. Adenosine triphosphate (ATP)

Free Induction Decay (FID) on QPU: first time high-field



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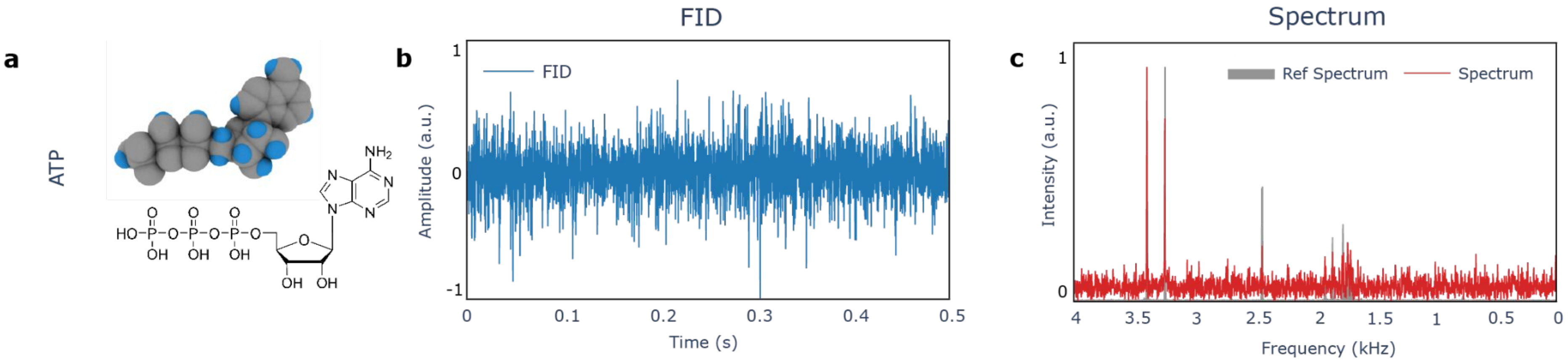
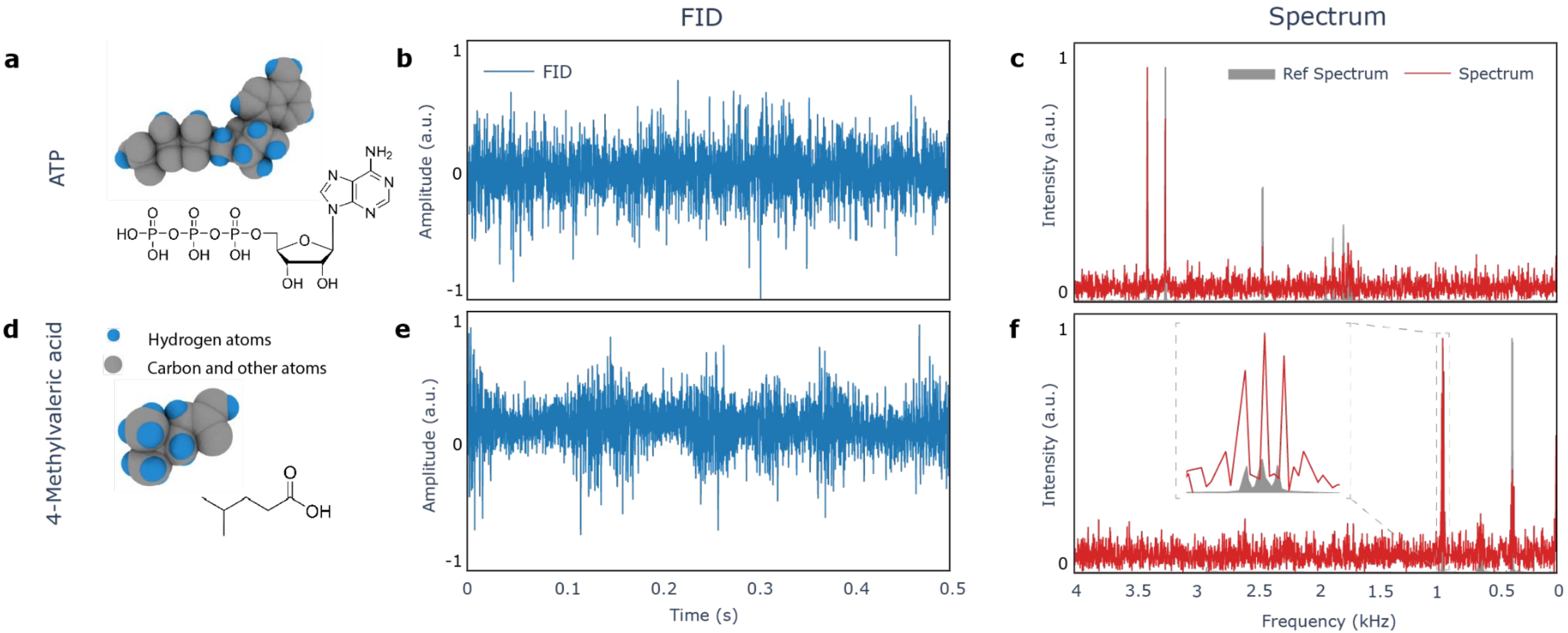
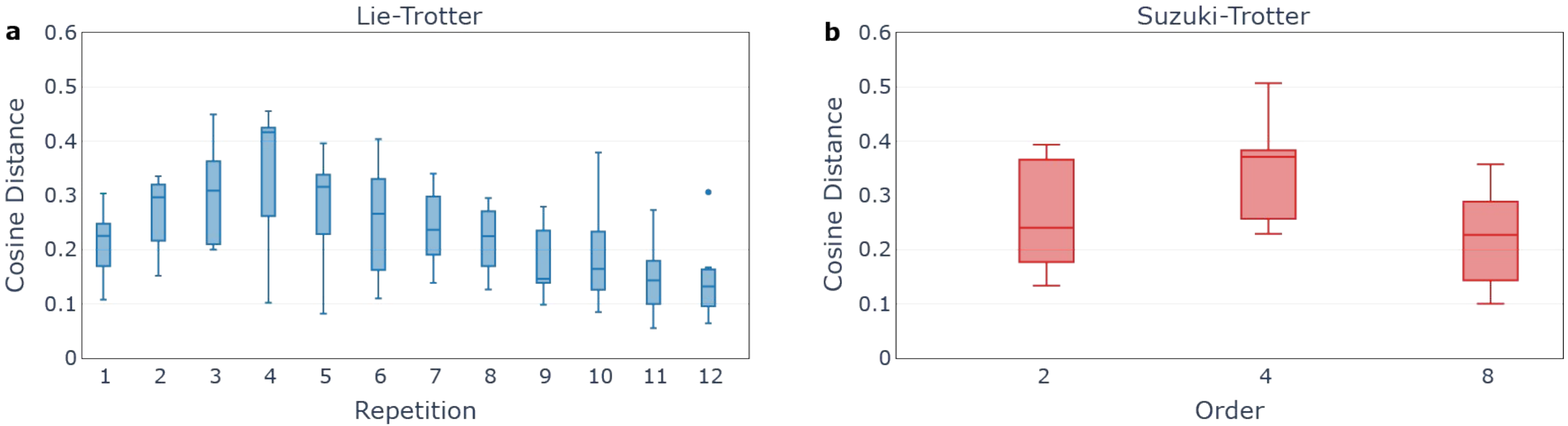


