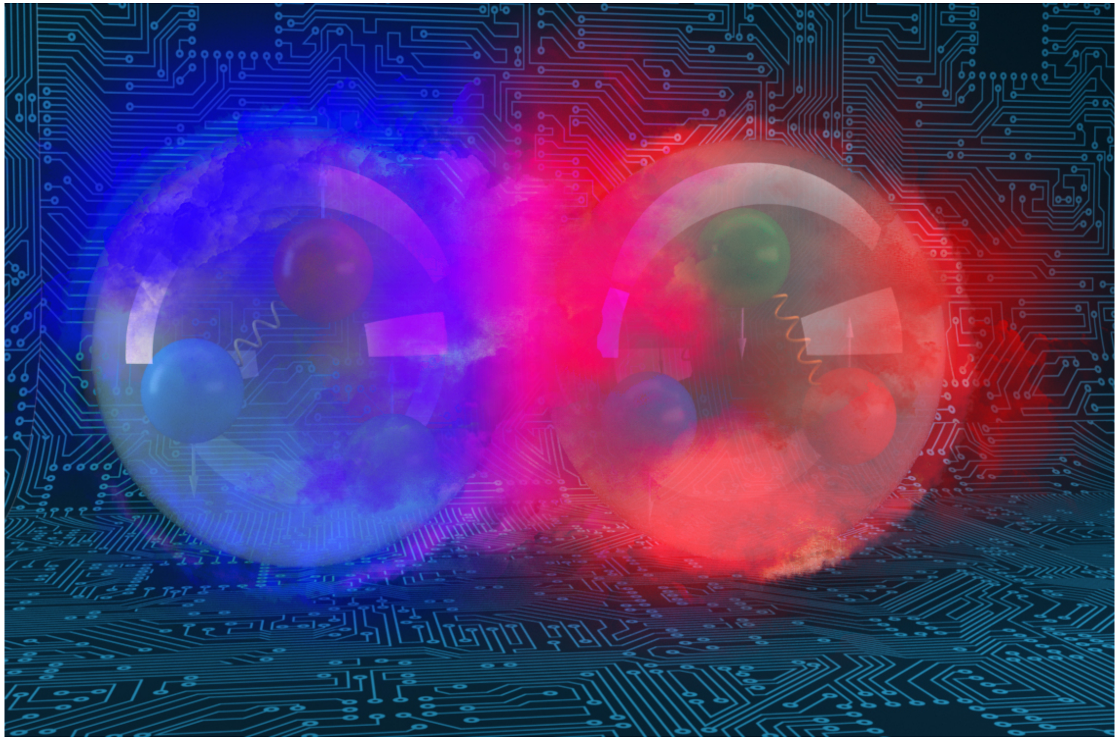
A quantum computation of an atomic nucleus



Gaute Hagen
Oak Ridge National Laboratory

Quantum computing and scientific research:
state of the art and potential impact in nuclear physics

CEA, Saclay, June 13th, 2019

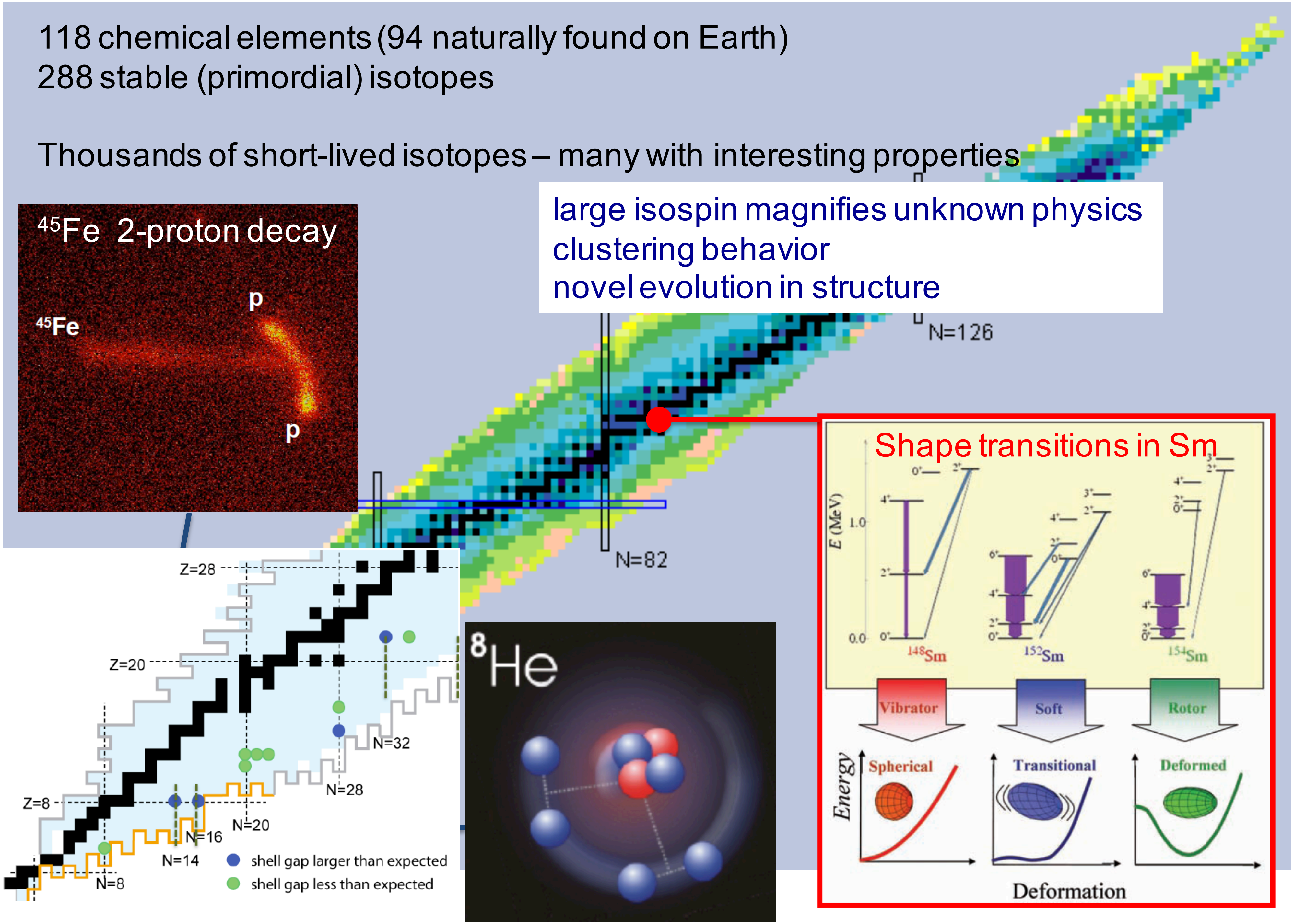
U.S. DEPARTMENT OF ENERGY NUCLEI Nuclear Computational Low-Energy Initiative

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Nuclei across the chart

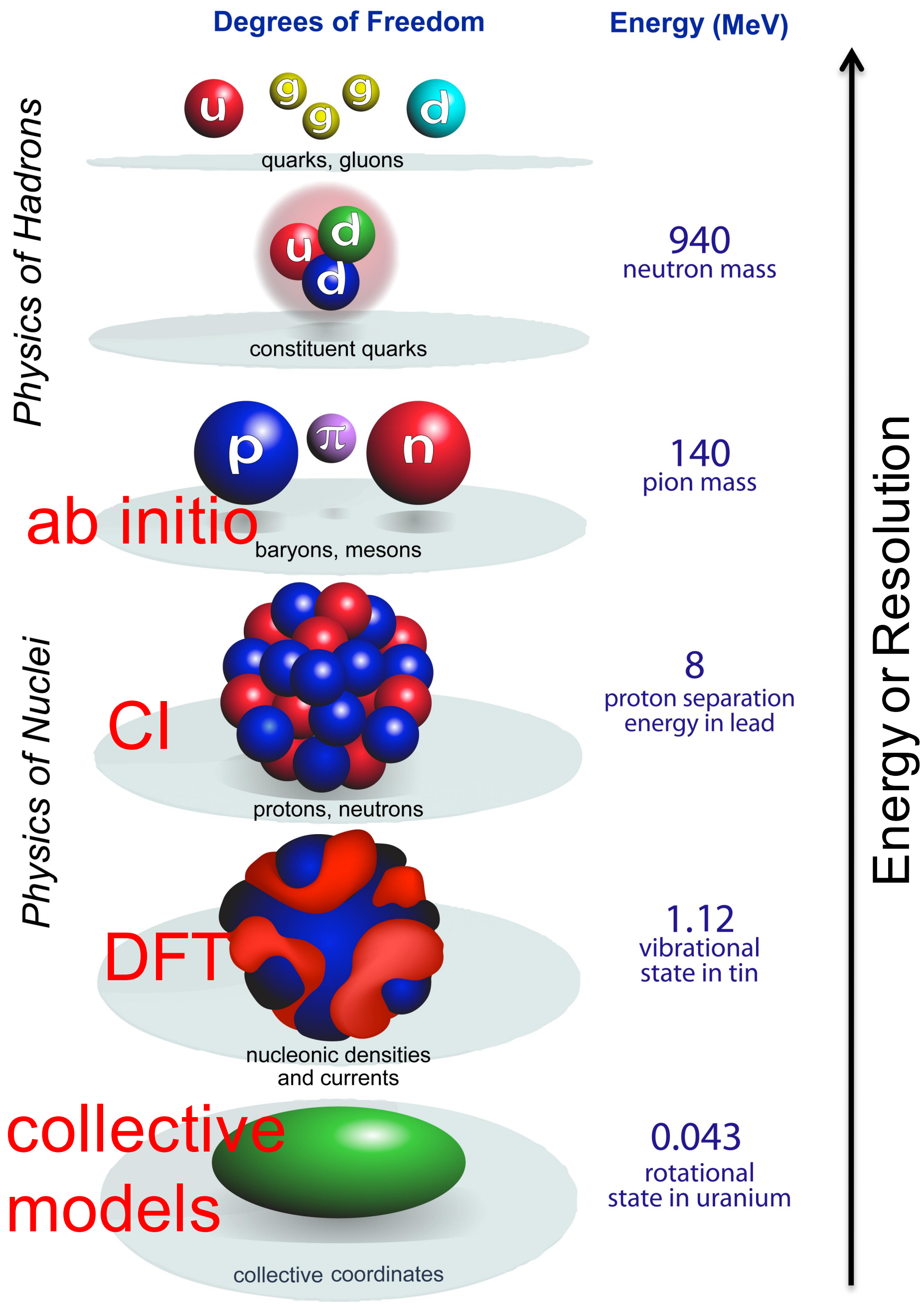
118 chemical elements (94 naturally found on Earth)
288 stable (primordial) isotopes

Thousands of short-lived isotopes – many with interesting properties



large isospin magnifies unknown physics
clustering behavior
novel evolution in structure

Energy scales and relevant degrees of freedom



Effective theories provide us with model independent approaches to atomic nuclei

Key: Separation of scales

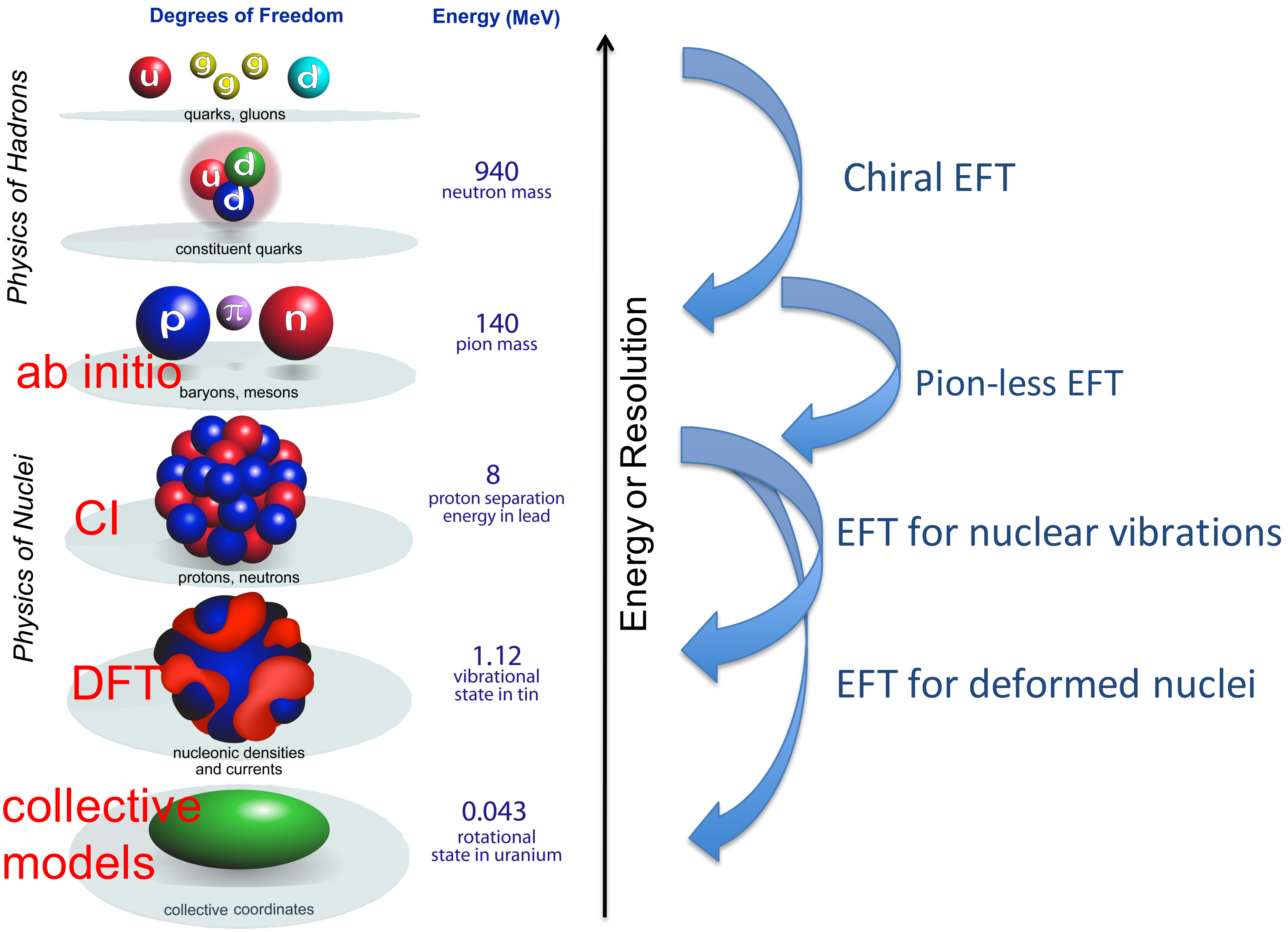
Ab-initio low-energy nuclear physics deals with nucleons (and pions) as dynamical degrees of freedom

Weinberg’s third law of Progress in theoretical Physics:

“You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you'll be sorry!”

