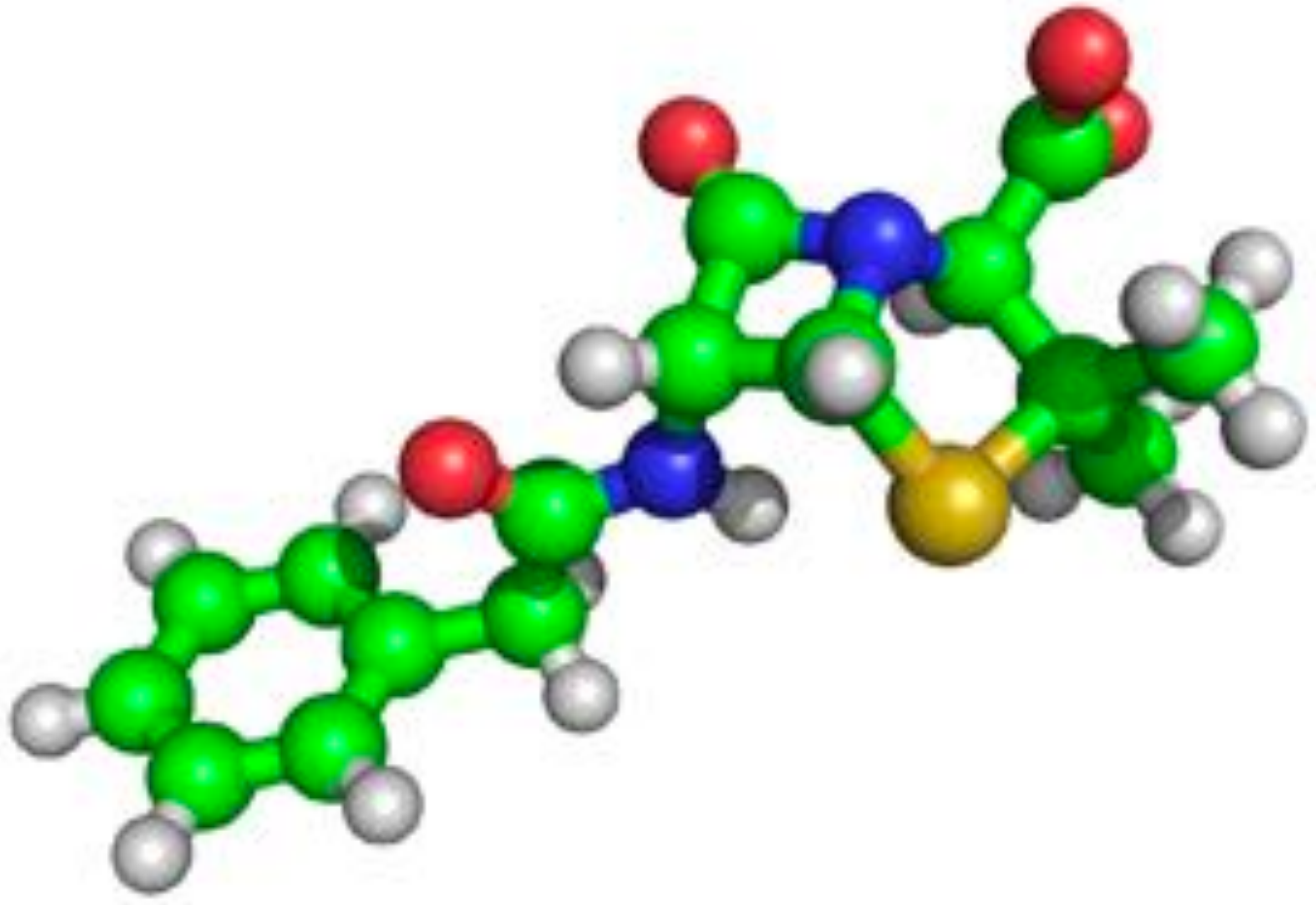
Quantum computing from life sciences to AI

Vedran Dunjko

⟨aQaL⟩
applied Quantum algorithms Leiden

LEIDEN
DRUG DEVELOPMENT
CONFERENCE

A story



Penicillin

- 120+ orbitals = 240+ electrons
  = 10^{73} configurations to consider.

- 300 exabytes (300 billion gigabytes) available today.
- **need over $10^{50} \times$ total memory on Earth.**

alternatively:

≈ 260 quantum bits (qubits)

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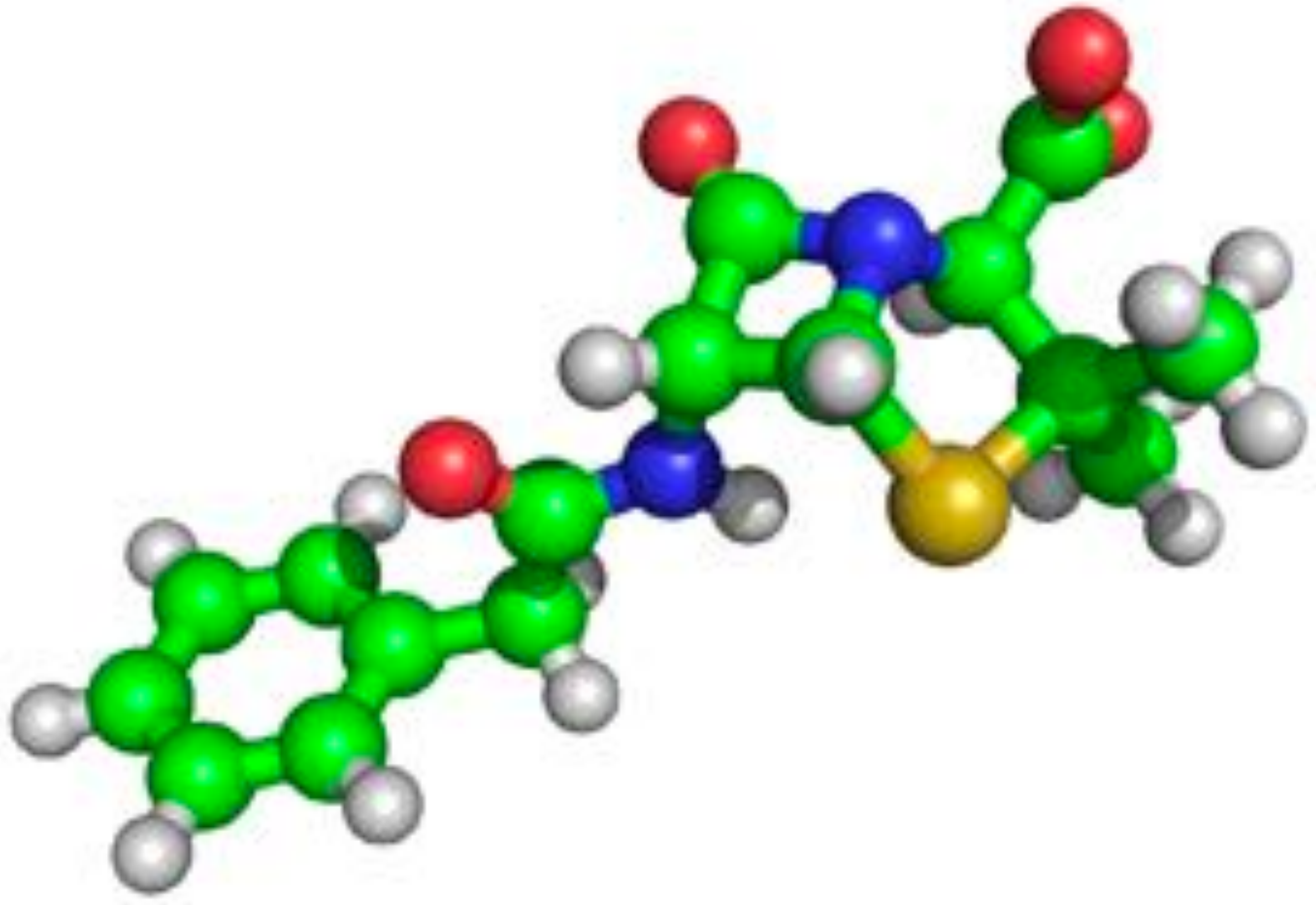
A story