e.g. benchmarked with experimental NMR data

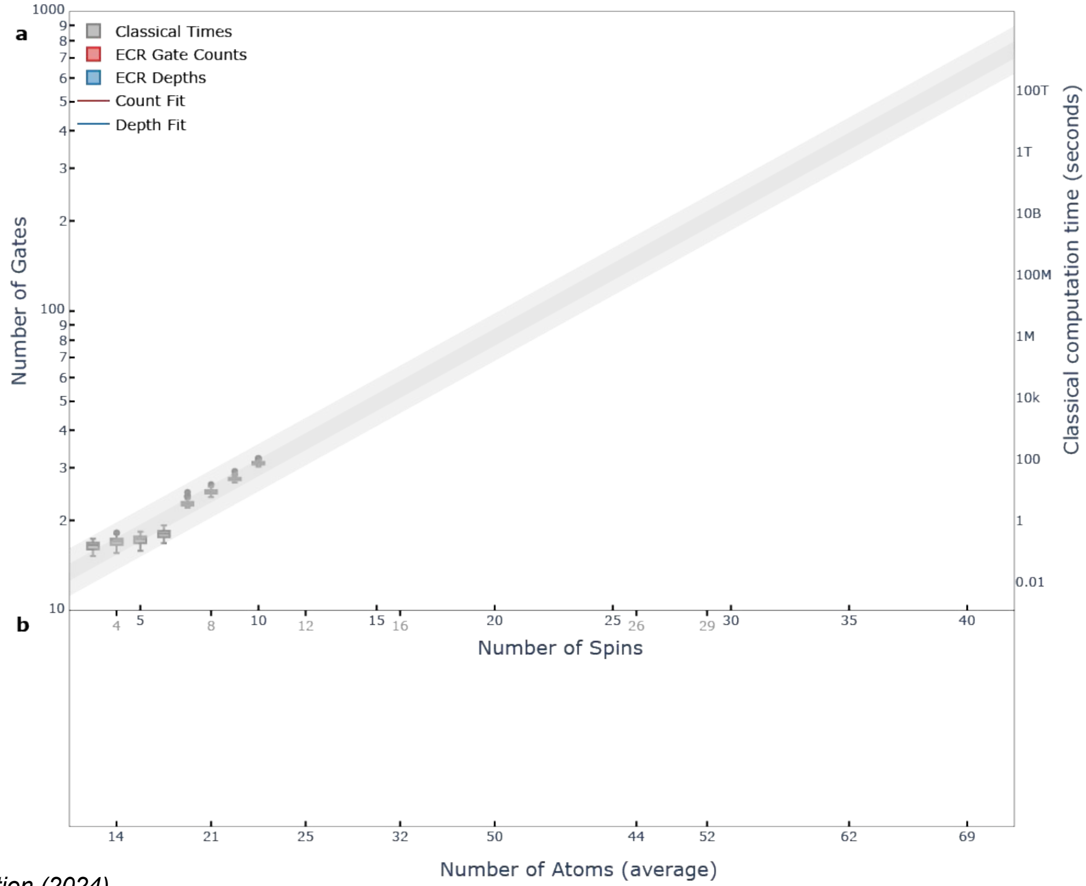
Free Induction Decay (FID) on QPU: first time high-field