Fig.: Bertsch, Dean, Nazarewicz, SciDAC review (2007)

Energy scales and relevant degrees of freedom



Degrees of Freedom	Energy (MeV)
quarks, gluons	
constituent quarks	940 neutron mass
baryons, mesons	140 pion mass
protons, neutrons	8 proton separation energy in lead
nucleonic densities and currents	1.12 vibrational state in tin
collective coordinates	0.043 rotational state in uranium

Physics of Hadrons

Physics of Nuclei

ab initio

CI

DFT

collective models

Energy or Resolution

Chiral EFT

Pion-less EFT

EFT for nuclear vibrations

EFT for deformed nuclei

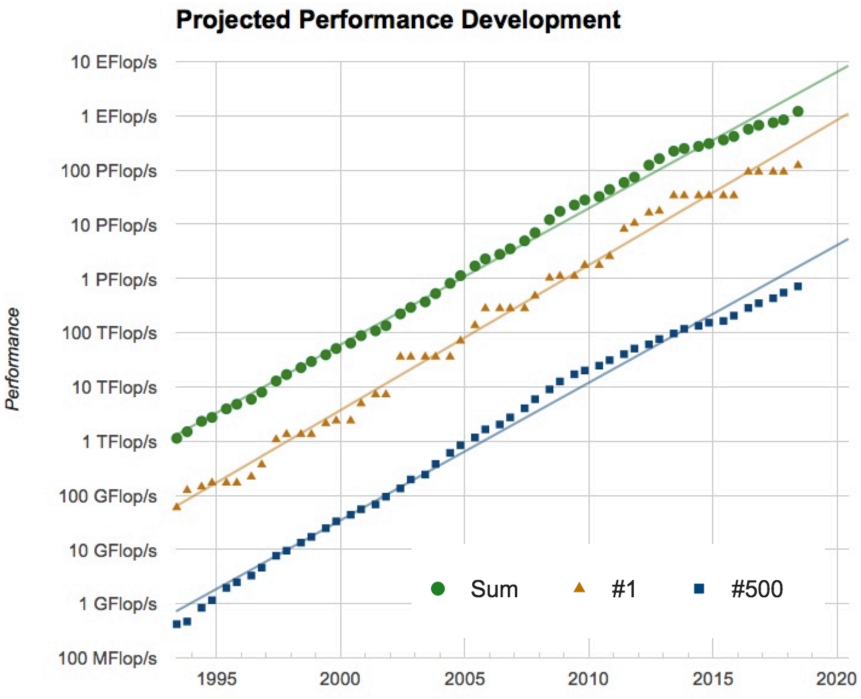
Fig.: Bertsch, Dean, Nazarewicz, SciDAC review (2007)

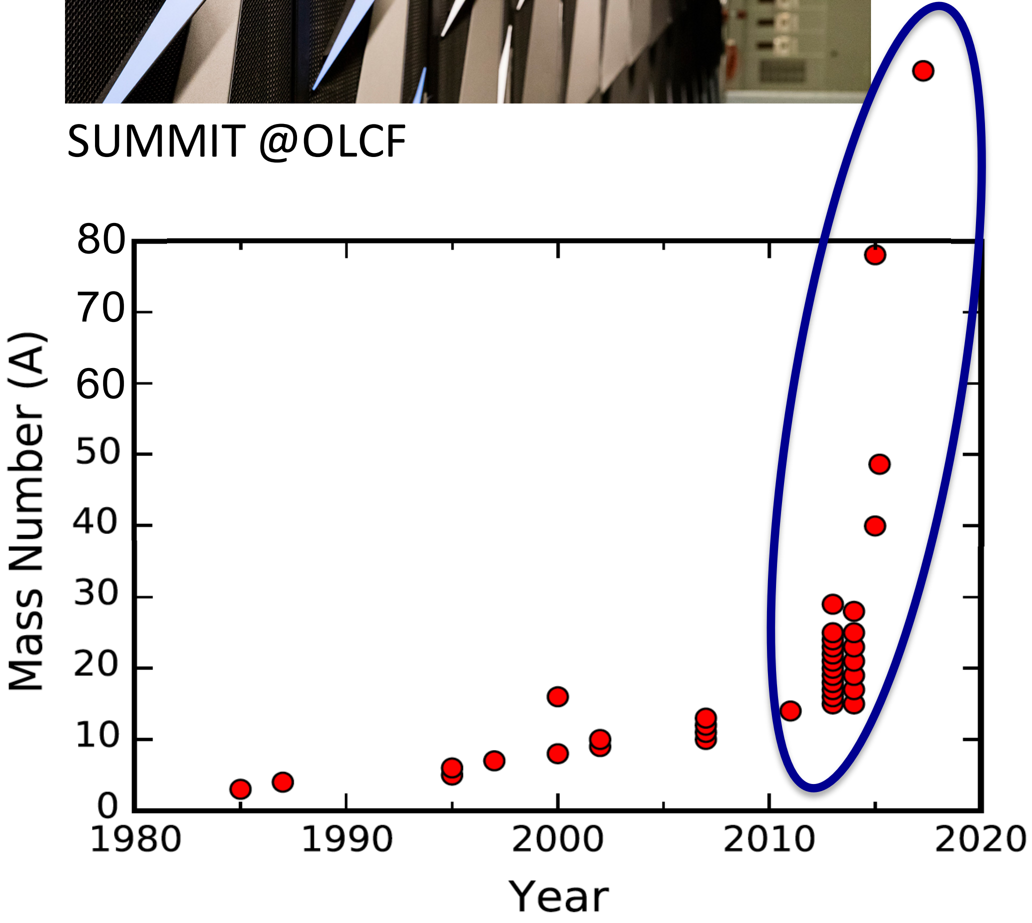
Trend in realistic ab-initio calculations

- Tremendous progress in recent years because of ideas from EFT and the renormalization group
- Computational methods with polynomial cost (coupled clusters 🙂 quantum computing 🤔)
- Ever-increasing computer power?

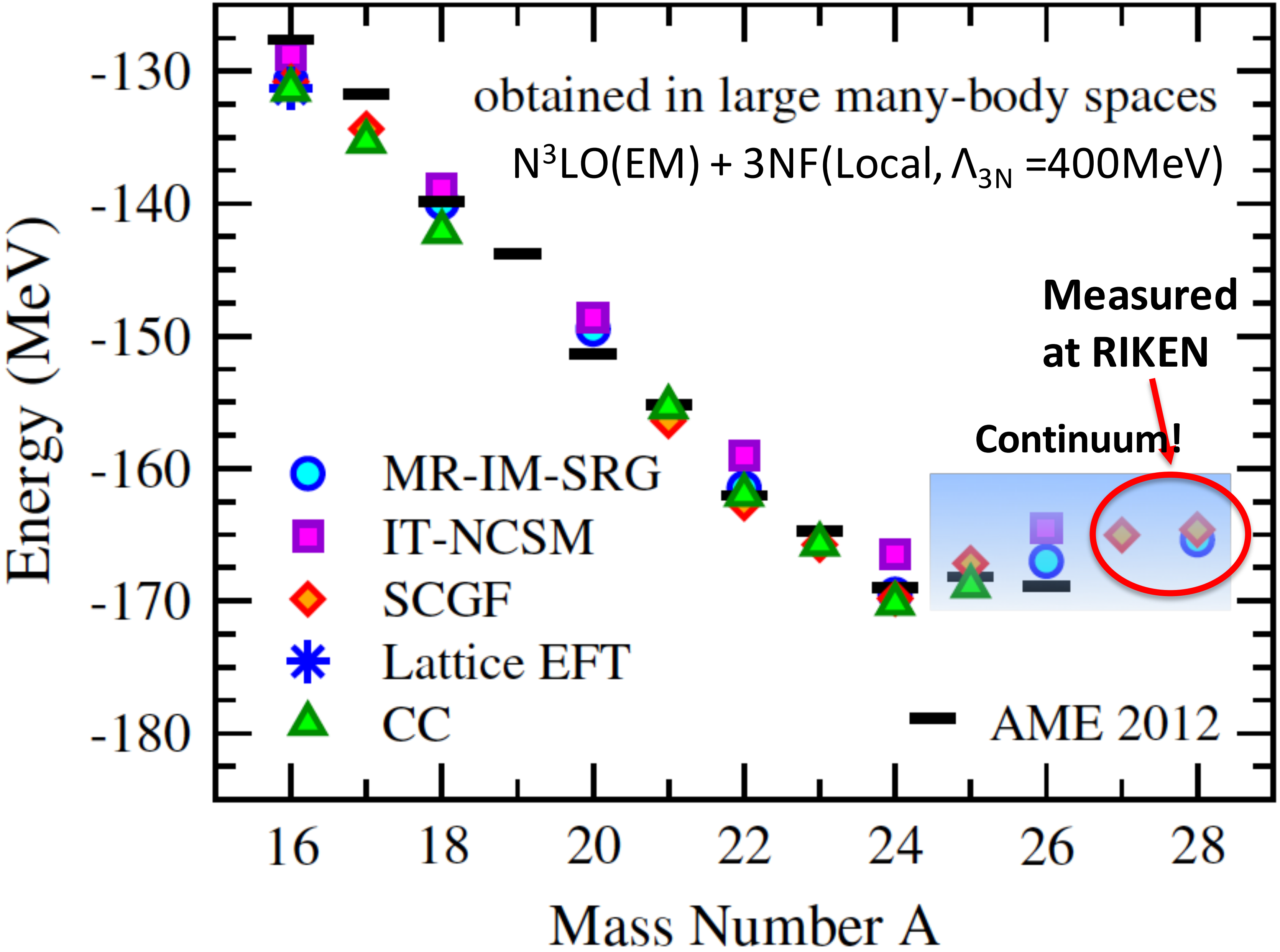
SUMMIT @OLCF

Development with time (top500.org)



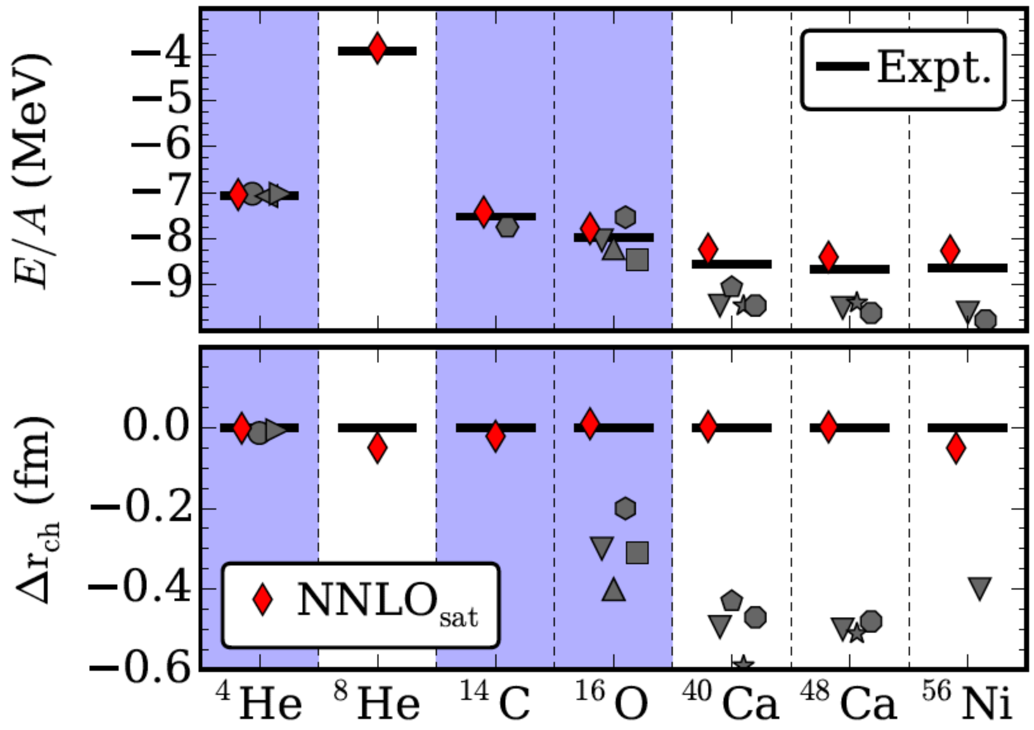


Oxgyen chain with interactions from chiral EFT



Hebeler, Holt, Menendez, Schwenk, Annu. Rev. Nucl. Part. Sci. 65, 457 (2015)

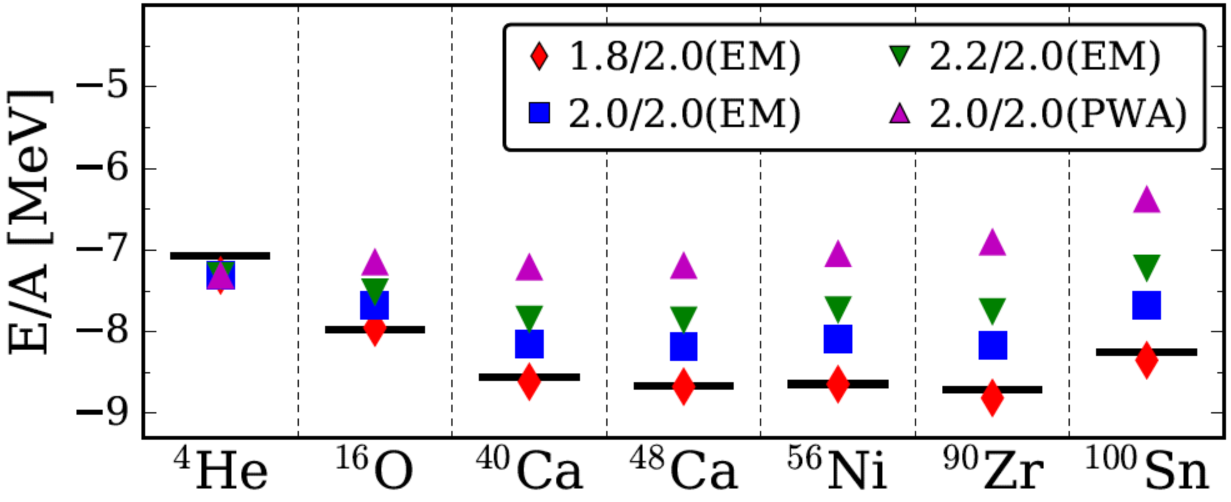
A family of interactions from chiral EFT



NNLO$_{sat}$: Accurate radii and BEs

- Simultaneous optimization of NN and 3NFs
- Include charge radii and binding energies of ^{3}H, ^{3,4}He, ^{14}C, ^{16}O in the optimization
- Harder interaction: difficult to converge beyond ^{56}Ni