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How valuable would such a technology be!?

A story

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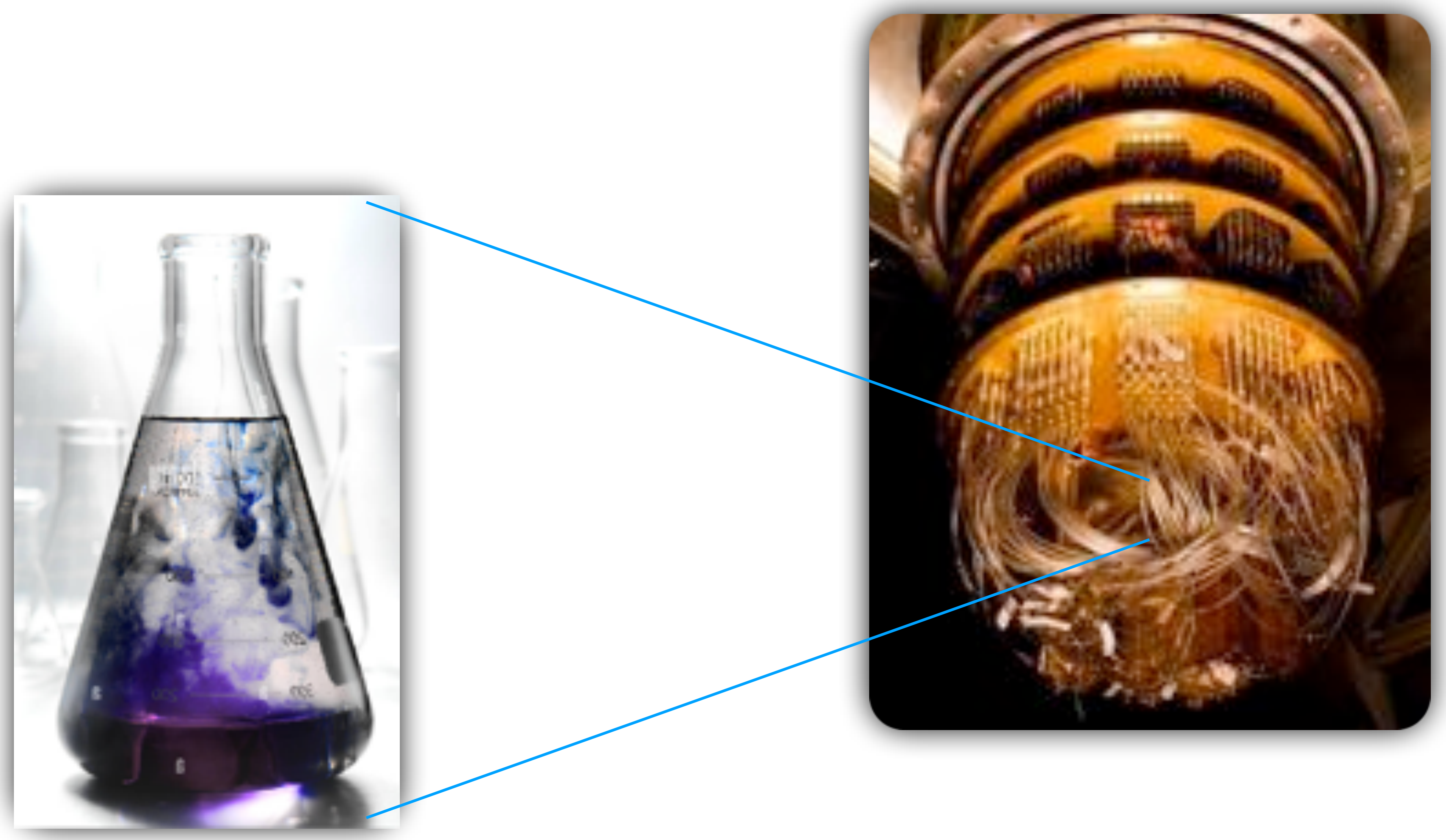
its (qubits)