Hamiltonian Simulation via product formula

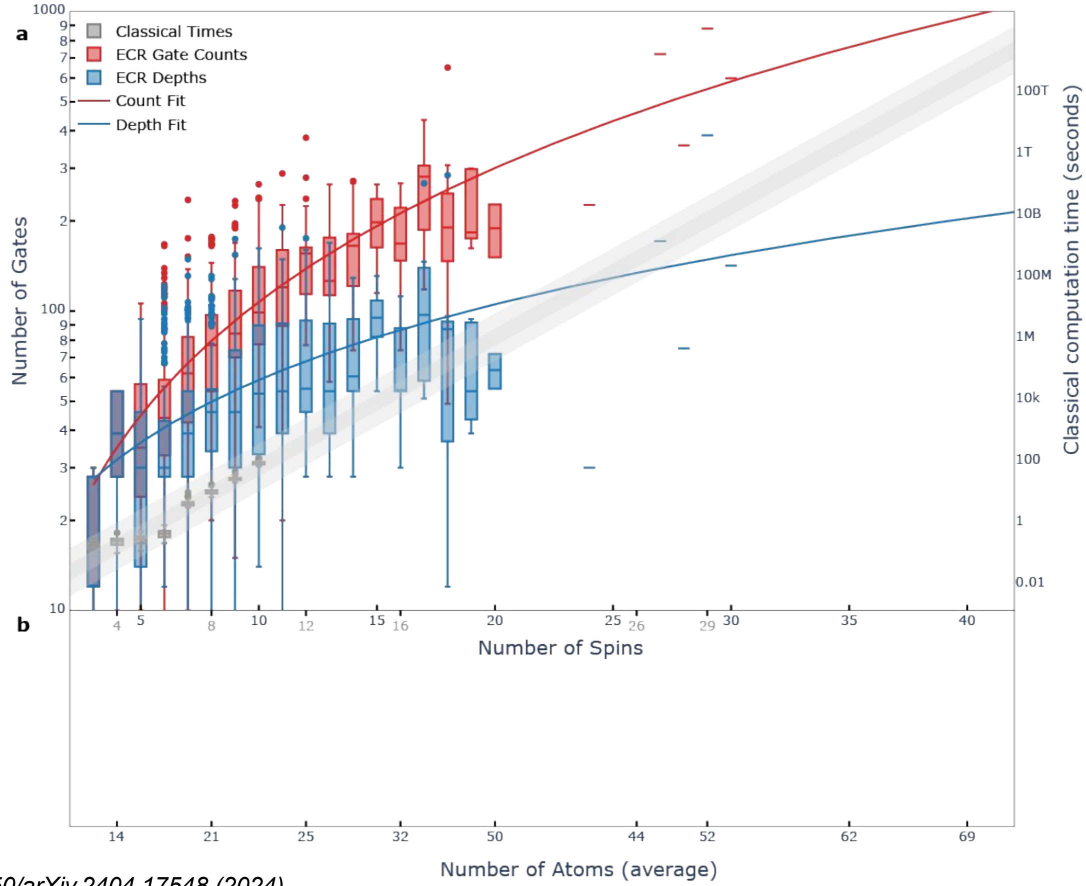


Resource estimation



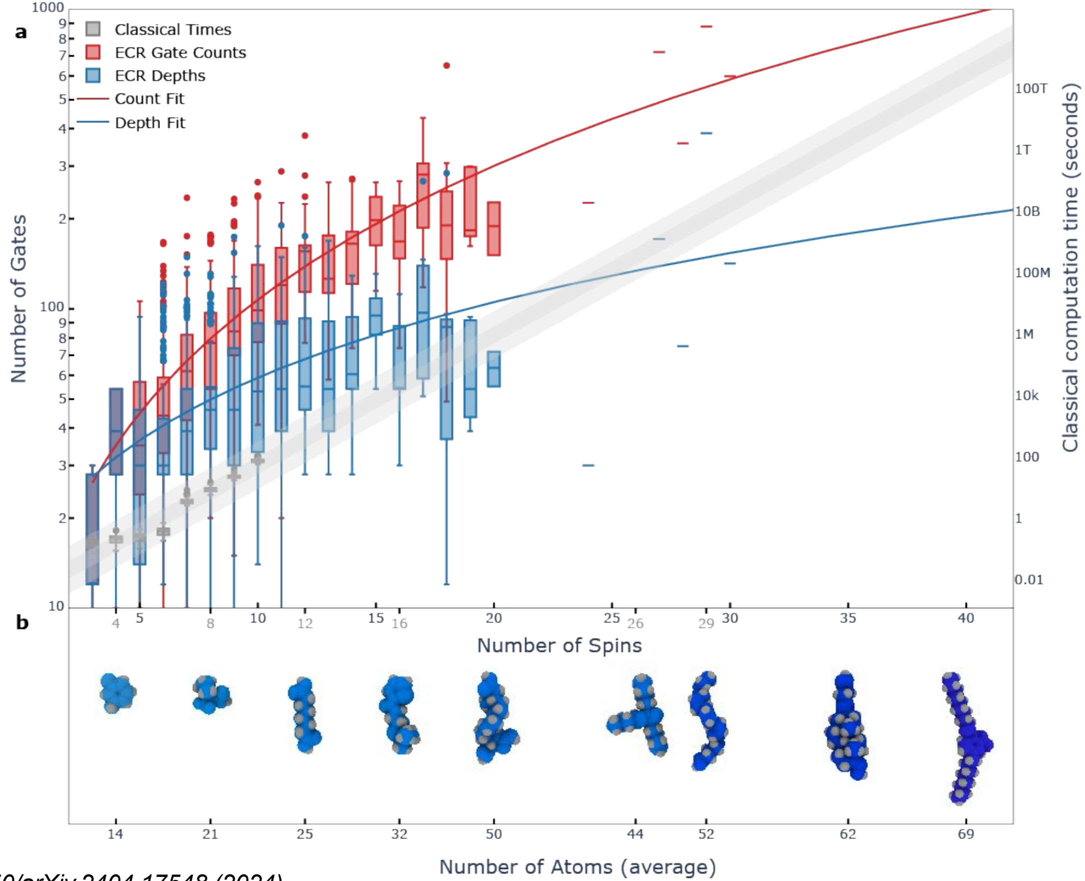
Burov et al., manuscript in preparation (2024)