A. Ekström *et al*, Phys. Rev. C **91**, 051301(R) (2015).

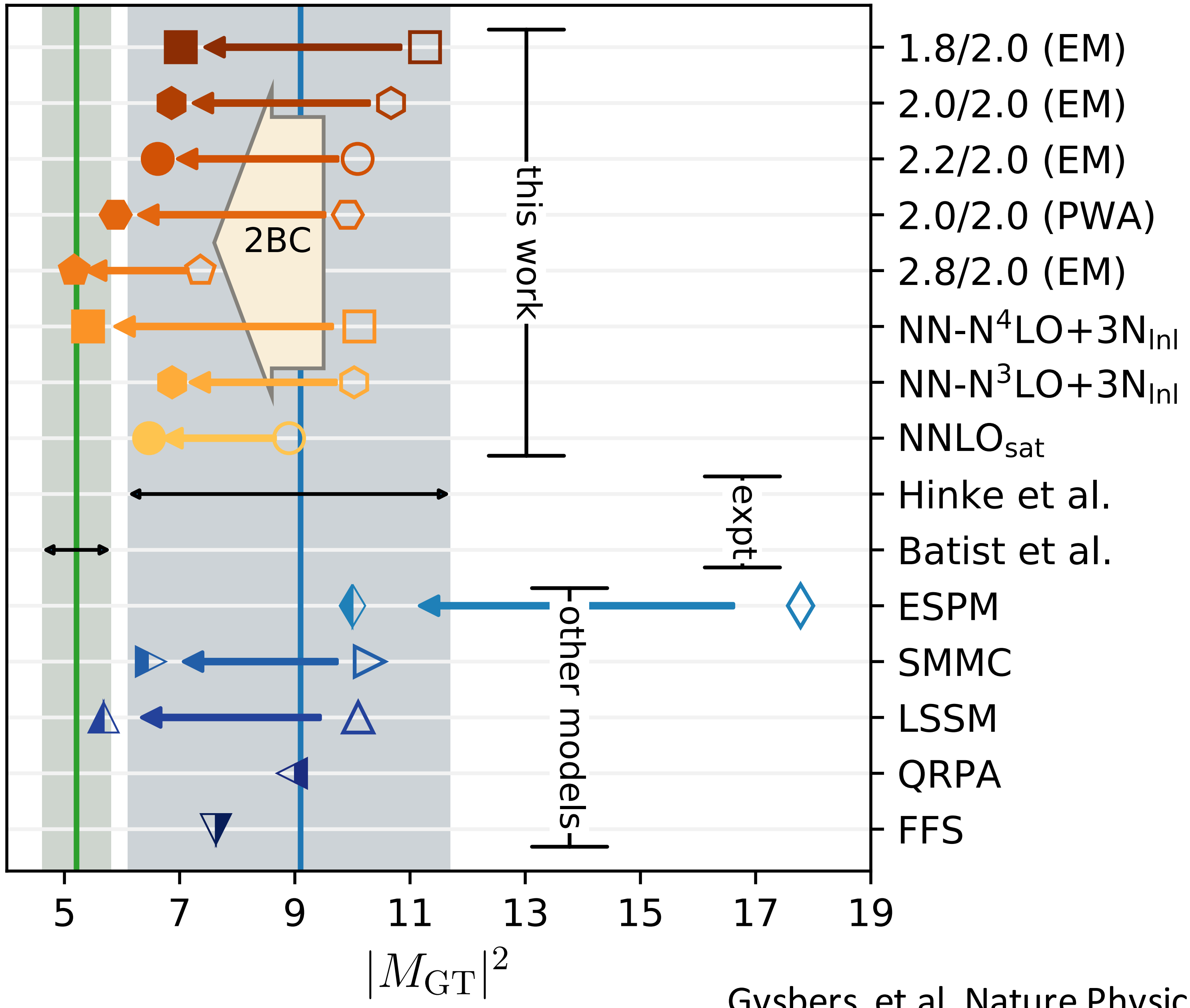


1.8/2.0(EM): Accurate BEs

Soft interaction: SRG NN from Entem & Machleidt with 3NF from chiral EFT

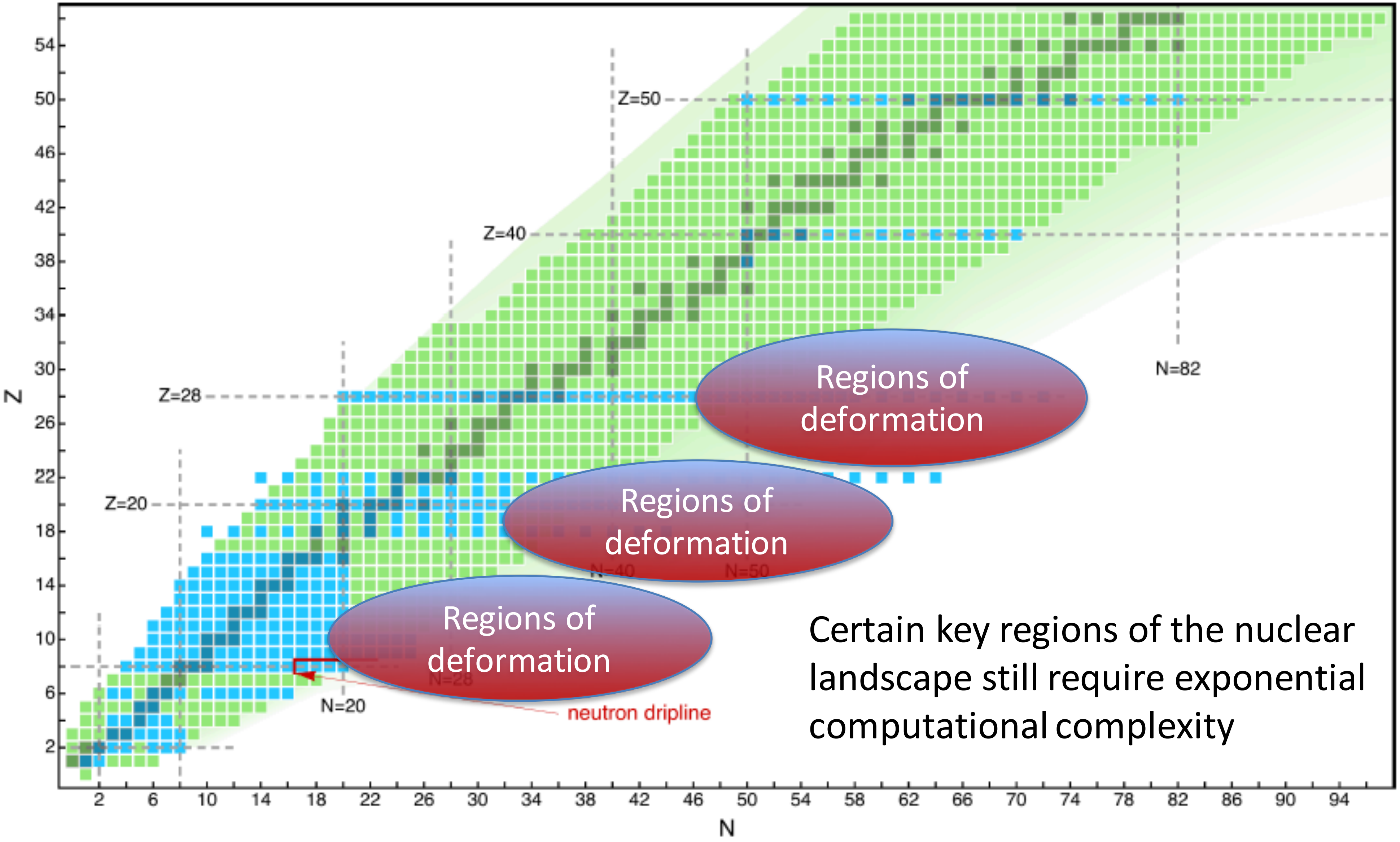
K. Hebeler *et al* PRC (2011).
T. Morris *et al*, PRL (2018).

Super allowed Gamow-Teller decay of ^{100}Sn



Gysbers, et al, Nature Physics, volume 15, pages 428–431 (2019)

Reach of ab-initio computations of nuclei



Regions of deformation

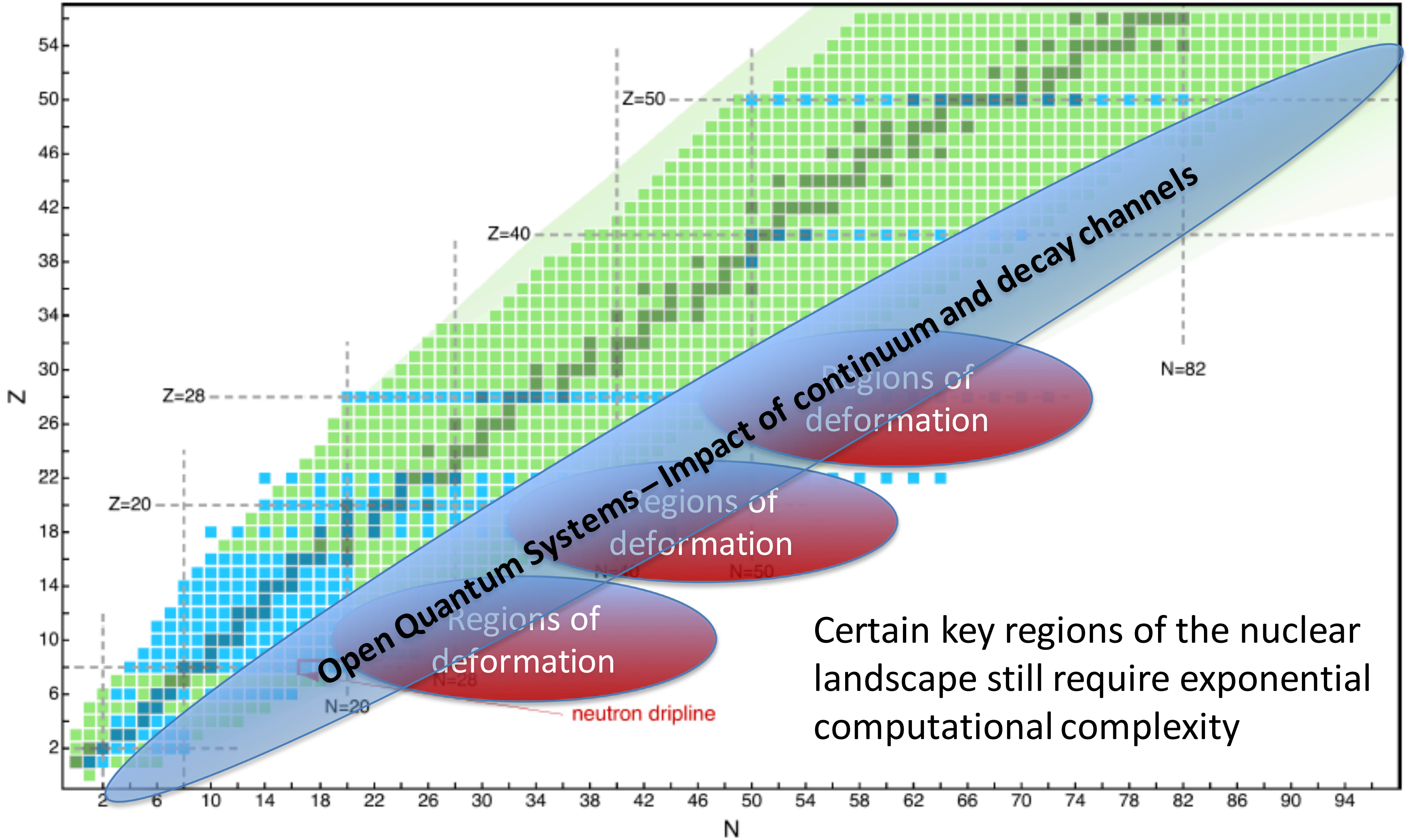
Regions of deformation

Regions of deformation

Certain key regions of the nuclear landscape still require exponential computational complexity

H. Hergert *et al*, Physics Reports 621, 165-222 (2016)

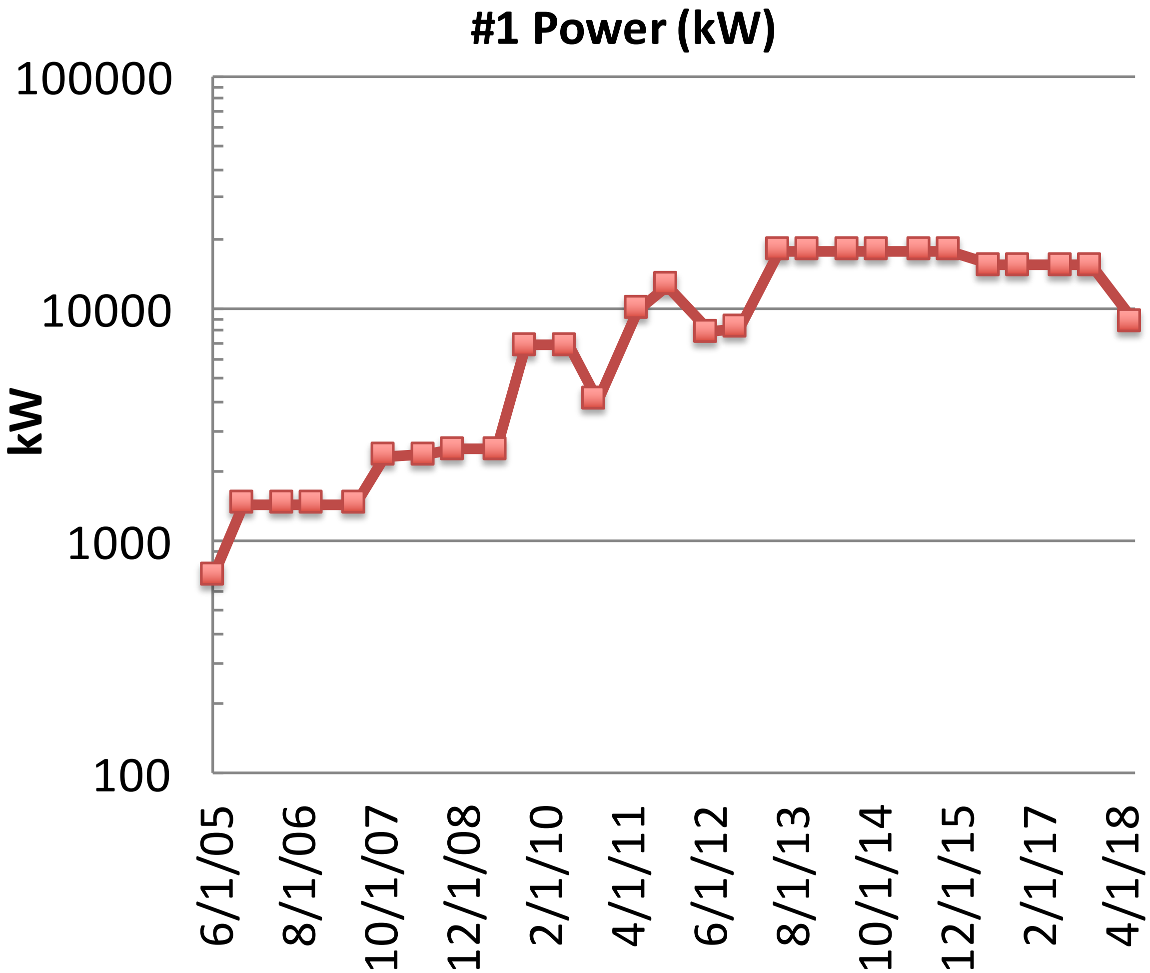
Reach of ab-initio computations of nuclei



Certain key regions of the nuclear landscape still require exponential computational complexity

H. Hergert *et al*, Physics Reports 621, 165-222 (2016)

A big issue: power



Incremental cost of running RHIC: $550k/week

Incremental cost of running Titan: $140k/week

Incremental cost of running Summit: $150k/week

(assume $0.1/kW-h)

June 2005 Tflop/kW = 0.191
June 2018 Tflop/kW = 13.88

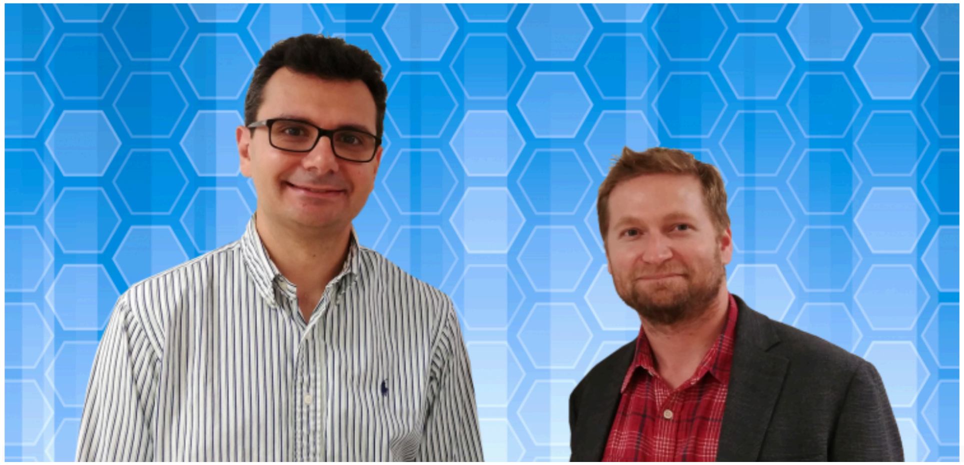
72x technology improvement

Nuclear Physics & Quantum Computing Collaboration at ORNL

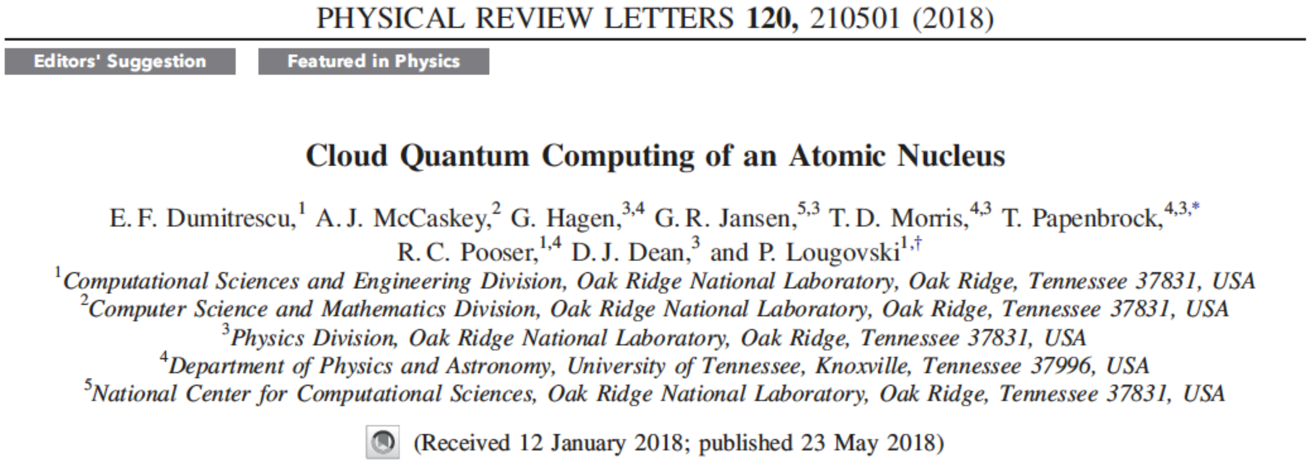
Two ORNL-led research teams receive $10.5 million to advance quantum computing for scientific applications (ORNL news, October 2017)


Eugene Dumitrescu


Alex McCaskey


Pavel Lougovski

Raphael Pooser


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,†]

[1]*Computational Sciences and Engineering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*
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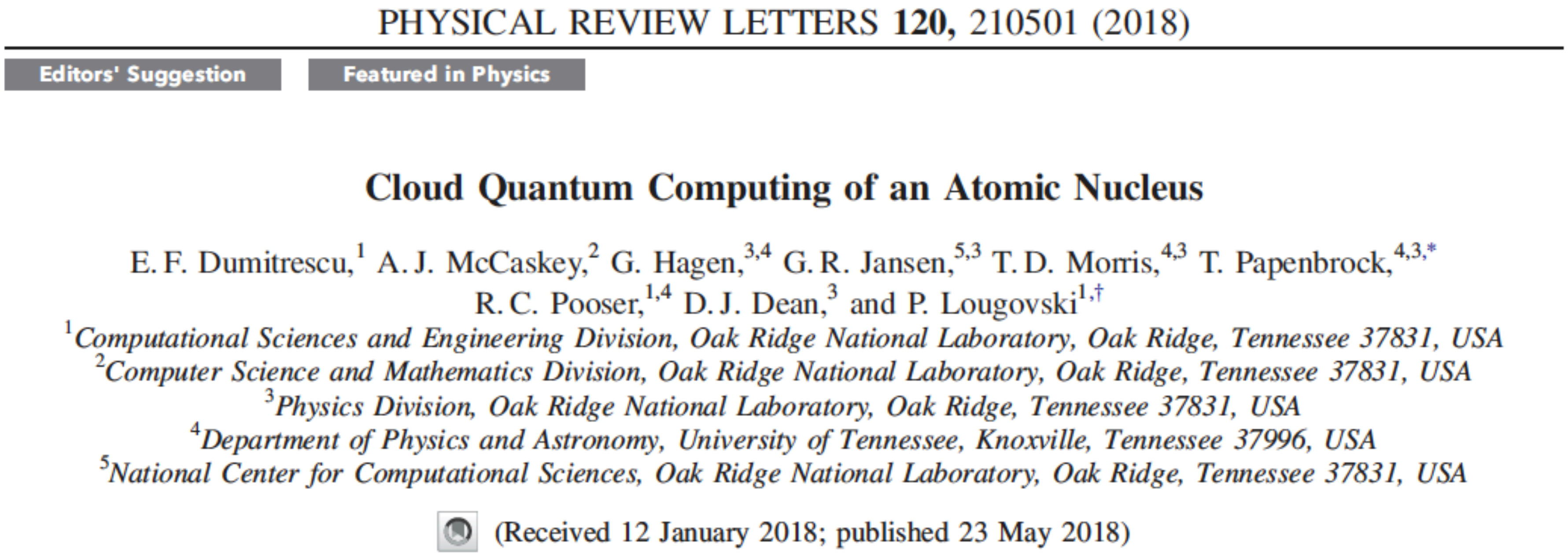
(Received 12 January 2018; published 23 May 2018)