Quantum computer is
a *universal simulator*
of all physics…

Feynman

Manin

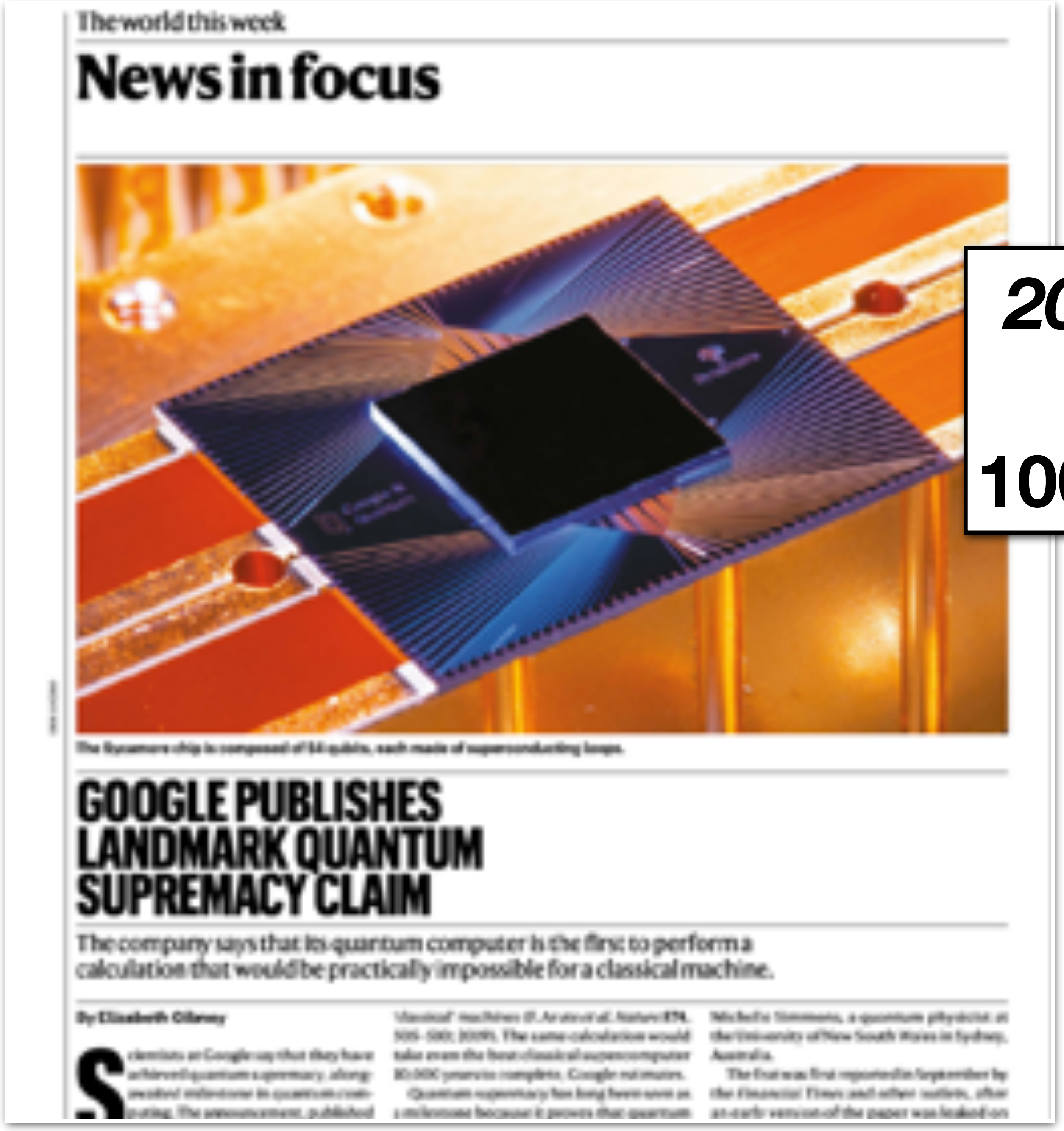
Given “Teraqubits”, “GigaQOPS”… sky is (not) the limit

“Quantum computers realized”

Theory: Game changer in data analysis, cryptanalysis, diff. equations

Technology: always 10 years away

until…



The world this week

News in focus

The Sycamore chip is composed of 54 qubits, each made of superconducting loops.

GOOGLE PUBLISHES LANDMARK QUANTUM SUPREMACY CLAIM

The company says that its quantum computer is the first to perform a calculation that would be practically impossible for a classical machine.

200 seconds **on quantum computer**

v.s.

