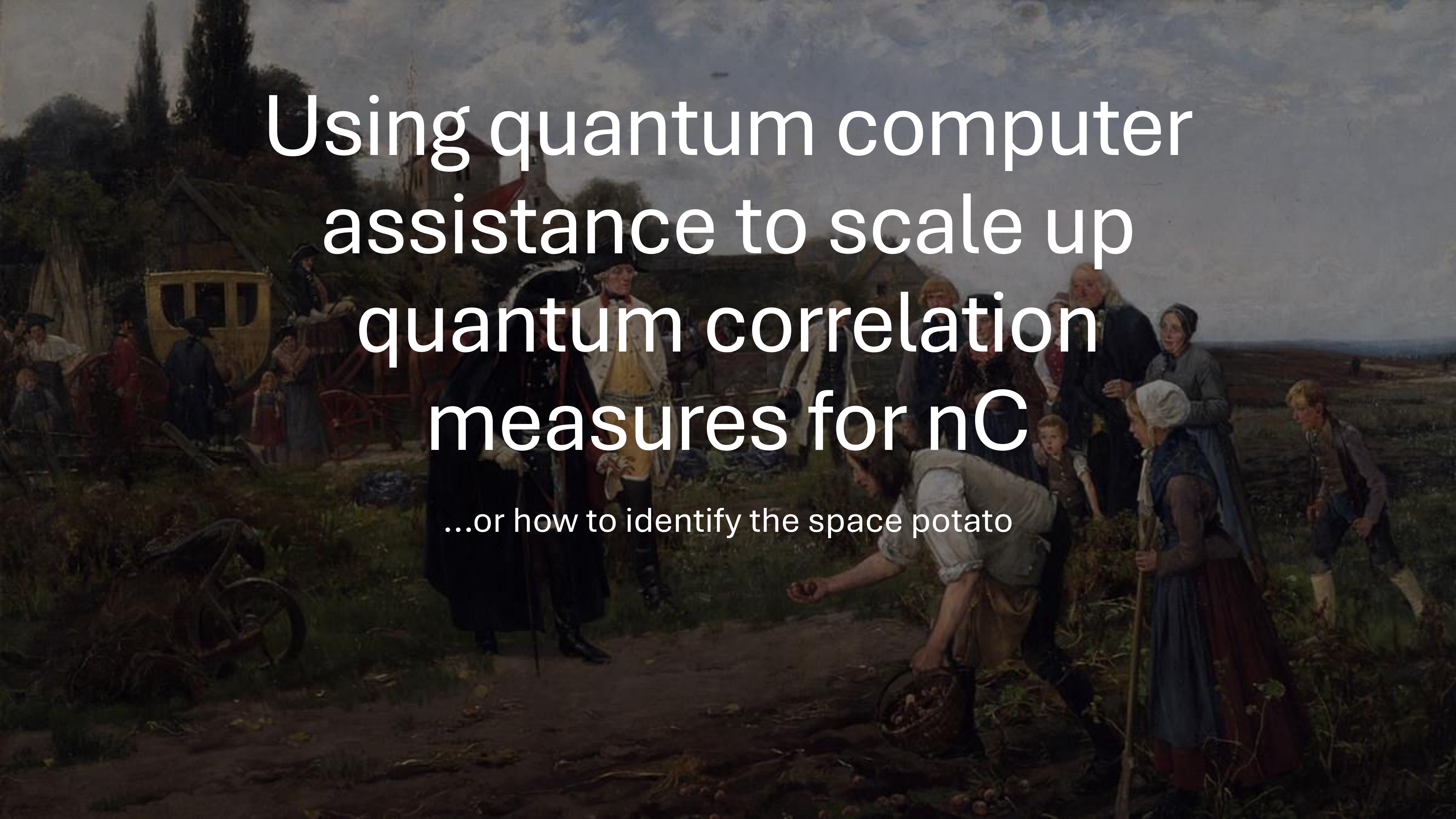


Using quantum computer assistance to scale up quantum correlation measures for nC

...or how to identify the space potato

Acknowledgements

K, Yurtseven, K. Aytemiz, C. Kehribar, Ö. Nazlı, Z. Çırnaz, T, Yücel,S. Sarikurt Malcioglu, O.B. Malcioglu