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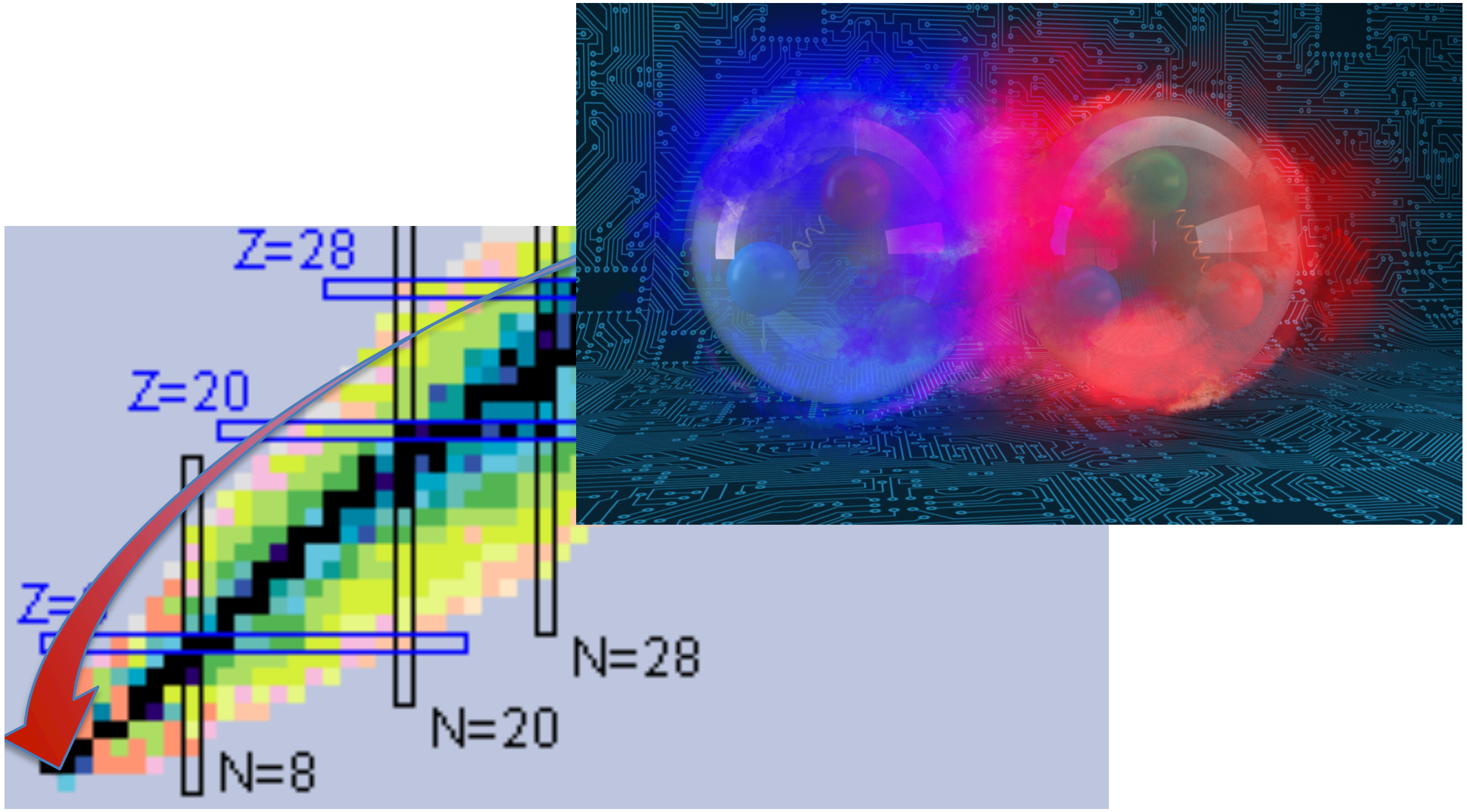
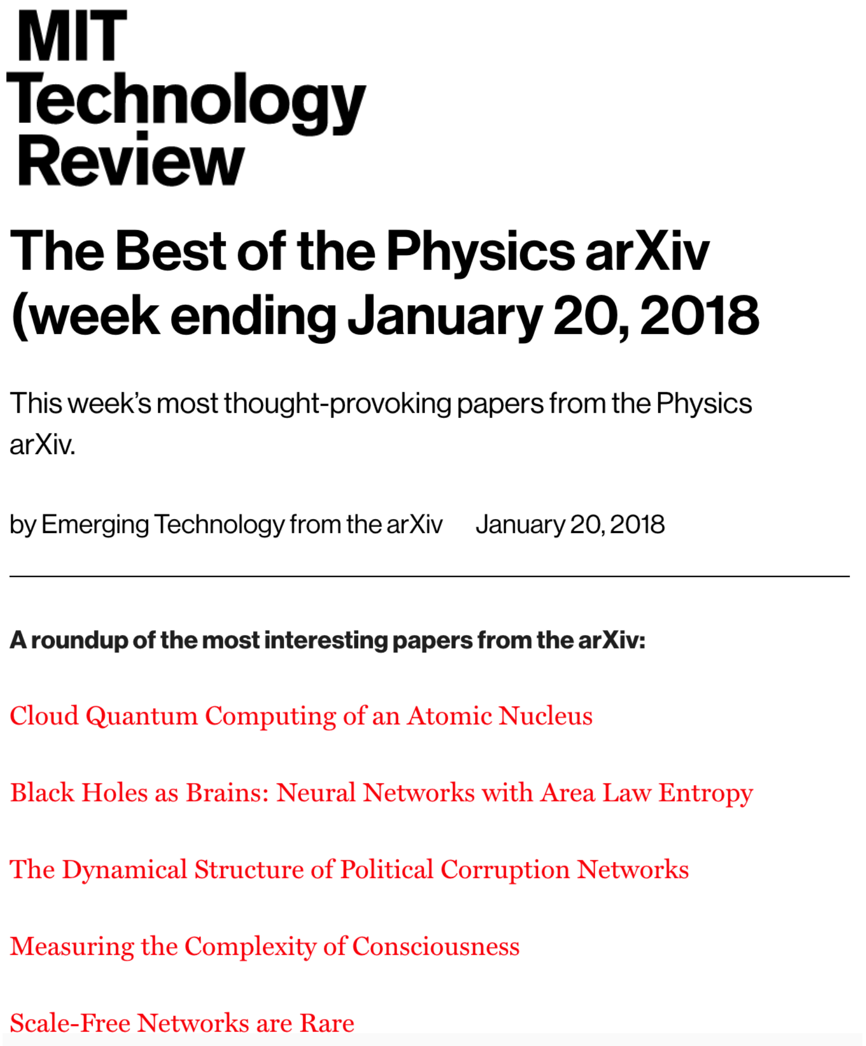


The deuteron is the lightest atomic nucleus consisting of a proton and neutron

Well studied and understood and suitable for existing quantum computers



MIT Technology Review

The Best of the Physics arXiv (week ending January 20, 2018

This week's most thought-provoking papers from the Physics arXiv.

by Emerging Technology from the arXiv January 20, 2018

A roundup of the most interesting papers from the arXiv:

Cloud Quantum Computing of an Atomic Nucleus

Black Holes as Brains: Neural Networks with Area Law Entropy

The Dynamical Structure of Political Corruption Networks

Measuring the Complexity of Consciousness

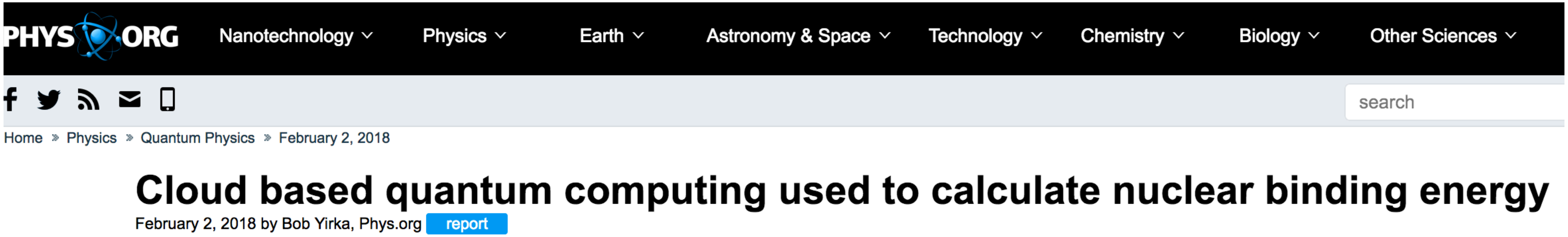
Scale-Free Networks are Rare

IOP Physics World - the member magazine of the Institute of Physics

physicsworld.com

Cloud quantum computing calculates nuclear binding energy

Jan 29, 2018



Cloud based quantum computing used to calculate nuclear binding energy

February 2, 2018 by Bob Yirka, Phys.org report

What can quantum computers possibly do well?

Some quantum algorithms outperform their classical counter parts:

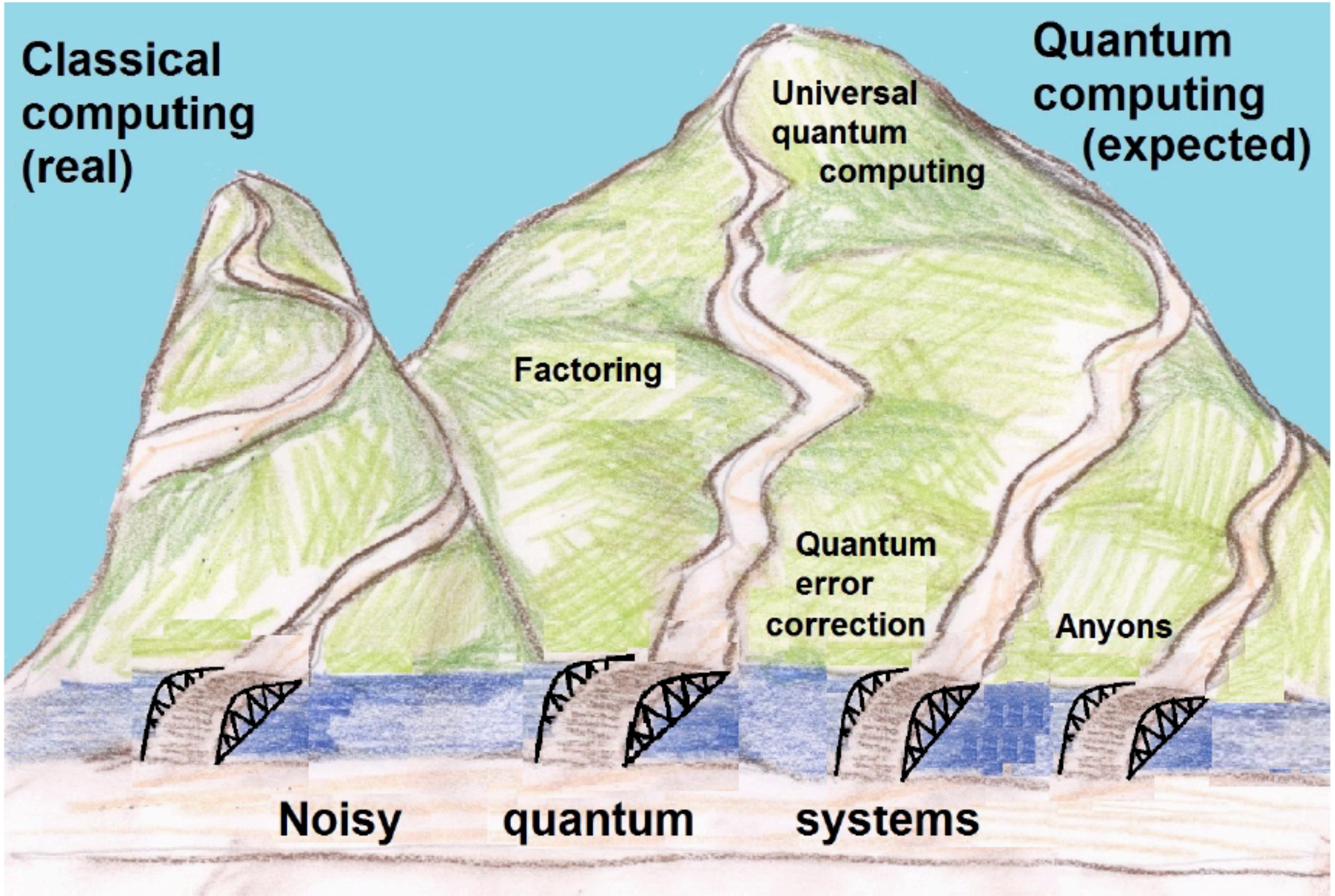
- Shor’s algorithm: factoring of integers
- Grover’s algorithm: inverting a function / searching an unordered list
- Quantum Fourier transform
- Quantum mechanics simulation: N qubits vs. 2^N complex numbers

Hope/expectation: quantum computing could solve problems with polynomial effort that are exponentially hard for classical computers.

Contrasting views:

1. We already have classical algorithms that yield approximate ground states for certain Hamiltonians/systems in polynomial time (e.g. DFT, coupled cluster method, IMSRG, Monte Carlo methods, …).
2. See Gil Kalai, arXiv:1605.00992 for a pessimistic view.

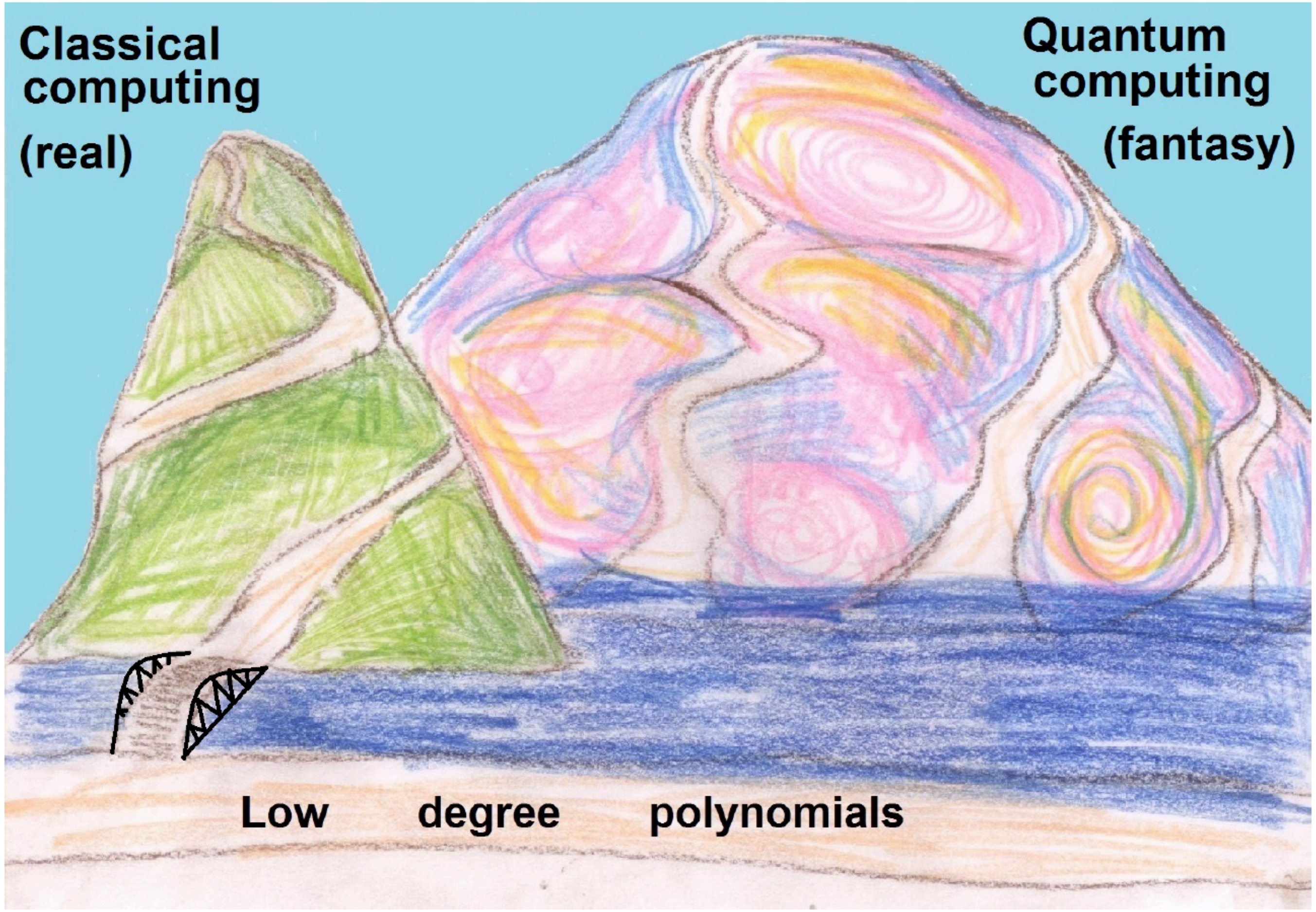
Optimistic view



Optimistic hypothesis: It is possible to realize universal quantum circuits with a small bounded error level regardless of the number of qubits. The effort required to obtain a bounded error level for universal quantum circuits increases moderately with the number of qubits. Therefore, <u>large-scale fault-tolerant quantum computers are possible</u>.