1000s years on best supercomputers

Theory, prototypes, applications

full prototypes

unforeseen applications

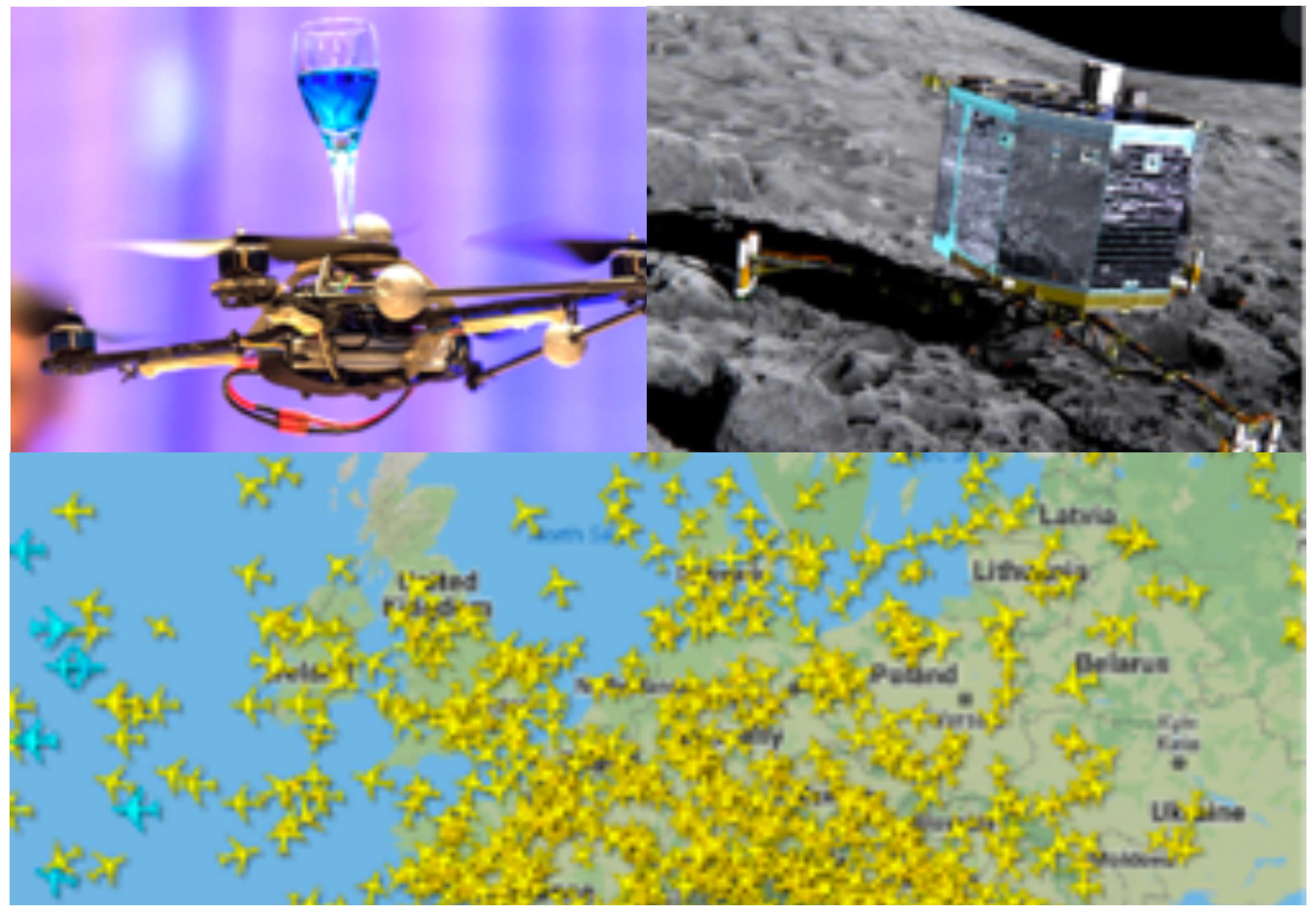
1903

1920s

1969

nowish

Theory, prototypes, applications



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Most algorithms for QCs

Theory, prototypes, applications

first approaches

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Today's QCs

Most algorithms for QCs

⟨aQa⟩

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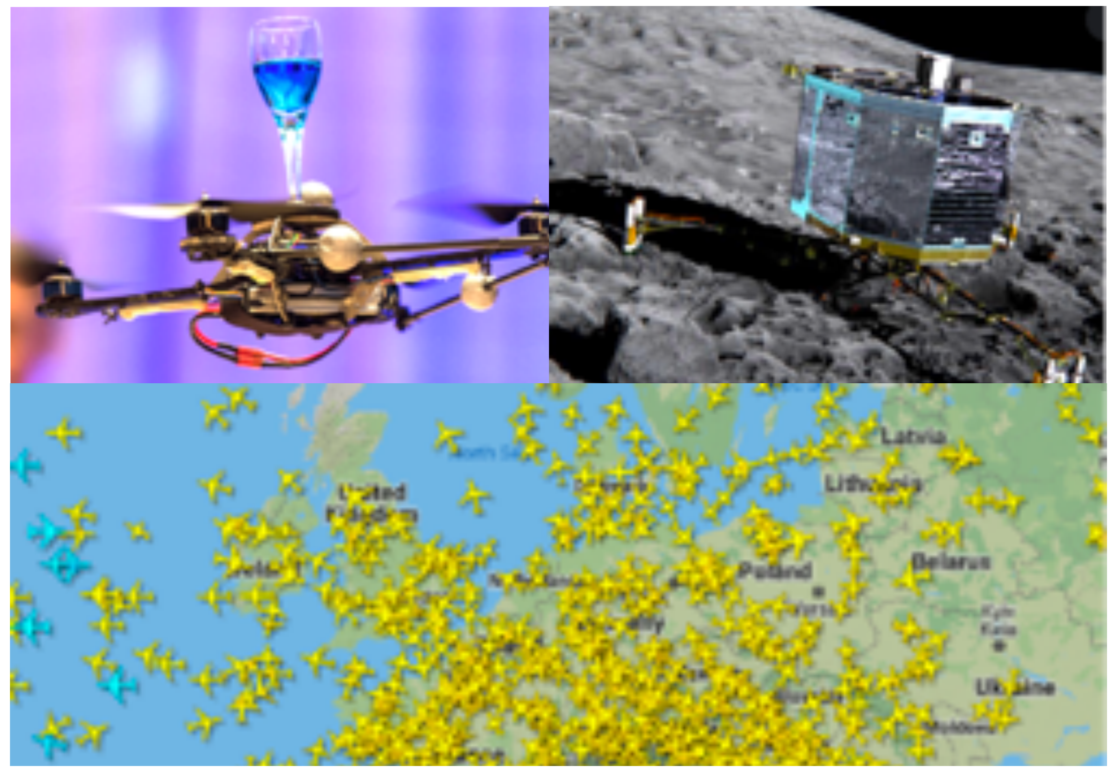

unforeseen applications

1890s

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Today's QCs

How to program them in the meantime?