O. Pusuluk

Building an open diverse & inclusive quantum future IBM

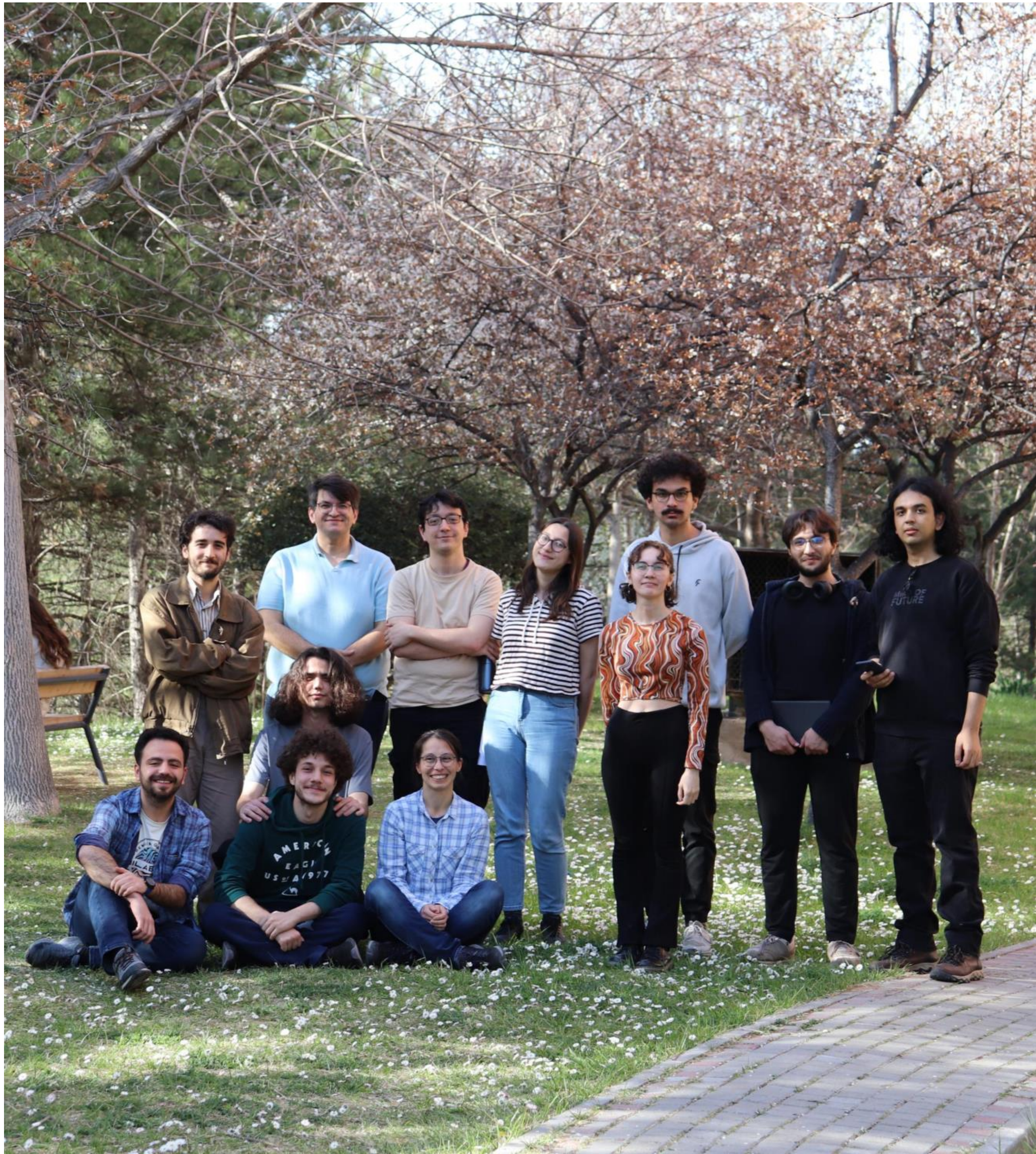
EURO²

TRUBA Turkish Science e-Infrastructure

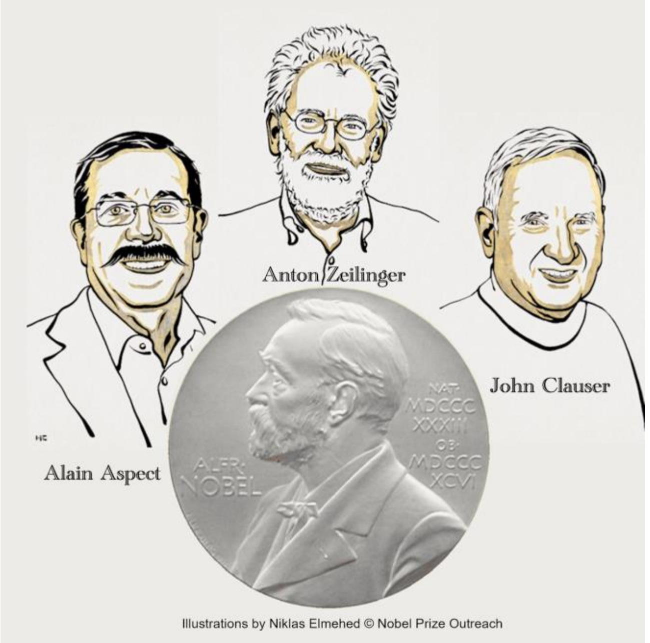
VEGA

The numerical calculations reported in this