Gil Kalai, arXiv:1605.00992

Pessimistic view



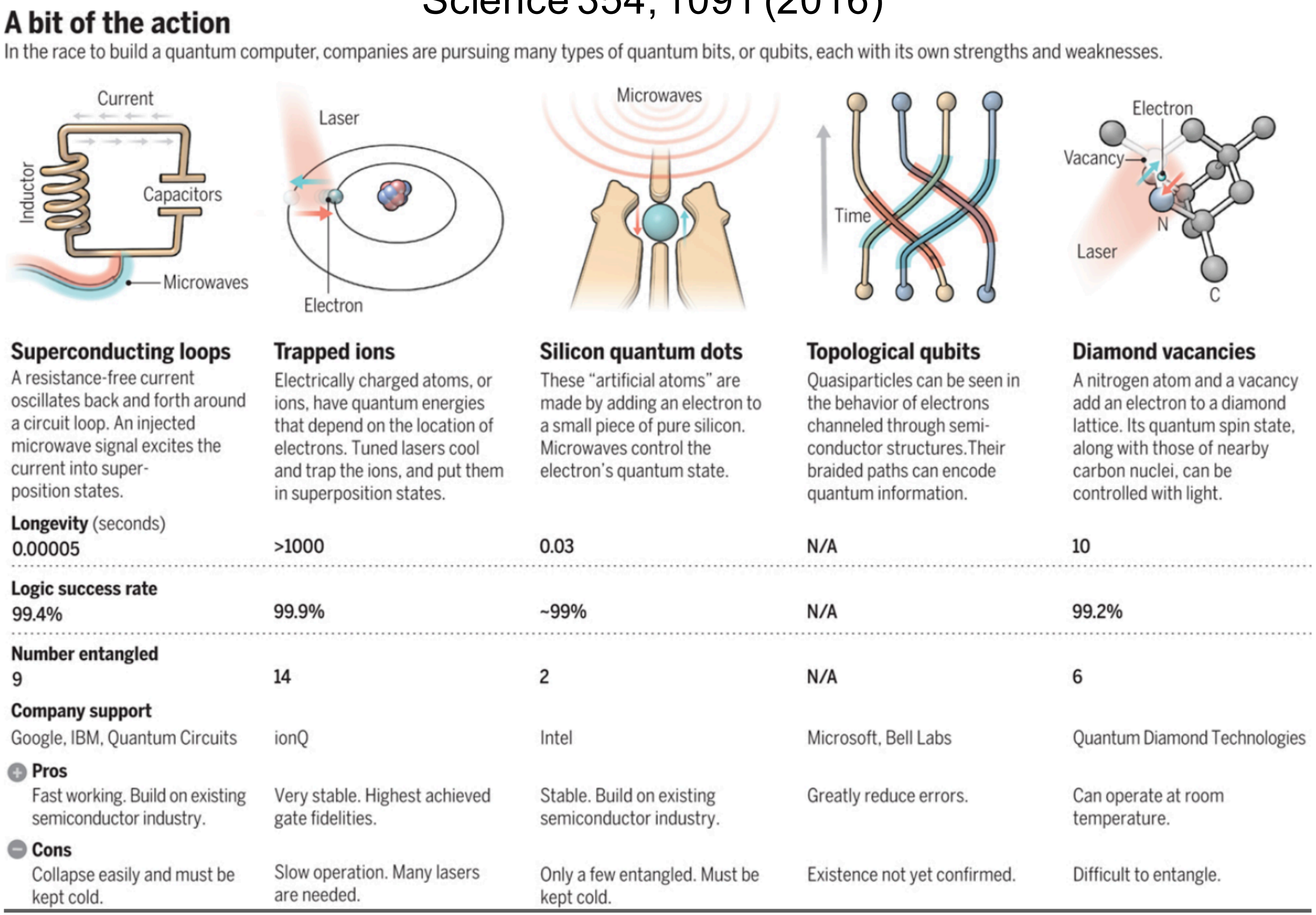
Pessimistic hypothesis: The error rate in every realization of universal quantum circuits scales up (at least) linearly with the number of qubits. The effort required to obtain a bounded error level for any implementation of universal quantum circuits increases (at least) exponentially with the number of qubits. Thus, quantum computers are not possible.

Gil Kalai, arXiv:1605.00992

How are QPUs realized?

Our work used transmon qubits (two-level system of Josephson junctions coupling an island with 0 or 1 Cooper pairs to a superconducting reservoir)

Science 354, 1091 (2016)

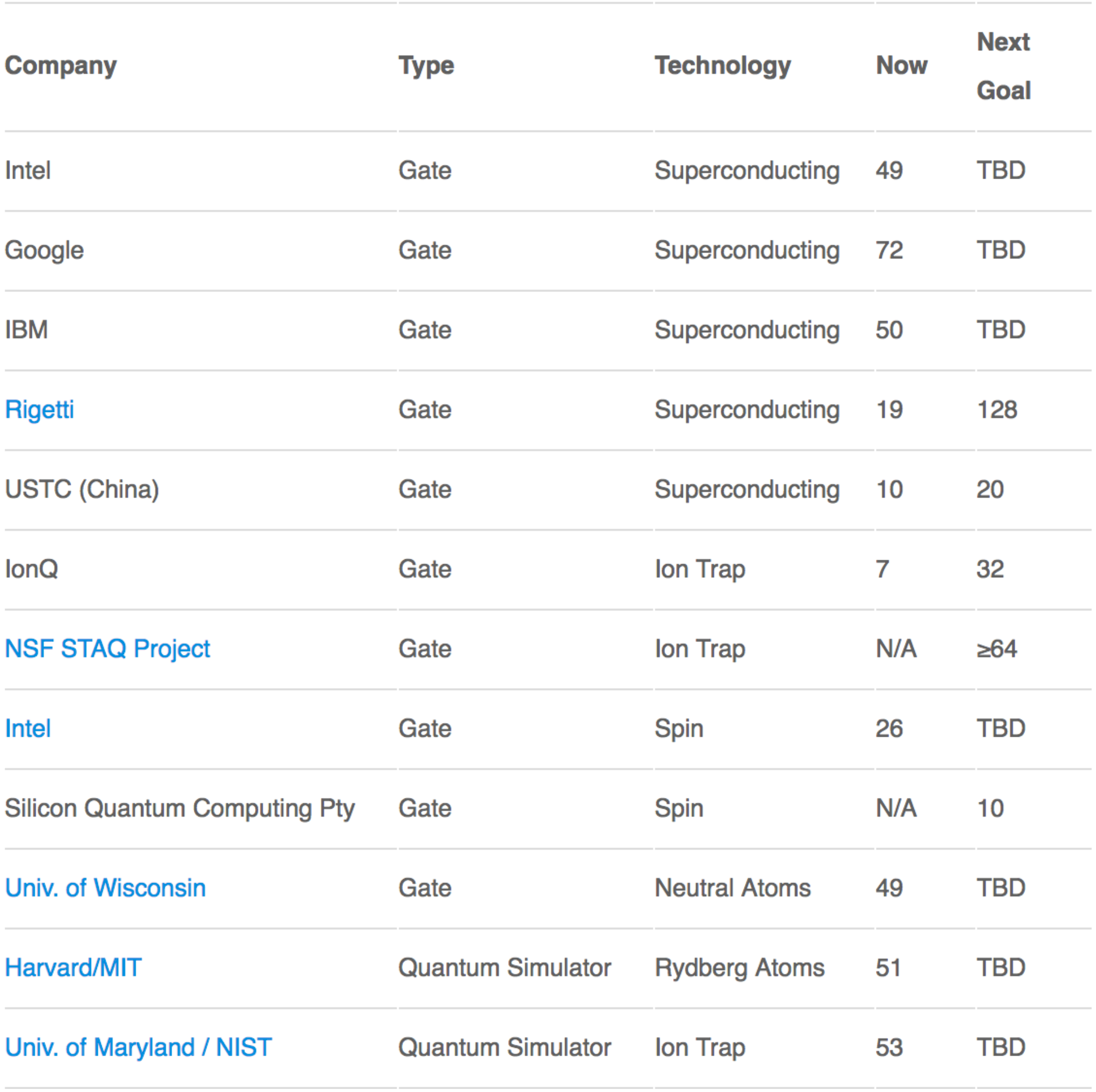


A bit of the action

In the race to build a quantum computer, companies are pursuing many types of quantum bits, or qubits, each with its own strengths and weaknesses.

	Superconducting loops	Trapped ions	Silicon quantum dots	Topological qubits	Diamond vacancies
	A resistance-free current oscillates back and forth around a circuit loop. An injected microwave signal excites the current into superposition states.	Electrically charged atoms, or ions, have quantum energies that depend on the location of electrons. Tuned lasers cool and trap the ions, and put them in superposition states.	These "artificial atoms" are made by adding an electron to a small piece of pure silicon. Microwaves control the electron's quantum state.	Quasiparticles can be seen in the behavior of electrons channeled through semiconductor structures. Their braided paths can encode quantum information.	A nitrogen atom and a vacancy add an electron to a diamond lattice. Its quantum spin state, along with those of nearby carbon nuclei, can be controlled with light.
Longevity (seconds)	0.00005	>1000	0.03	N/A	10
Logic success rate	99.4%	99.9%	~99%	N/A	99.2%
Number entangled	9	14	2	N/A	6
Company support	Google, IBM, Quantum Circuits	ionQ	Intel	Microsoft, Bell Labs	Quantum Diamond Technologies
⊕ **Pros**	Fast working. Build on existing semiconductor industry.	Very stable. Highest achieved gate fidelities.	Stable. Build on existing semiconductor industry.	Greatly reduce errors.	Can operate at room temperature.
⊖ **Cons**	Collapse easily and must be kept cold.	Slow operation. Many lasers are needed.	Only a few entangled. Must be kept cold.	Existence not yet confirmed.	Difficult to entangle.

Quantum computing – who's doing it?



Company	Type	Technology	Now	Next Goal
Intel	Gate	Superconducting	49	TBD
Google	Gate	Superconducting	72	TBD
IBM	Gate	Superconducting	50	TBD
Rigetti	Gate	Superconducting	19	128
USTC (China)	Gate	Superconducting	10	20
IonQ	Gate	Ion Trap	7	32
NSF STAQ Project	Gate	Ion Trap	N/A	≥64
Intel	Gate	Spin	26	TBD
Silicon Quantum Computing Pty	Gate	Spin	N/A	10
Univ. of Wisconsin	Gate	Neutral Atoms	49	TBD
Harvard/MIT	Quantum Simulator	Rydberg Atoms	51	TBD
Univ. of Maryland / NIST	Quantum Simulator	Ion Trap	53	TBD

Many more are building a quantum chip.

Source: QuantumComputingReport.com

Quantum computing

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: H2 molecule on two qubits [O'Malley et al., Phys. Rev. X 6, 031007 (2016)]; BeH2 on six qubits [Kandala et al., Nature 549, 242 (2017)]; ...

The scientific works were collaborations between theorists and hardware specialists (owners/operators of quantum chips).

Quantum computation of H_2 molecule using a hybrid quantum/classical algorithm

SCALABLE QUANTUM SIMULATION OF MOLECULAR ENERGIES PHYS. REV. X **6**, 031007 (2016)

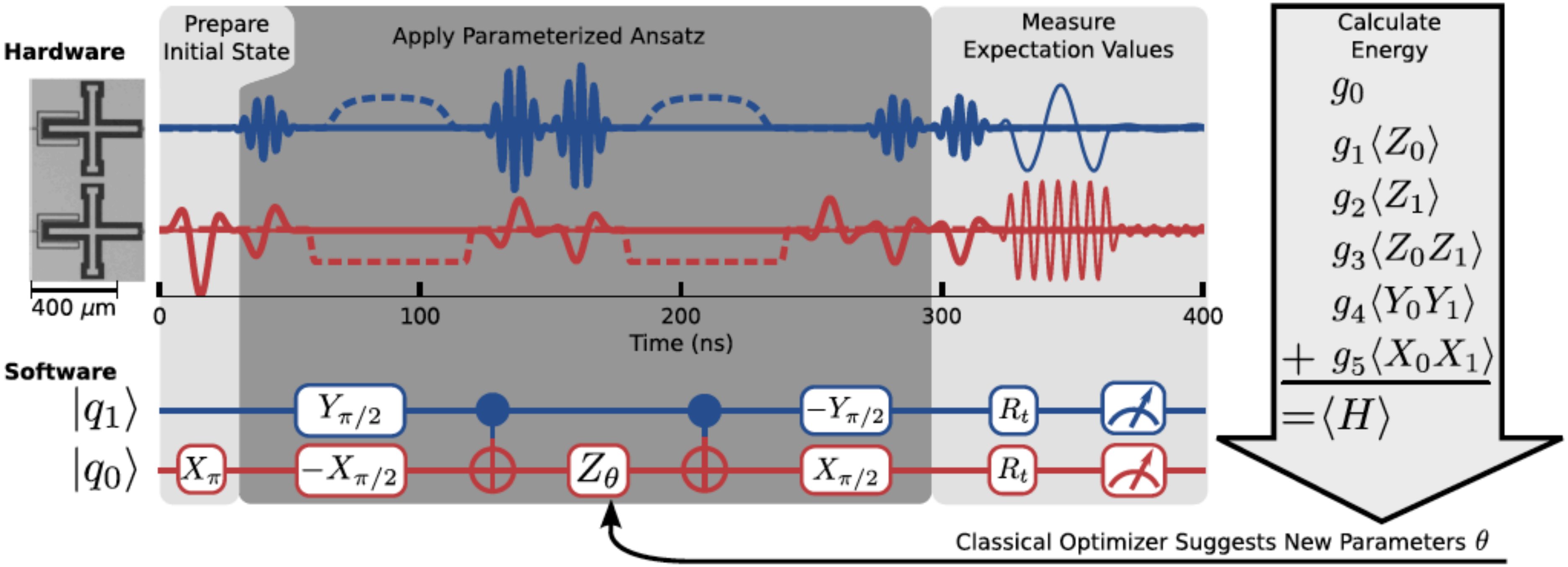
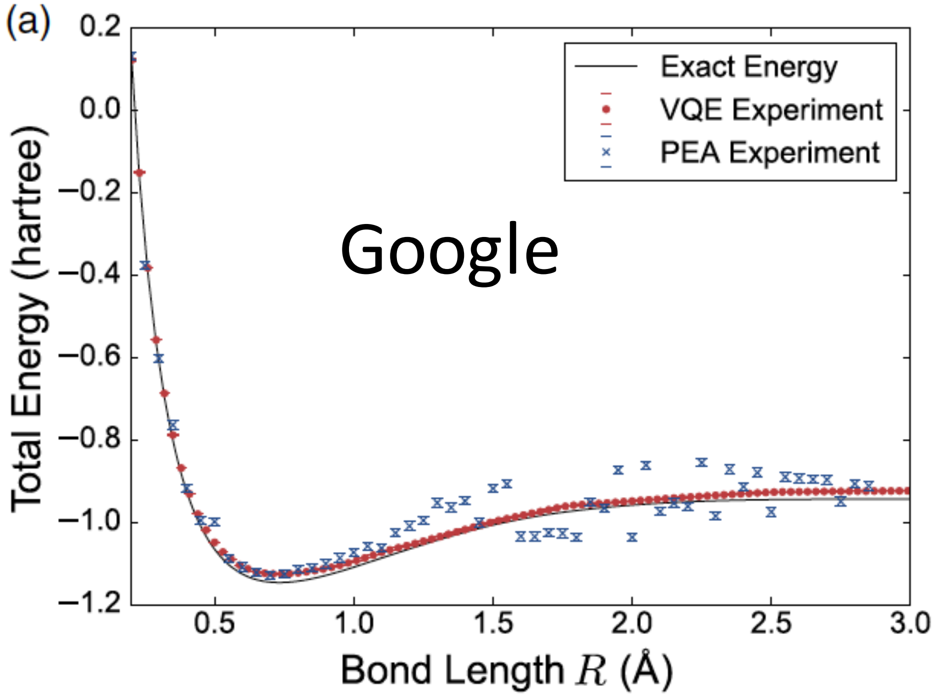