Most algorithms for QCs

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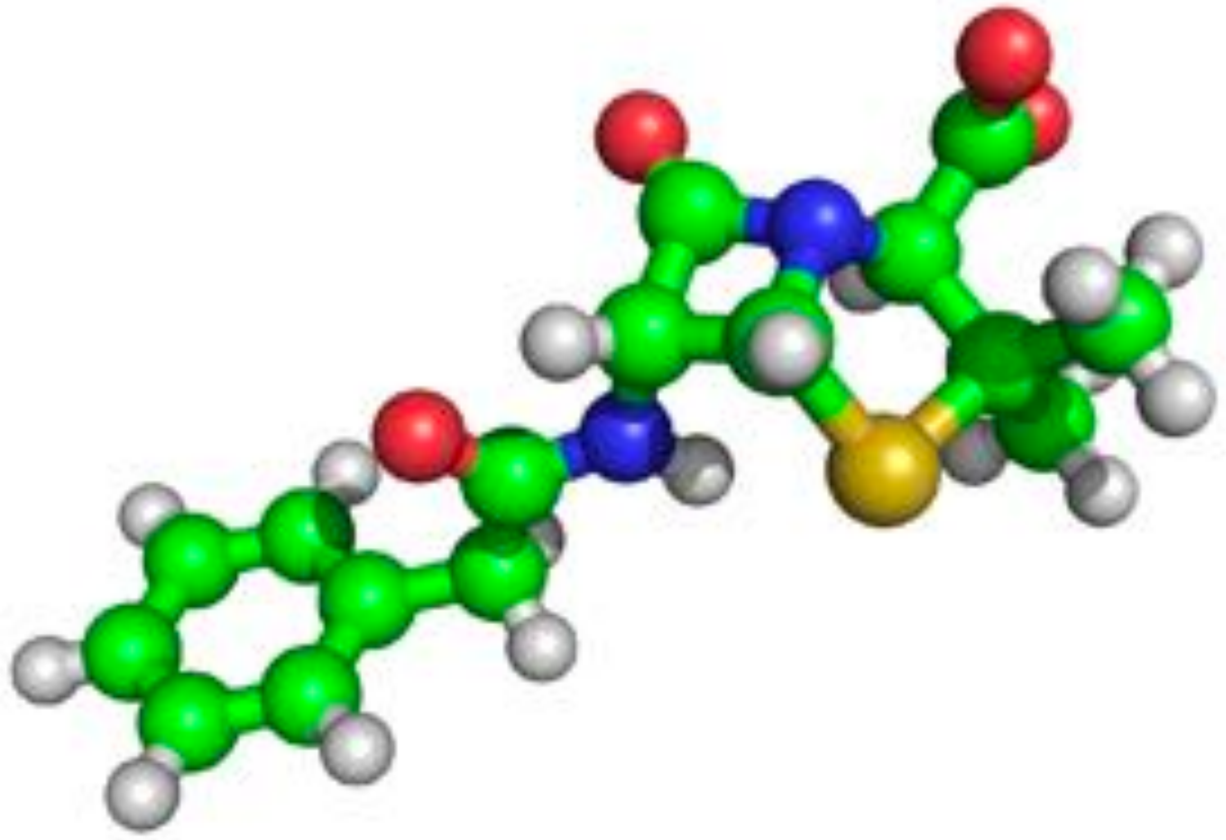
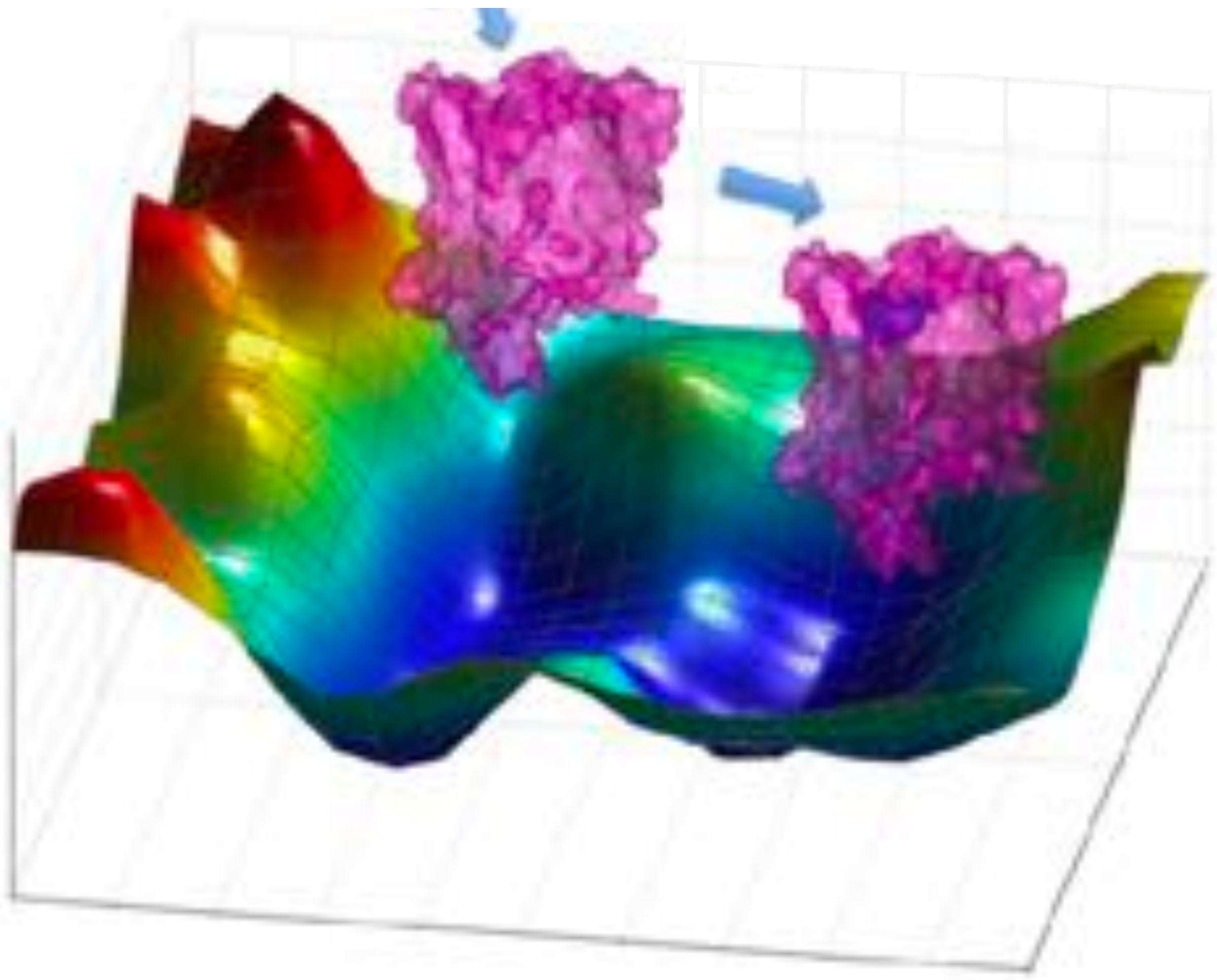
The (mainstream) quantum computing challenge

small (1000-100000)
perhaps very noisy

current focus:
- *computing ground energies*
  esp. electronic structure problem

applications in:
- binding affinities (e.g. hits)
- molecular dynamics (e.g. docking)





Vaidehi N., Jain A., J. Phys. Chem. B (2015), 119, 4, 1233–1242

The (mainstream) quantum computing challenge

Ground states
hard even for QC!

heuristics;
bigger QCs needed
and new ideas needed

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Conventional methods
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New kids on the block:

AlphaFold

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New kids on the block:

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New ideas arising daily. The field is only getting started

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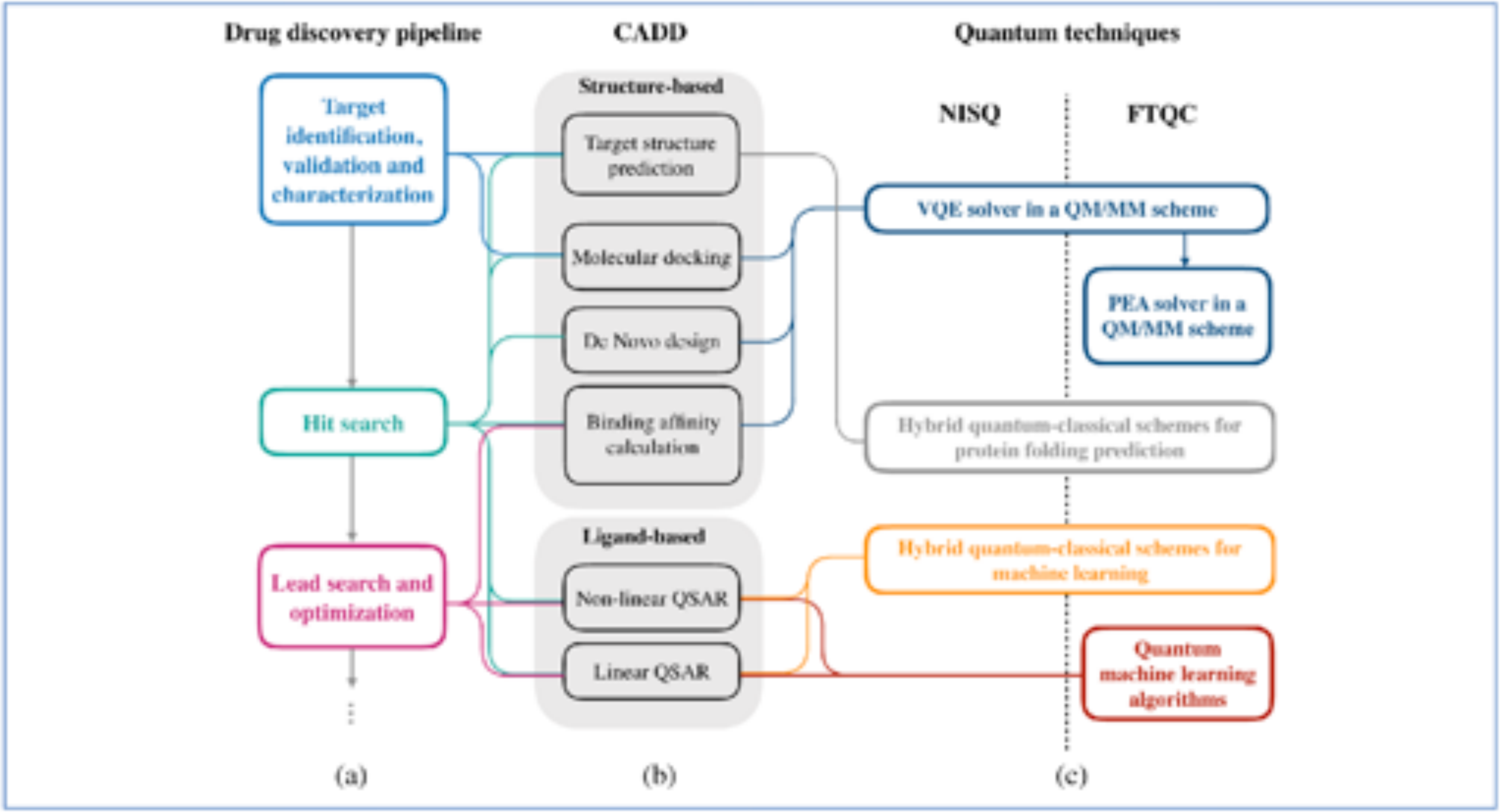