Resource estimation



Burov et al., *https://doi.org/10.48550/arXiv.2404.17548 (2024)*

Resource estimation



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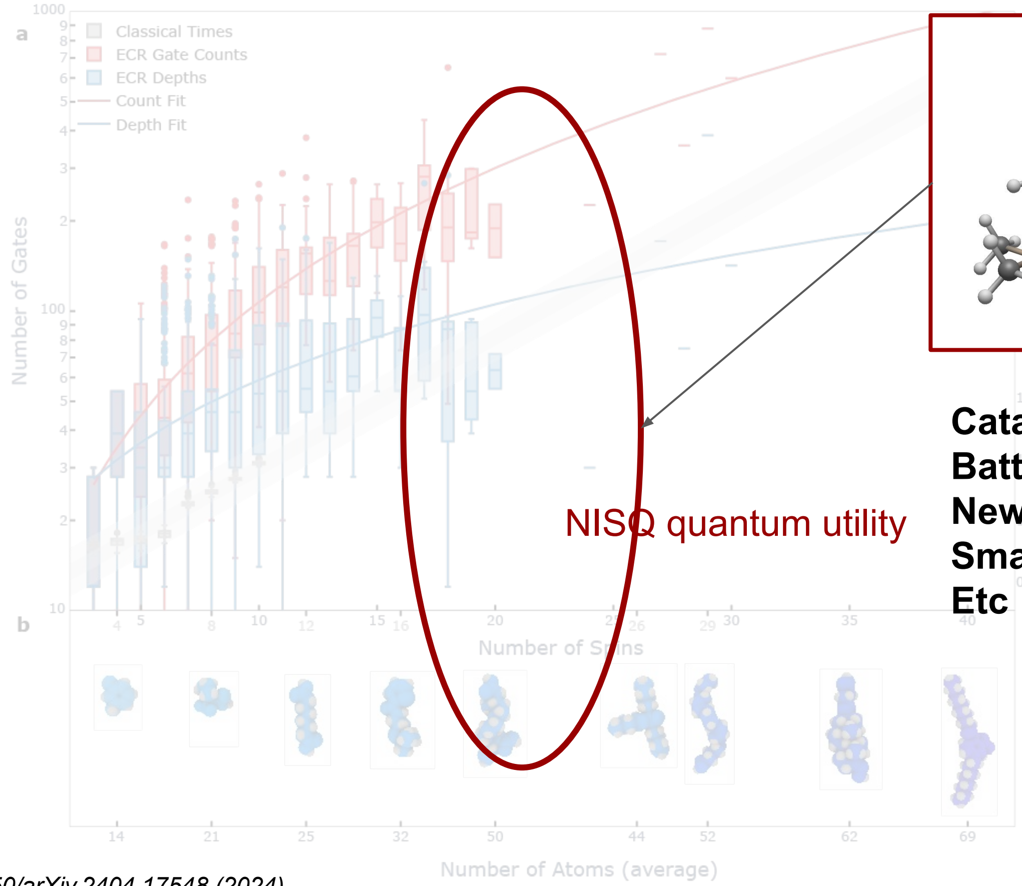
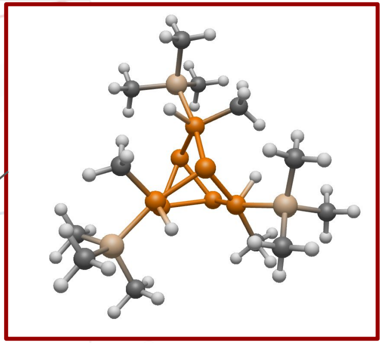
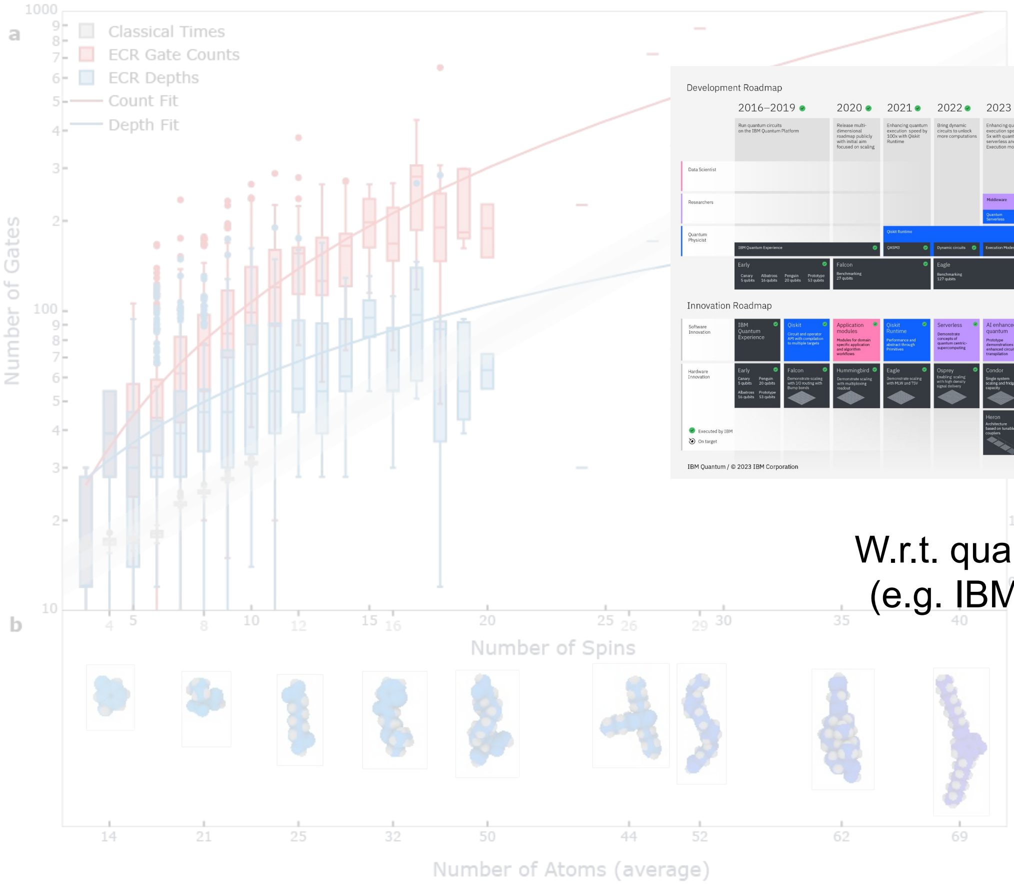