FIG. 1. Hardware and software schematic of the variational quantum eigensolver. (Hardware) micrograph shows two Xmon transmon qubits and microwave pulse sequences to perform single-qubit rotations (thick lines), dc pulses for two-qubit entangling gates (dashed lines), and microwave spectroscopy tones for qubit measurements (thin lines). (Software) quantum circuit diagram shows preparation of the Hartree-Fock state, followed by application of the unitary coupled cluster ansatz in Eq. (3) and efficient partial tomography (R_t) to measure the expectation values in Eq. (1). Finally, the total energy is computed according to Eq. (4) and provided to a classical optimizer which suggests new parameters

$$H = g_0 \mathbb{1} + g_1 Z_0 + g_2 Z_1 + g_3 Z_0 Z_1 + g_4 Y_0 Y_1 + g_5 X_0 X_1$$

Quantum computation of H_2 molecule using a hybrid quantum/classical algorithm

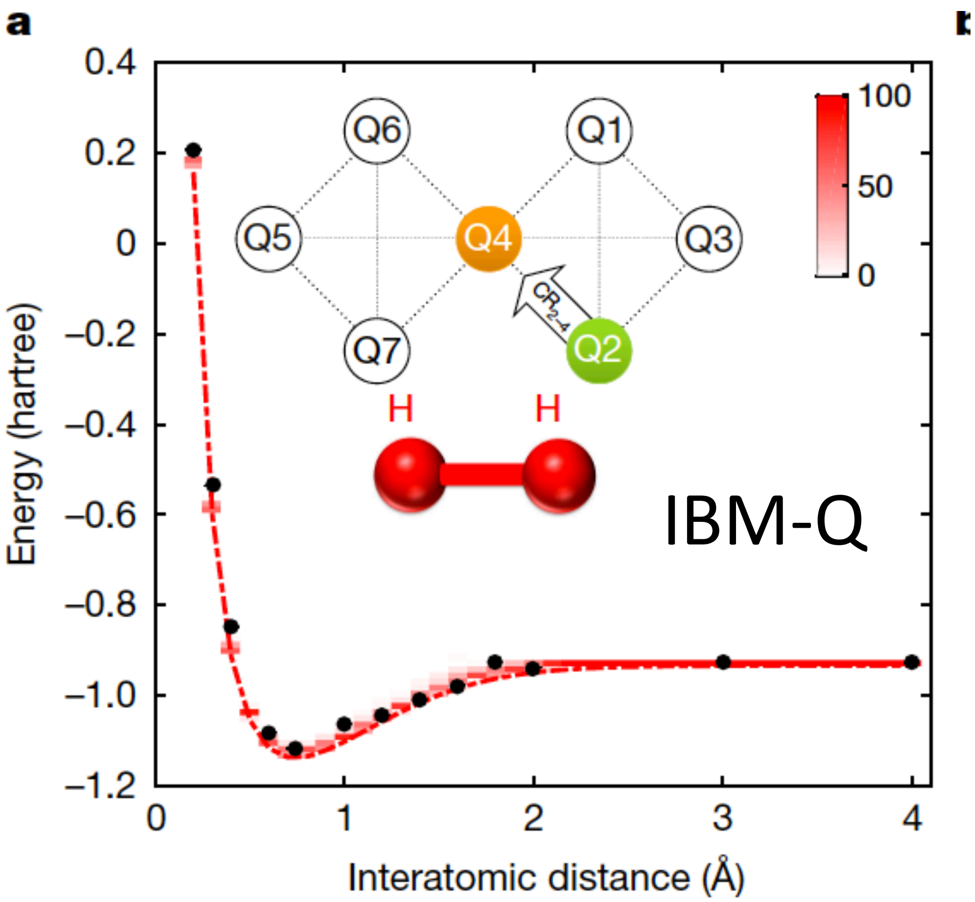
O'Malley et al. Phys. Rev. X 6, 031007 (2016)



Google

Kandala et al used 10^5 measurements on the IBM-Q for the BeH_2 molecule. The Hamiltonian consisted of more than hundred Pauli terms

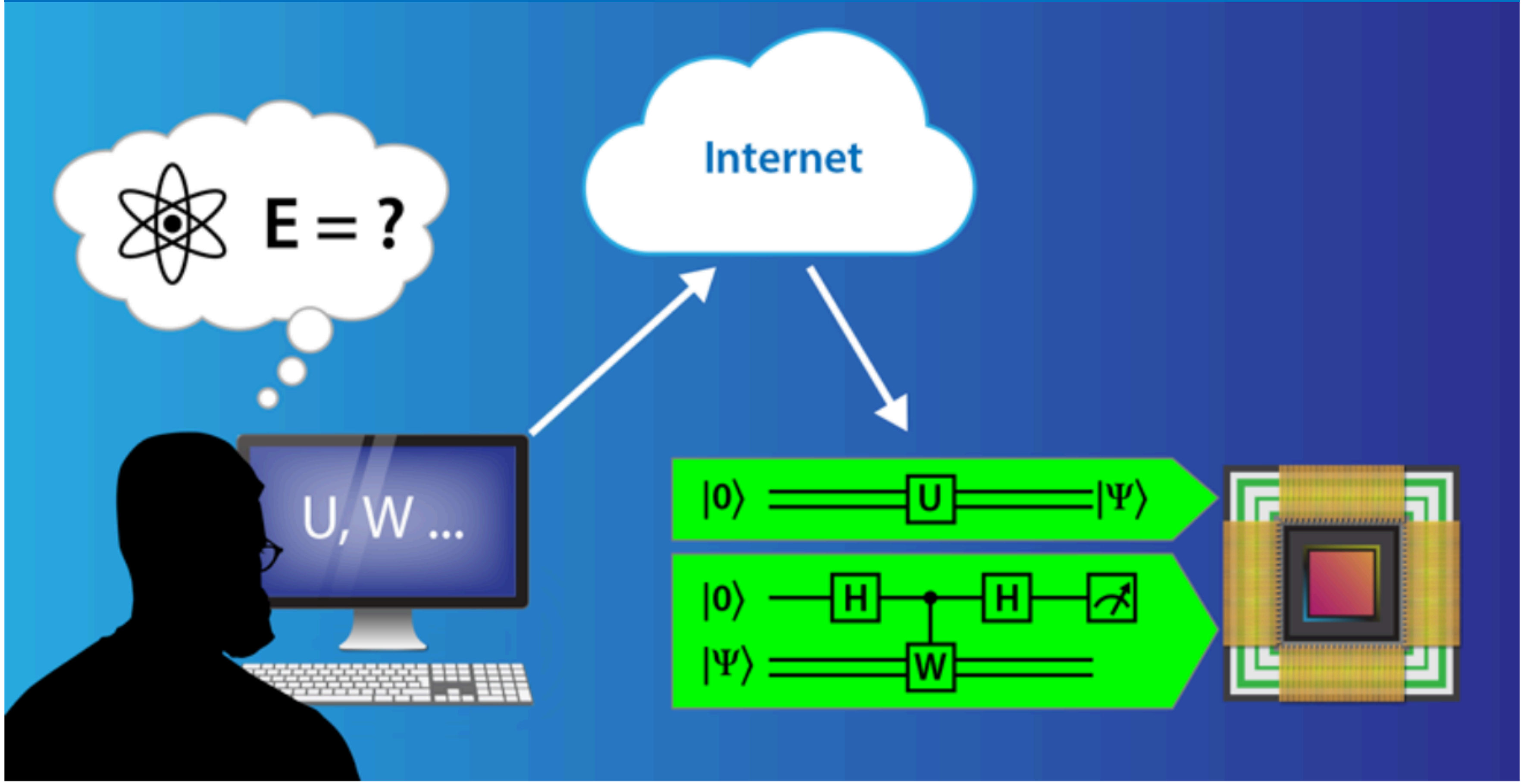
Kandala et al., Nature 549, 242-246 (2017)



IBM-Q

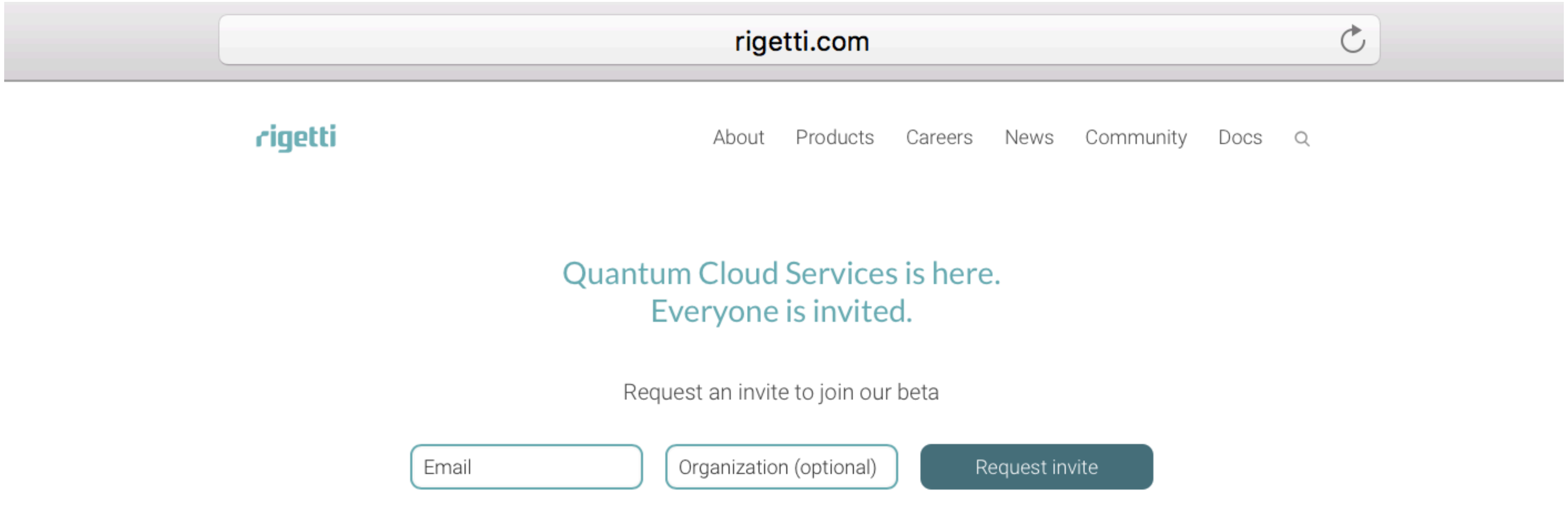
Cloud access to quantum computers/simulators

Now: Cloud access possible; no insider knowledge required!
[Dumitrescu, McCaskey, Hagen, Jansen, Morris, TP, Pooser, Dean, Lougovski,
Phys. Rev. Lett. **120**, 210501 (2018)]



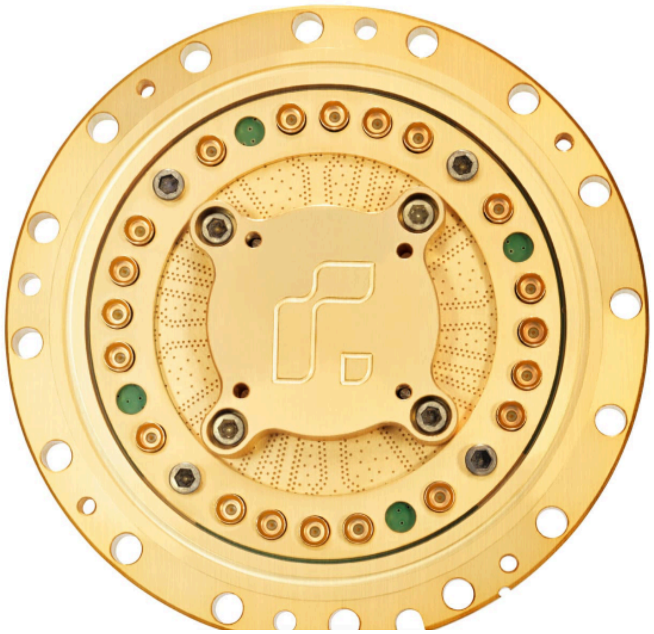
Source: S. Gandofli, Physics Viewpoint,
https://physics.aps.org/articles/v11/51

Cloud access to quantum computers/simulators



Quantum Cloud Services is here.
Everyone is invited.

Request an invite to join our beta

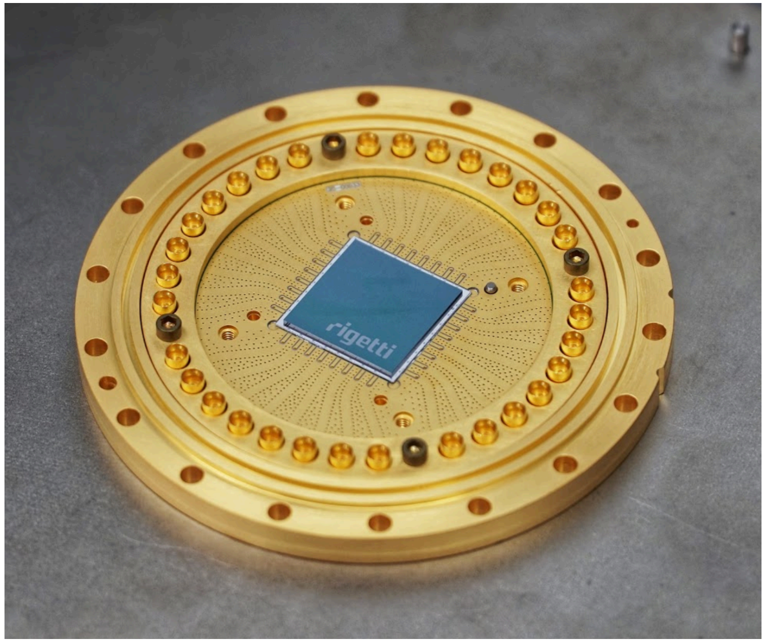


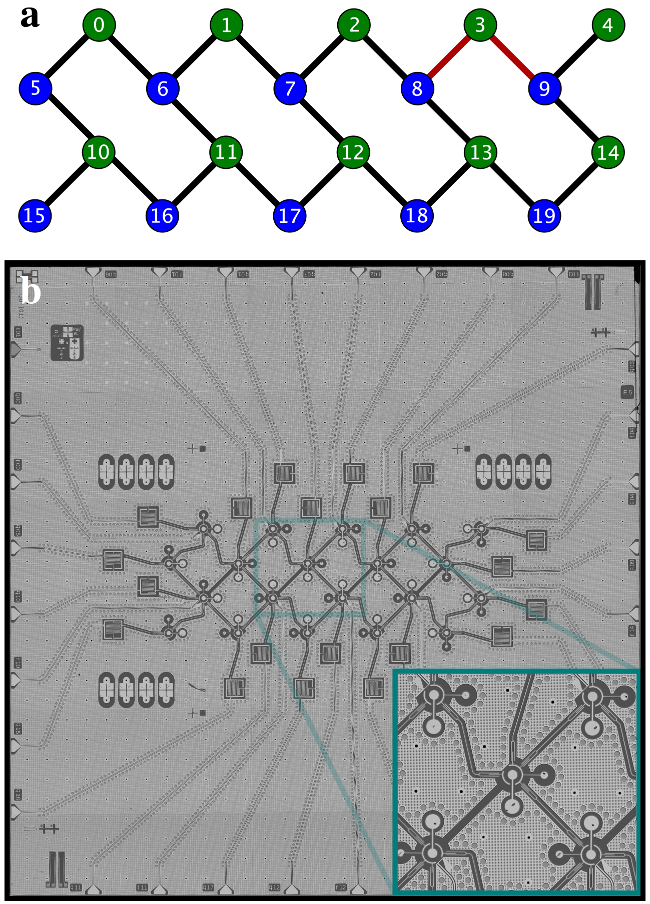
Can quantum computing live up to the hype?