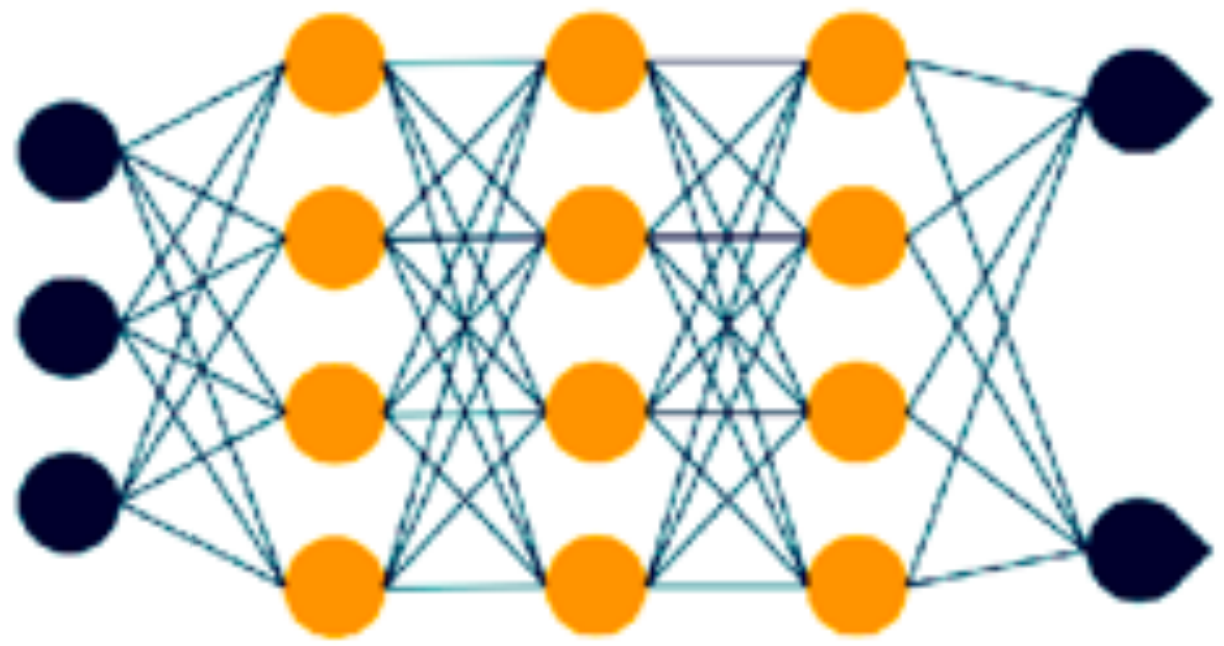
Cao, Y., Fontalvo, J. R., & Aspuru-Guzik, A. (2018). *Potential of quantum computing for drug discovery. IBM Journal of Research and Development, 1–1.* doi:10.1147/jrd.2018.2888987

A new idea: quantum machine learning

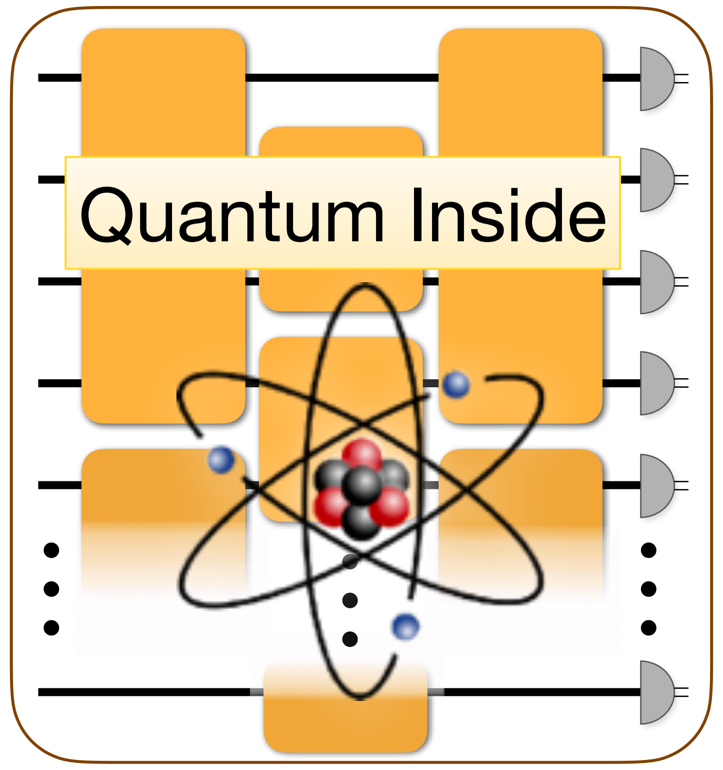
Challenge: how to optimally program the limited quantum computers