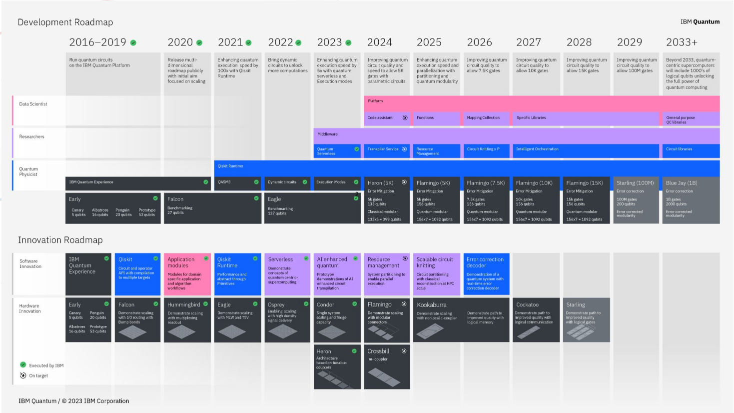


Catalysts
Batteries
New materials
Small drugs
Etc

Burov et al., https://doi.org/10.48550/arXiv.2404.17548 (2024)

Resource estimation

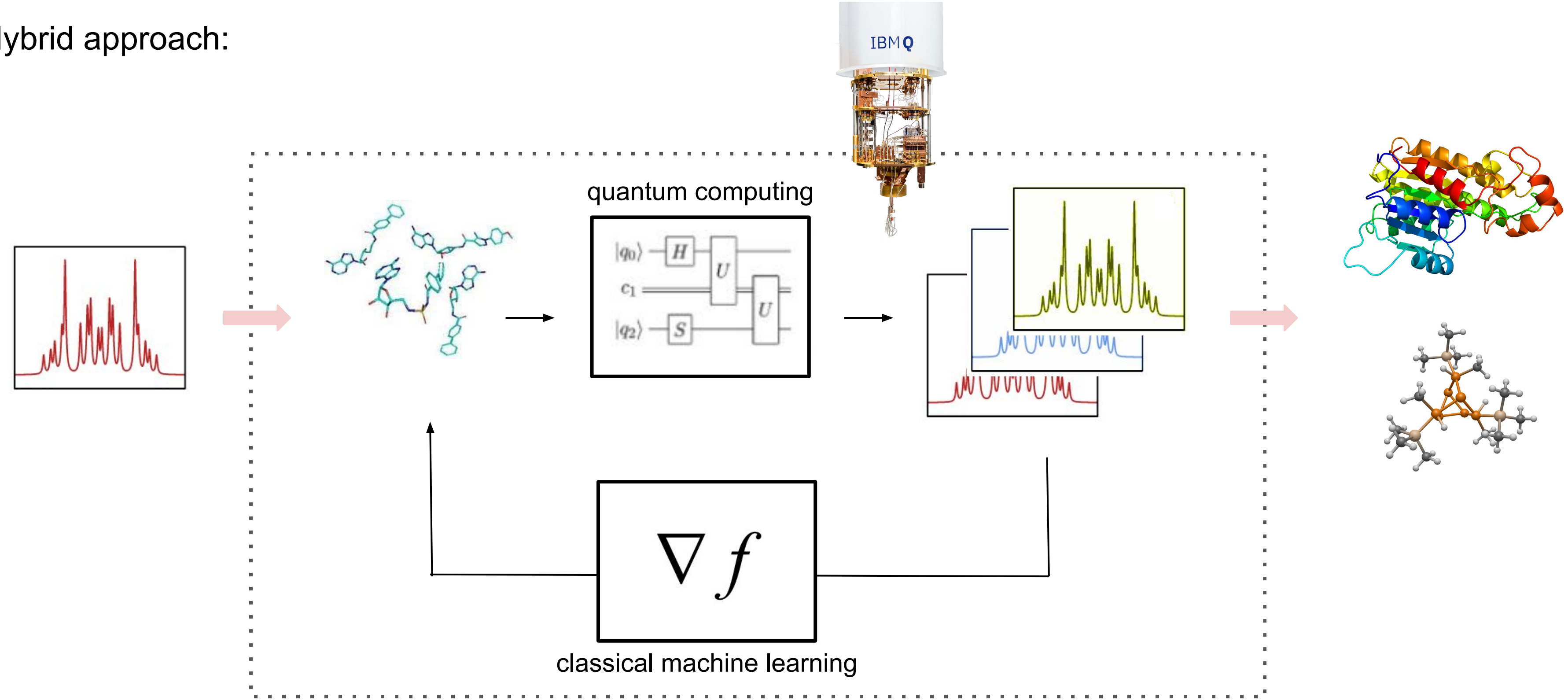




W.r.t. quantum roadmaps
(e.g. IBM, Quantinuum)

MatterDecoder: from spectroscopic data to molecular structure

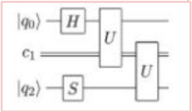
Hybrid approach:



MatterDecoder: from spectroscopic data to molecular structure

Chemical compound to be elucidated (liquid, powder, solid-state, etc)

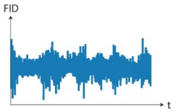
NMR spectrometer



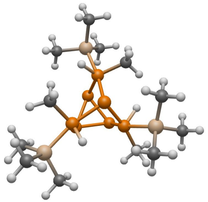
Quantum circuit

Quantum processor

$$|\psi(0)\rangle \xrightarrow[\text{Hamiltonian Simulation}]{\exp\left\{\frac{-i\hat{H}t}{\hbar}\right\}}$$



Nuclear spin dynamics

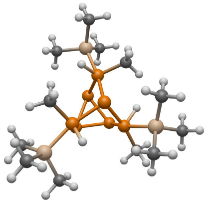


Elucidated molecular (catalyst, battery, pharmaceuticals, etc) structure; or dynamics, interaction, etc.

MatterDecoder: from spectroscopic data to molecular structure

Chemical compound to be elucidated (liquid, powder, solid-state, etc)

Towards automating NMR
Deciphering spectroscopic data on NISQ quantum computers



Elucidated molecular (catalyst, battery, pharmaceuticals, etc) structure; or dynamics, interaction, etc.

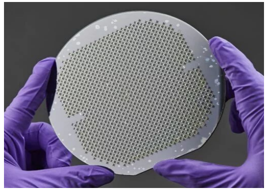
For other spin systems in sensing (NV-centers etc)

To be made available through *MatterDecoder* (spin-off technology)

Applications in solid-state NMR, material development, pharmaceuticals, sensing, etc

Radio pharmaceuticals, isotopes

Next generation of medical quantum sensors for healthcare



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Questions?
What can we solve together?

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