$1 million prize for the first conclusive demonstration of quantum advantage on QCS

Rigetti 19Q

Superconducting qubits

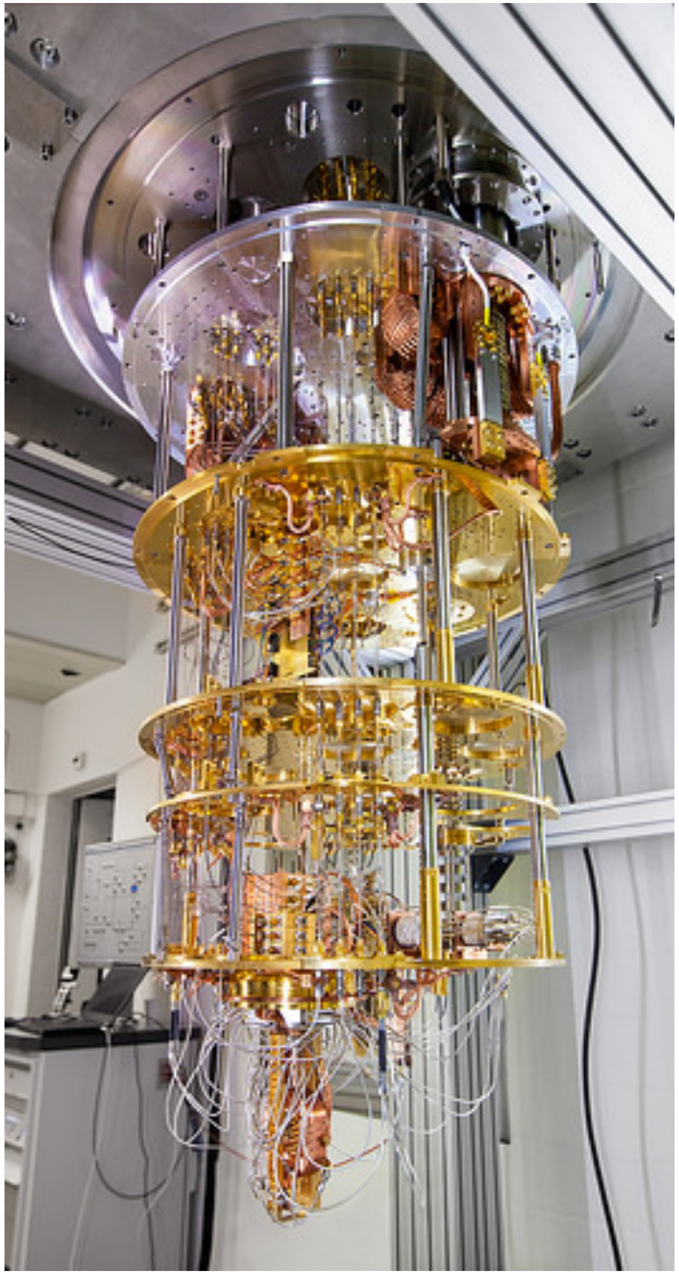


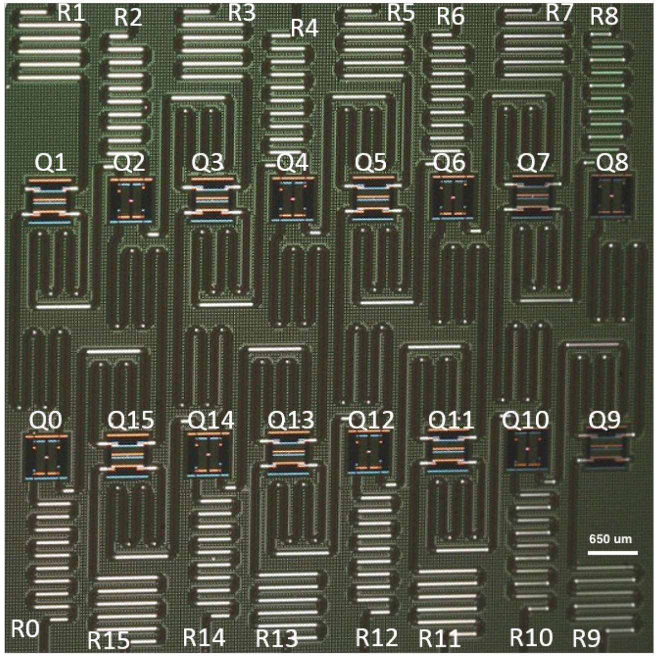


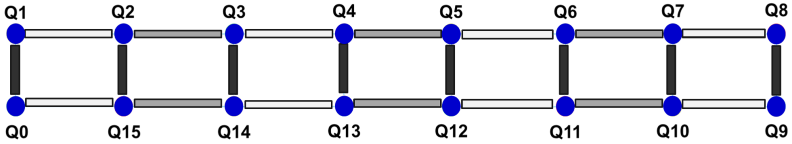
Connectivity of Rigetti 19Q.
a, *Chip schematic showing tunable transmons (green circles) capacitively coupled to fixed-frequency transmons (blue circles).*
b, *Optical chip image. Note that some couplers have been dropped to produce a lattice with three-fold, rather than four-fold connectivity.*

Otterbach et al, arXiv:1712.05771

IBM QX5 (16 qubits)

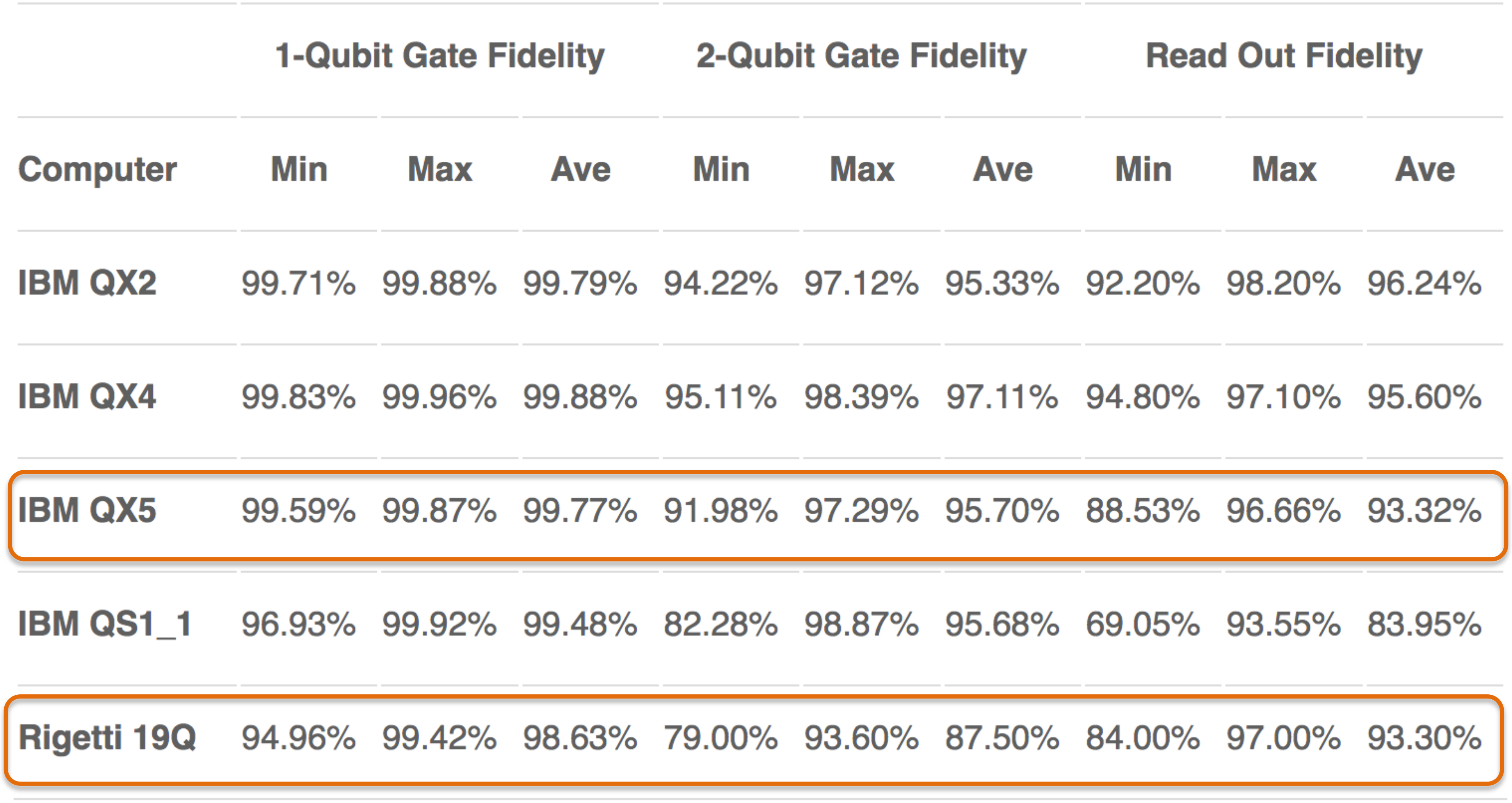






→ IBM Q Experience

Qubit fidelities



	1-Qubit Gate Fidelity			2-Qubit Gate Fidelity			Read Out Fidelity		
Computer	**Min**	**Max**	**Ave**	**Min**	**Max**	**Ave**	**Min**	**Max**	**Ave**
IBM QX2	99.71%	99.88%	99.79%	94.22%	97.12%	95.33%	92.20%	98.20%	96.24%
IBM QX4	99.83%	99.96%	99.88%	95.11%	98.39%	97.11%	94.80%	97.10%	95.60%
IBM QX5	99.59%	99.87%	99.77%	91.98%	97.29%	95.70%	88.53%	96.66%	93.32%
IBM QS1_1	96.93%	99.92%	99.48%	82.28%	98.87%	95.68%	69.05%	93.55%	83.95%
Rigetti 19Q	94.96%	99.42%	98.63%	79.00%	93.60%	87.50%	84.00%	97.00%	93.30%

Sources: QuantumComputingReport.com; Rigetti.com

Mitigating exisiting constraints

1. Gate errors, decoherence → low-depth circuit
2. Limited connectivity of qubits → tailored, simple Hamiltonian
3. Cloud access → only expectation values on QPU
4. Limited fidelity → noise correction

Game plan

1. Hamiltonian from pionless EFT at leading order; fit to deuteron binding energy; constructed in harmonic-oscillator basis of $^3S_1$ partial wave [à la Binder et al. (2016); **Aaina Bansal et al. (2017)**]; cutoff at about 150 MeV.

$$H_N = \sum_{n,n'=0}^{N-1} \langle n'|(T+V)|n\rangle a^\dagger_{n'} a_n \qquad \langle n'|V|n\rangle = V_0 \delta^0_n \delta^{n'}_n$$

$$V_0 = -5.68658111 \text{ MeV}$$

For example the $N = 2$ Hamiltonian is given by:

$$H_2 = \begin{bmatrix} -1.677 & 2.339 \\ 2.339 & 22.242 \end{bmatrix}$$

Easily diagonalized on a piece of paper.

Game plan

2. Map single-particle states |n⟩ onto qubits using |0⟩ = |↑⟩ and |1⟩ = |↓⟩. This is an analog of the Jordan-Wigner transform.

$$a_p^\dagger \leftrightarrow \sigma_-^{(p)} \equiv \frac{1}{2}(X_p - iY_p) \qquad a_p \leftrightarrow \sigma_+^{(p)} \equiv \frac{1}{2}(X_p + iY_p)$$

$$H_2 = \begin{bmatrix} -1.677 & 2.339 \\ 2.339 & 22.242 \end{bmatrix} =$$

$$5.9067I + 0.21729Z_0 - 0.125Z_1 - 2.143(X_0X_1 + Y_0Y_1)$$

3. Solve H_1, H_2 (and H_3) and extrapolate to infinite space using harmonic oscillator variant of Lüscher's formula [More, Furnstahl, Papenbrock (2013)]

$$E_N = -\frac{\hbar^2 k^2}{2m}\left(1 - 2\frac{\gamma^2}{k}e^{-2kL} - 4\frac{\gamma^4 L}{k}e^{-4kL}\right) + \frac{\hbar^2 k\gamma^2}{m}\left(1 - \frac{\gamma^2}{k} - \frac{\gamma^4}{4k^2} + 2w_2 k\gamma^4\right)e^{-4kL}$$

Variational wave function

Wave functions on two qubits

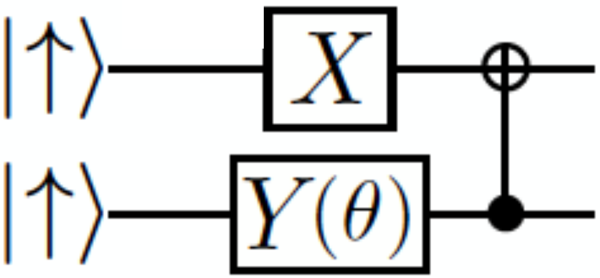
$$U(\theta)|{\downarrow\uparrow}\rangle \qquad U(\theta) \equiv e^{\theta\left(a_0^\dagger a_1 - a_1^\dagger a_0\right)} = e^{i\frac{\theta}{2}(X_0 Y_1 - X_1 Y_0)}$$

Wave functions on three qubits

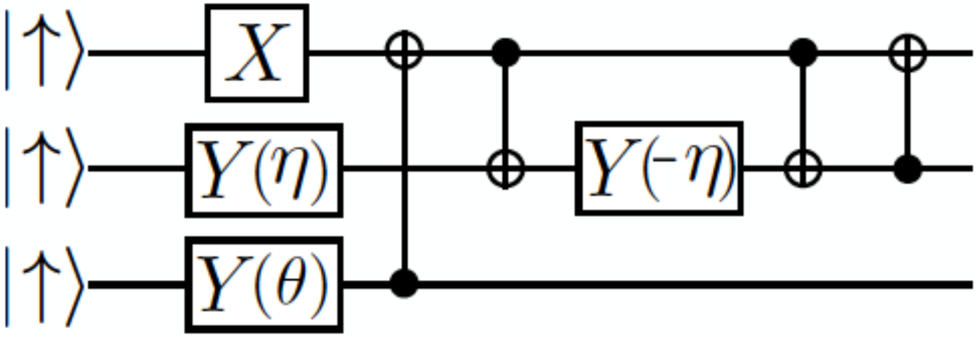
$$U(\eta,\theta)|{\downarrow\uparrow\uparrow}\rangle \qquad U(\eta,\theta) \equiv e^{\eta\left(a_0^\dagger a_1 - a_1^\dagger a_0\right) + \theta\left(a_0^\dagger a_2 - a_2^\dagger a_0\right)}$$

Minimize number of two-qubit CNOT operations to mitigate low two-qubit fidelities (construct a “low-depth circuit”)

$U(\theta)$

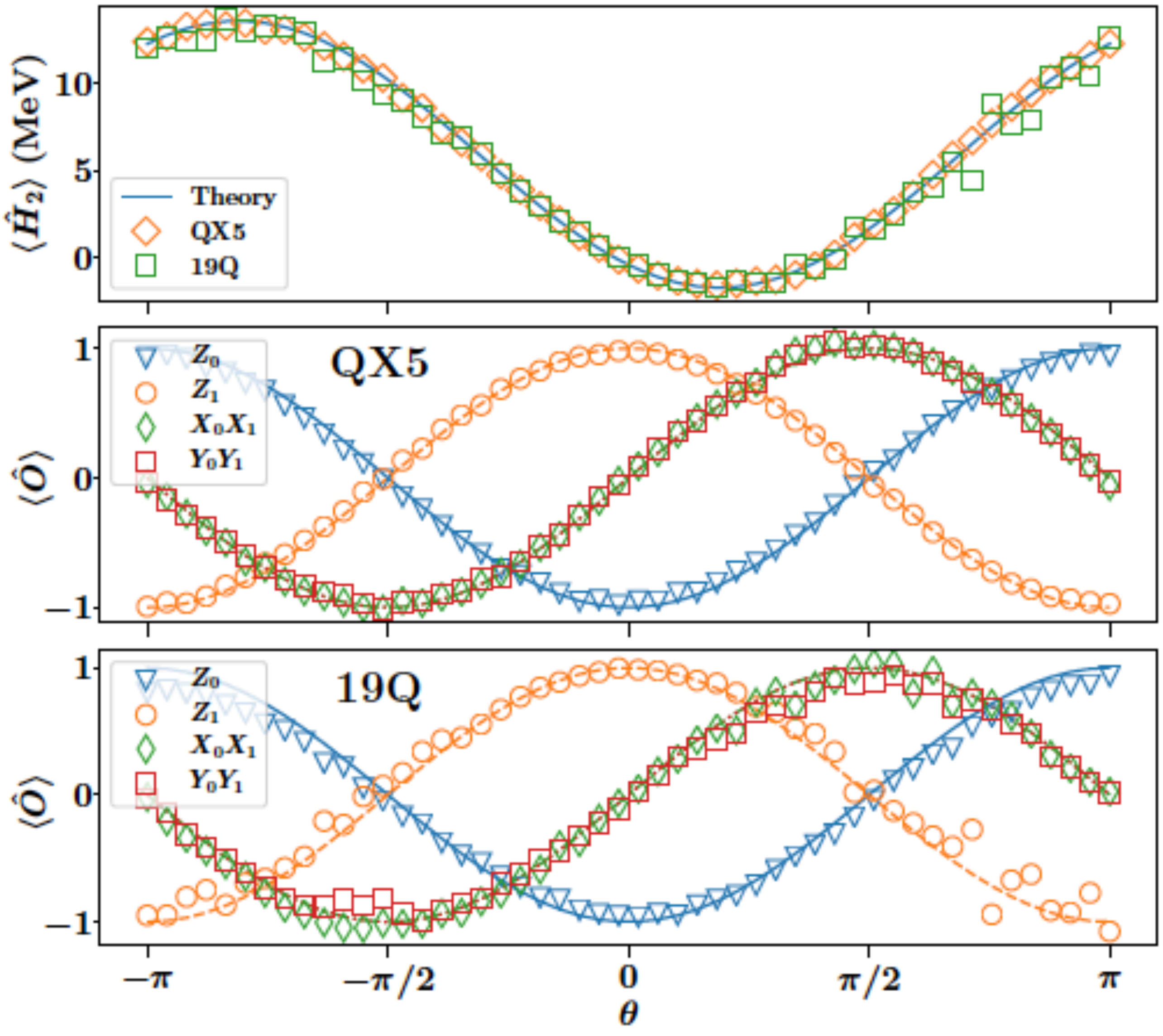


$U(\eta,\theta)$



Hamiltonian on two qubits

$$H_2 = 5.906709 I + 0.218291 Z_0 - 6.125 Z_1 - 2.143304 \left(X_0 X_1 + Y_0 Y_1 \right)$$