Machine learning: useful results *without explicit programming*

Near-term Quantum ML: Deep neural networks → Quantum Neural Networks



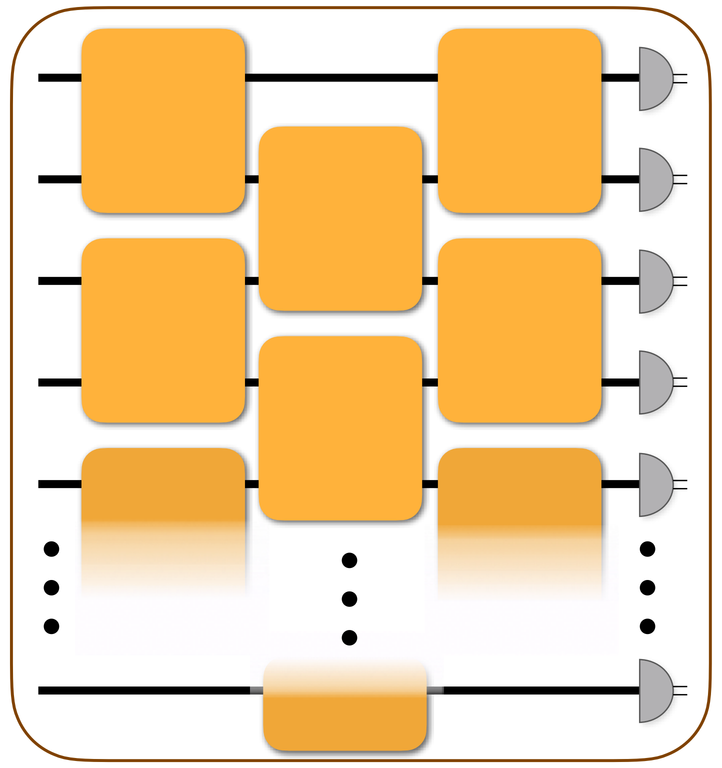
V.S.



But are they *better*? On real problems? In drug design?

Progress in quantum machine learning

What *are* Quantum Neural Networks



We study:
- classification of all types
- learning capabilities
- trainability

Gyurik, C., Dunjko, V.,arXiv:2208.06339 (2022)
Jerbi, S. et al, arXiv:2110.13162 (2021)

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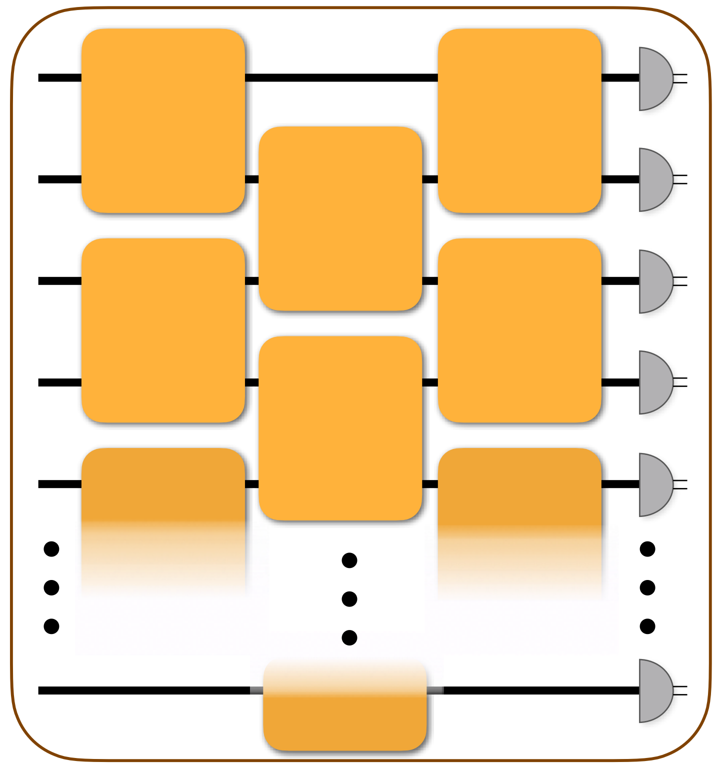

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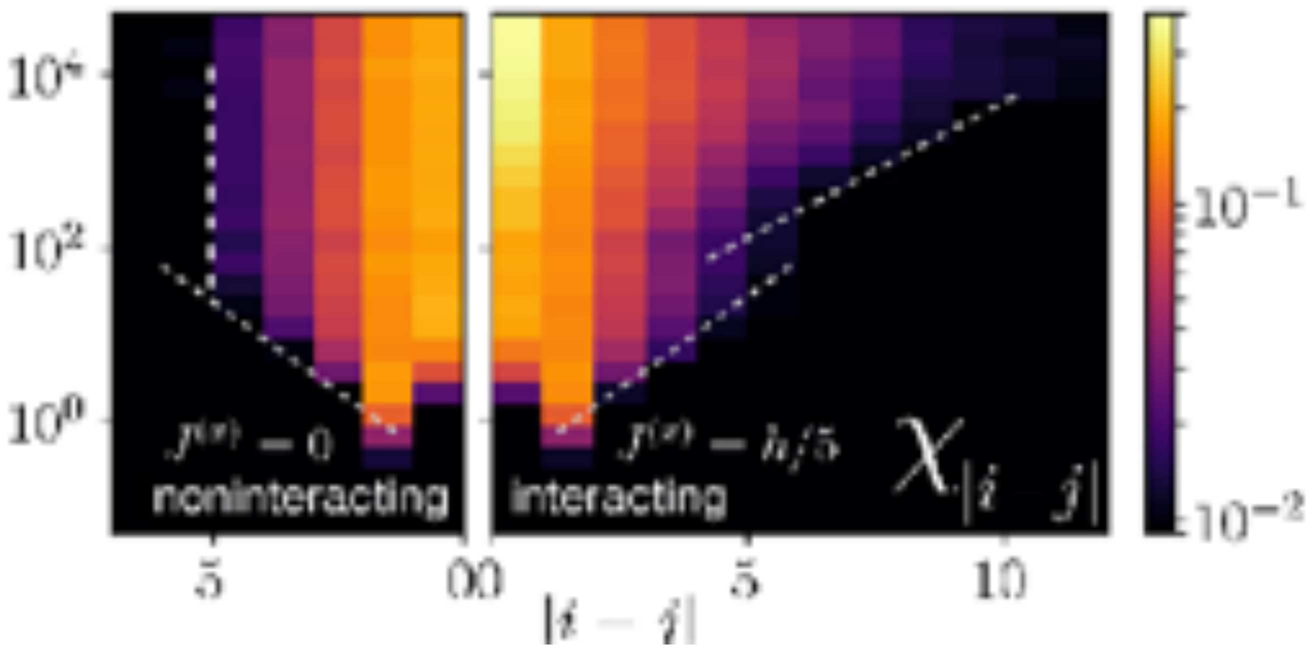
Do we *need* quantum neural networks?



Recent result:
- if data is generated by a“general” quantum process quantum learning is *necessary*
- Condensed matter? High-energy? **Drug design?**

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Image: Phys. Rev. Lett. 127, 050601 (2021)

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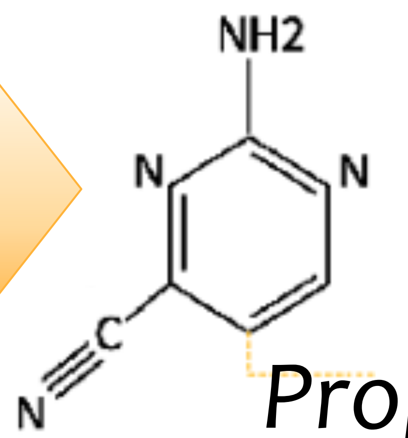
But the proof is in the pudding

Theory ≠ practice… except in theory… .