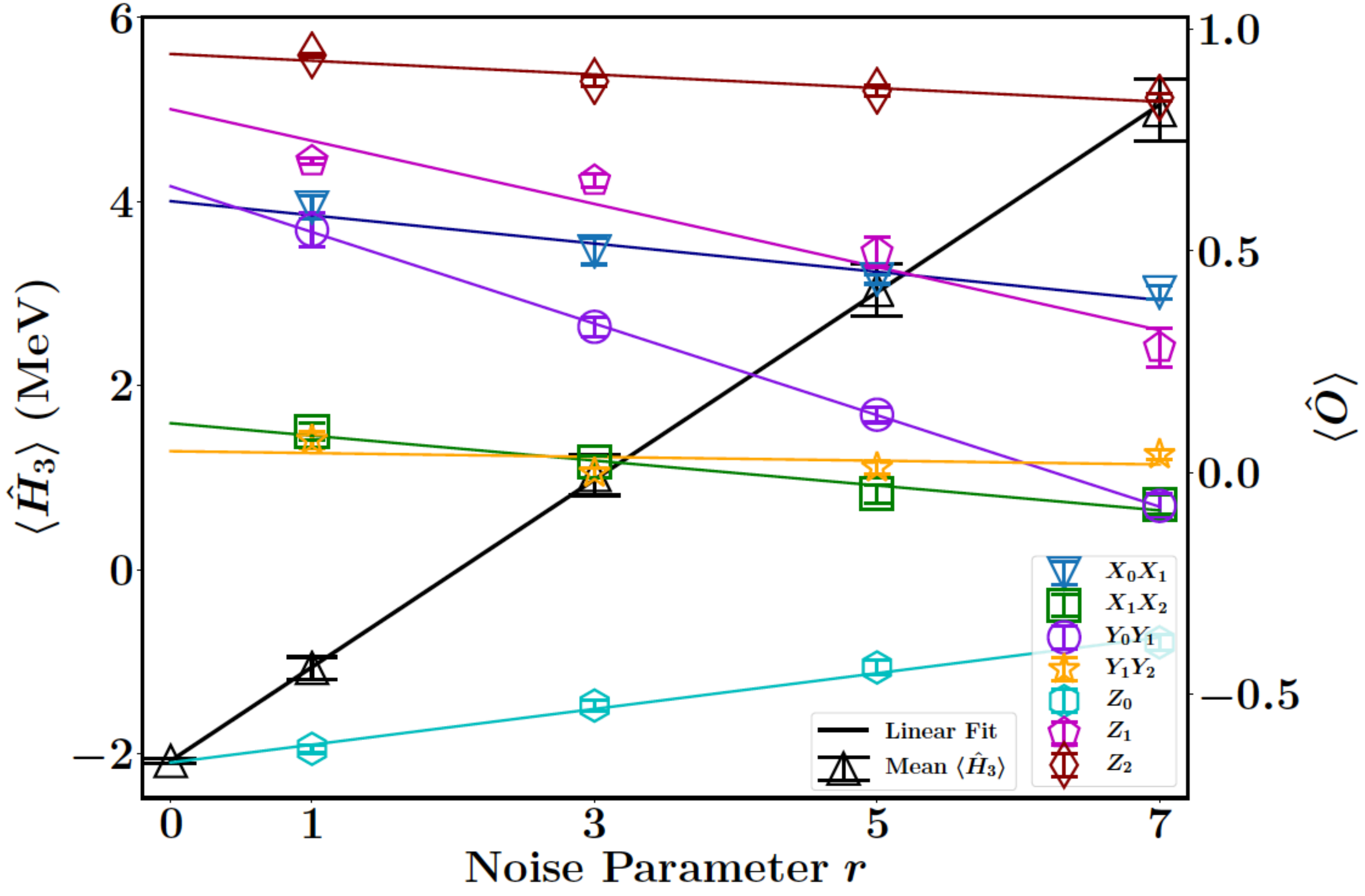
Quantum-classical hybrid algorithm VQE [Peruzzo et al. 2014; McClean et al 2016]:

Expectation values on QPU. Minimization on CPU.

To manage noise we performed 8,192 (10,000) measurements on QX5 (19Q)

Three qubits

$$H_3 = H_2 + 9.625(I - Z_2) - 3.913119\,(X_1X_2 + Y_1Y_2)$$



Three qubits have more noise. Insert pairs of CNOT (unity operators) to extrapolate to *r*=0. [See, e.g., Ying Li & S. C. Benjamin 2017]

Final results

Deuteron ground-state energies from a quantum computer compared to the exact result, E_∞=-2.22 MeV.

E from exact diagonalization

N	E_N	$\mathcal{O}(e^{-2kL})$	$\mathcal{O}(kLe^{-4kL})$	$\mathcal{O}(e^{-4kL})$
2	-1.749	-2.39	-2.19	
3	-2.046	-2.33	-2.20	-2.21

E from quantum computing

N	E_N	$\mathcal{O}(e^{-2kL})$	$\mathcal{O}(kLe^{-4kL})$	$\mathcal{O}(e^{-4kL})$
2	$-1.74(3)$	$-2.38(4)$	$-2.18(3)$	
3	$-2.08(3)$	$-2.35(2)$	$-2.21(3)$	$-2.28(3)$

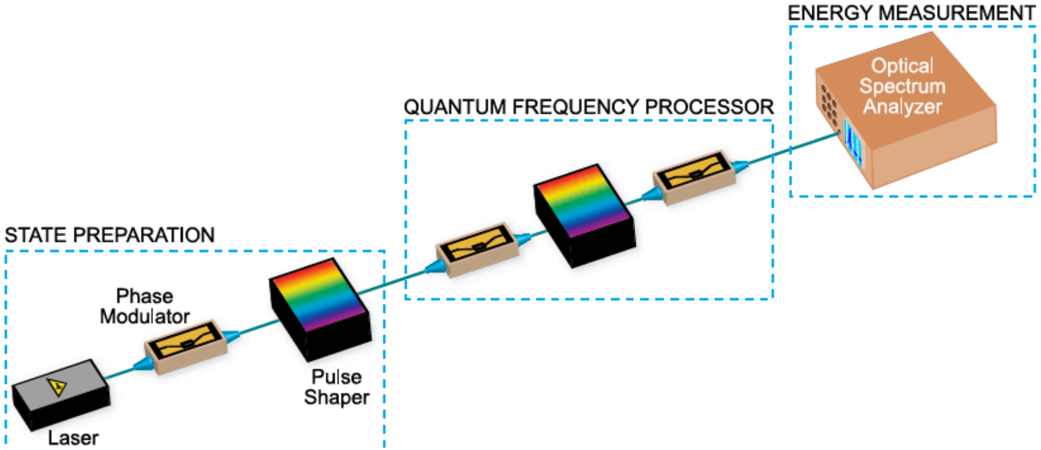
$$E_N = -\frac{\hbar^2 k^2}{2m}\left(1 - 2\frac{\gamma^2}{k}e^{-2kL} - 4\frac{\gamma^4 L}{k}e^{-4kL}\right) + \frac{\hbar^2 k\gamma^2}{m}\left(1 - \frac{\gamma^2}{k} - \frac{\gamma^4}{4k^2} + 2w_2 k\gamma^4\right)e^{-4kL}$$

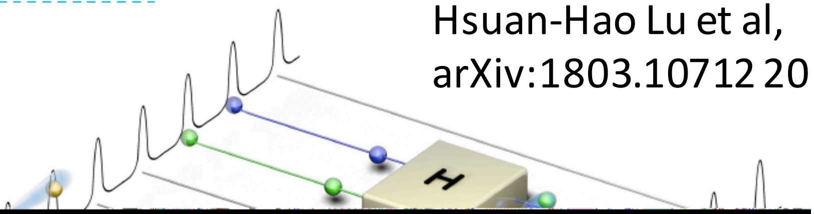
[Dumitrescu, McCaskey, Hagen, Jansen, Morris, TP, Pooser, Dean, Lougovski,
Phys. Rev. Lett. **120**, 210501 (2018)]

Simulations of atomic nuclei on a quantum frequency processor

Use an all-optical quantum frequency processor (QFP), to compute the ground-state energies of the light nuclei with a record-high 68-dimensional Hilbert space

- Encode qubits into narrow frequency bins
- Prepare quantum state by use a pulse shaper to modulate amplitude and phase of each frequency
- Use QFP to mix adjacent frequency bins equivalent to measure the density matrix
- Calculate expectation value





Hsuan-Hao Lu et al, arXiv:1803.10712 2018)

[redacted]

Hsuan-Hao Lu, Natalie Klco, Joseph M. Lukens, Titus D. Morris, et al, arXiv:1810.03959 (2018)

Simulating atomic nuclei on a QFP

Use pion-less EFT at NLO with contact parameters adjusted to effective range and deuteron/triton binding energies

Map Hamiltonian onto QFP:

$$H_{QFP} = \sum_{k=0}^{N-1} h_{kk}\hat{c}_k^\dagger \hat{c}_k + \sum_{\substack{i,j=0 \\ i<j}}^{N-1} [h_{ij}\hat{c}_i^\dagger \hat{c}_j + h_{ji}^* \hat{c}_j^\dagger \hat{c}_i].$$

Use VQE and with a unitary coupled-cluster ansatz:

$$|\Psi\rangle = \exp\left(\sum_{k=1}^{N-1} \theta_k [\hat{c}_0^\dagger \hat{c}_k - \hat{c}_k^\dagger \hat{c}_0]\right) |10\cdots 0\rangle$$

Measure the expectation value on the QFP:

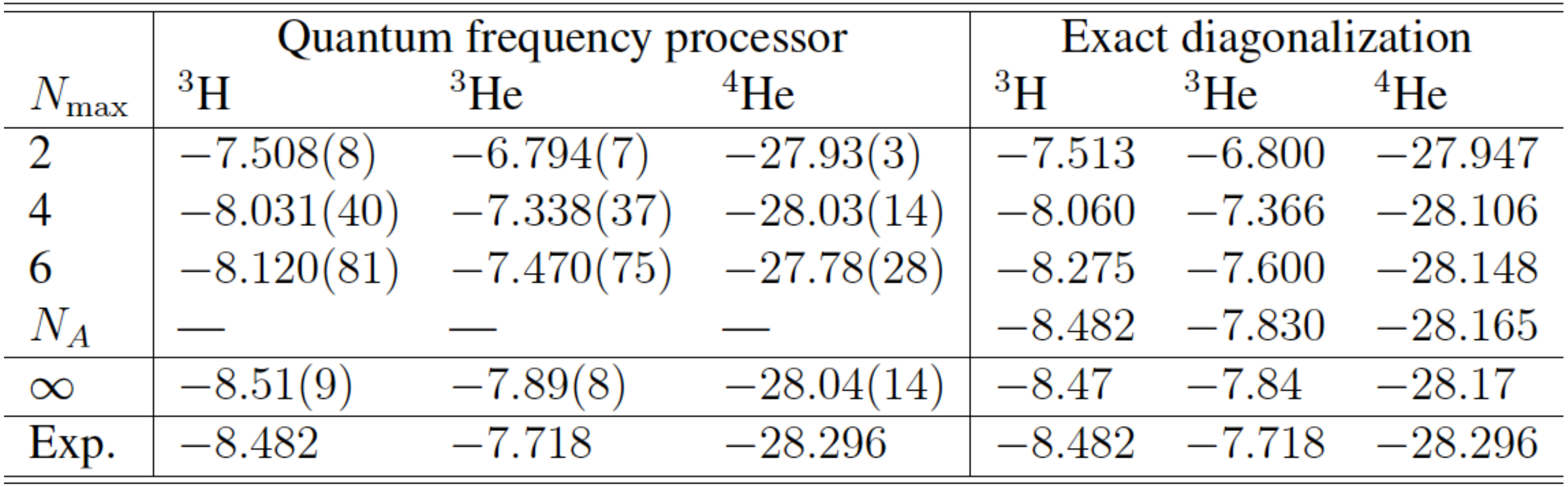
$$\langle H_{QFP}\rangle = \mathrm{Tr}[\rho H_{QFP}] = \sum_j \rho_{ij} h_{ji}$$

Extrapolate to infinite model-space using the Lüscher like formula:

$$E(L) = E_\infty + a e^{-2k_\infty L} \qquad k_\infty = \frac{1}{\hbar}\sqrt{-2m[E_\infty(A) - E_\infty(A-1)]}$$

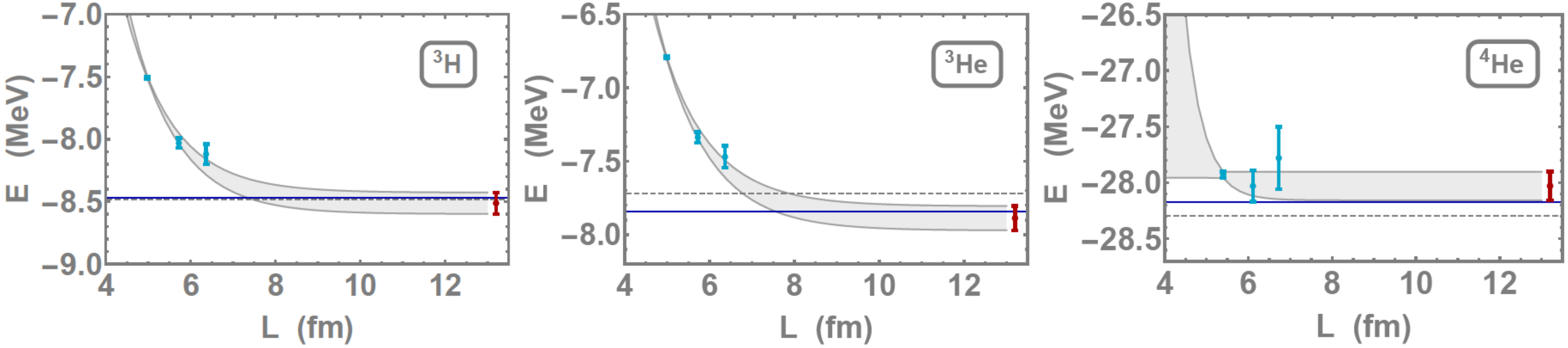
Hsuan-Hao Lu, Natalie Klco, Joseph M. Lukens, Titus D. Morris, et al, arXiv:1810.03959 (2018)

Simulating atomic nuclei on a QFP



	Quantum frequency processor			Exact diagonalization		
$N_{\max}$	^{3}H	^{3}He	^{4}He	^{3}H	^{3}He	^{4}He
2	−7.508(8)	−6.794(7)	−27.93(3)	−7.513	−6.800	−27.947
4	−8.031(40)	−7.338(37)	−28.03(14)	−8.060	−7.366	−28.106
6	−8.120(81)	−7.470(75)	−27.78(28)	−8.275	−7.600	−28.148
N_A	—	—	—	−8.482	−7.830	−28.165
∞	−8.51(9)	−7.89(8)	−28.04(14)	−8.47	−7.84	−28.17
Exp.	−8.482	−7.718	−28.296	−8.482	−7.718	−28.296

Matrix dimensions: d(A=3) = 5,15, 34 & d(A=4) = 5,20, 64



Hsuan-Hao Lu, Natalie Klco, Joseph M. Lukens, Titus D. Morris, et al,
arXiv:1810.03959 (2018)

Summary

- First step towards scalable nuclear structure calculations on a quantum processors accessed via the cloud
- Cloud quantum computation of atomic nuclei now possible
- 100 error corrected qubits could potentially revolutionize nuclear shell model calculations
- Largest photonic based quantum simulations to date

Is a Quantum Winter coming?

Collaborators

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