First tiny studies

Quantum Generative Models



Proposal molecule

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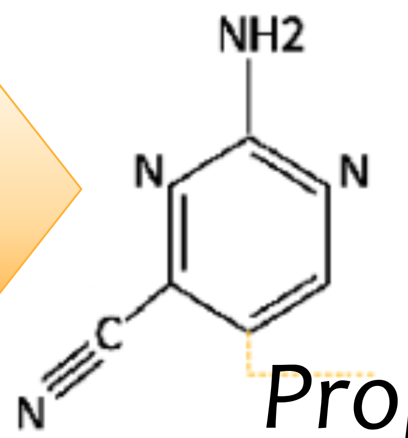
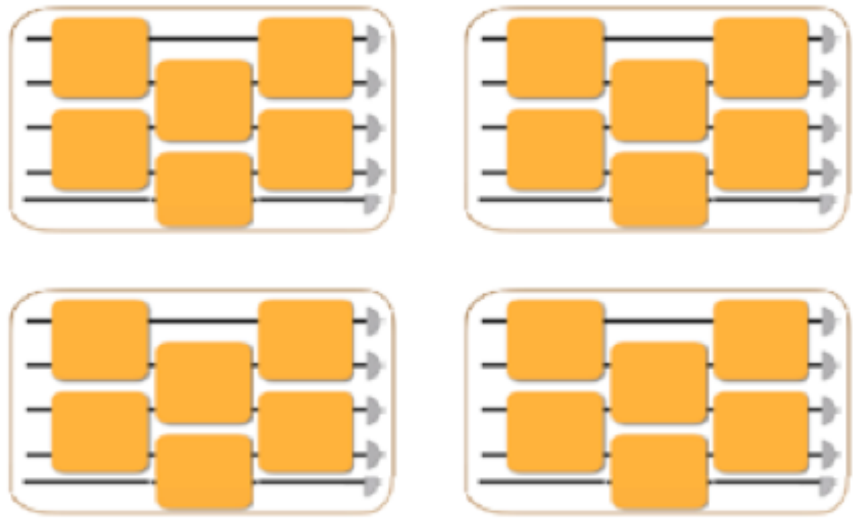


Proposal molecule

Go beyond tiny: "*Divide & Quantum*"

classical pre-processing



classical post-processing

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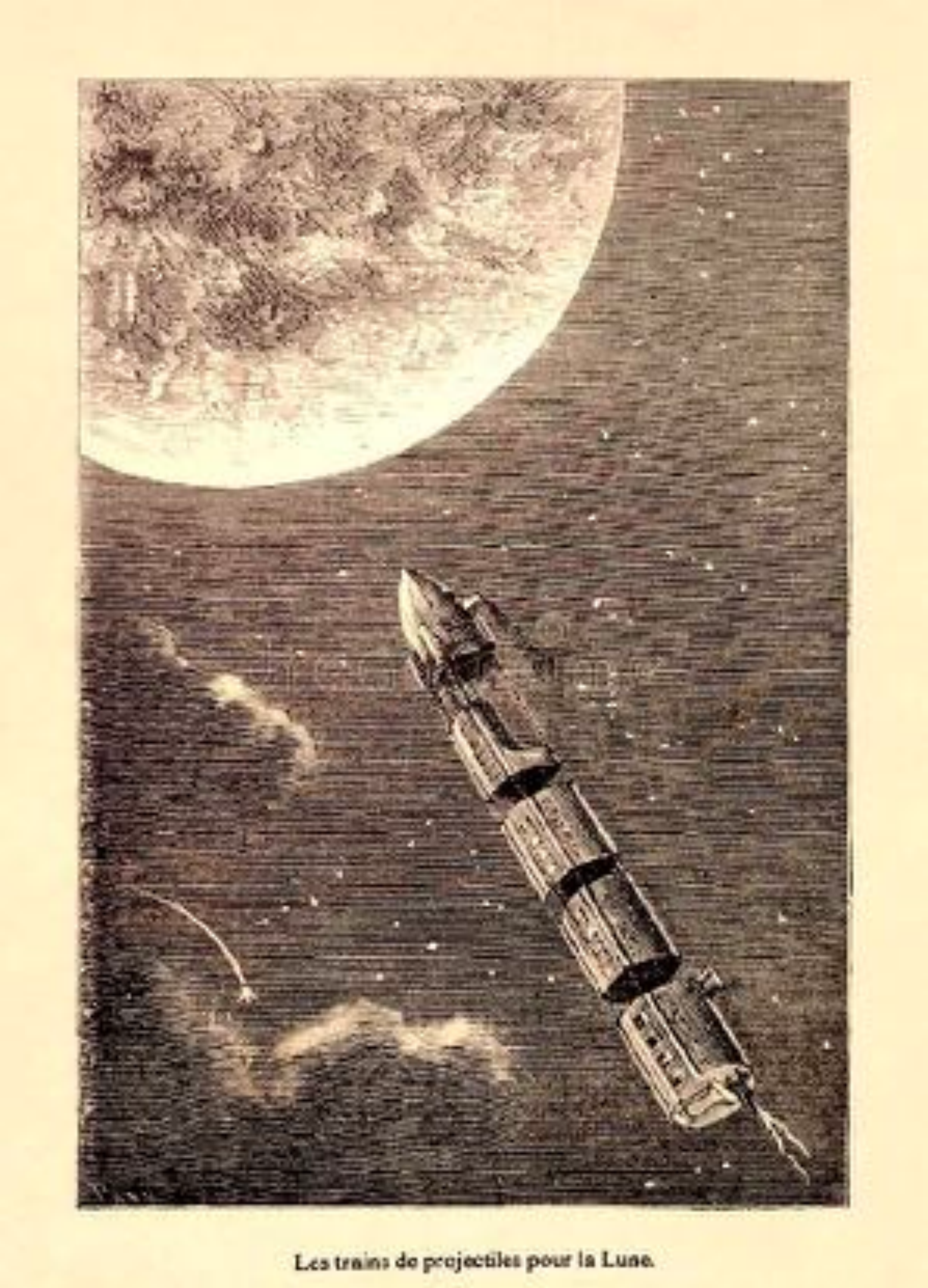
Up next: quantum computational discovery

Theory, experiment, and industry exploring **real world quantum solutions** on **real problems**

applied Quantum algorithms Leiden



Verne’s way to the moon

Year 2000 as viewed from 1900