paper were partially performed at TUBITAK ULAKBIM, and in VEGA HPC through EuroHPC benchmark access

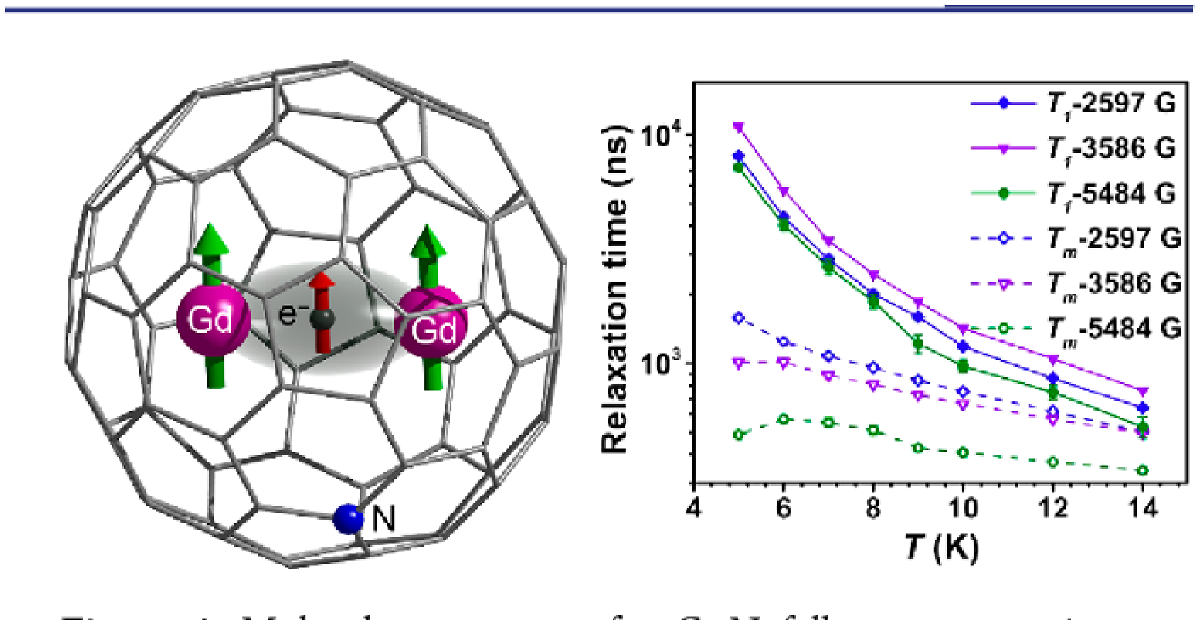
https://obm.physics.metu.edu.tr



Second Quantum Revolution: Quantum correlations as a precious resource



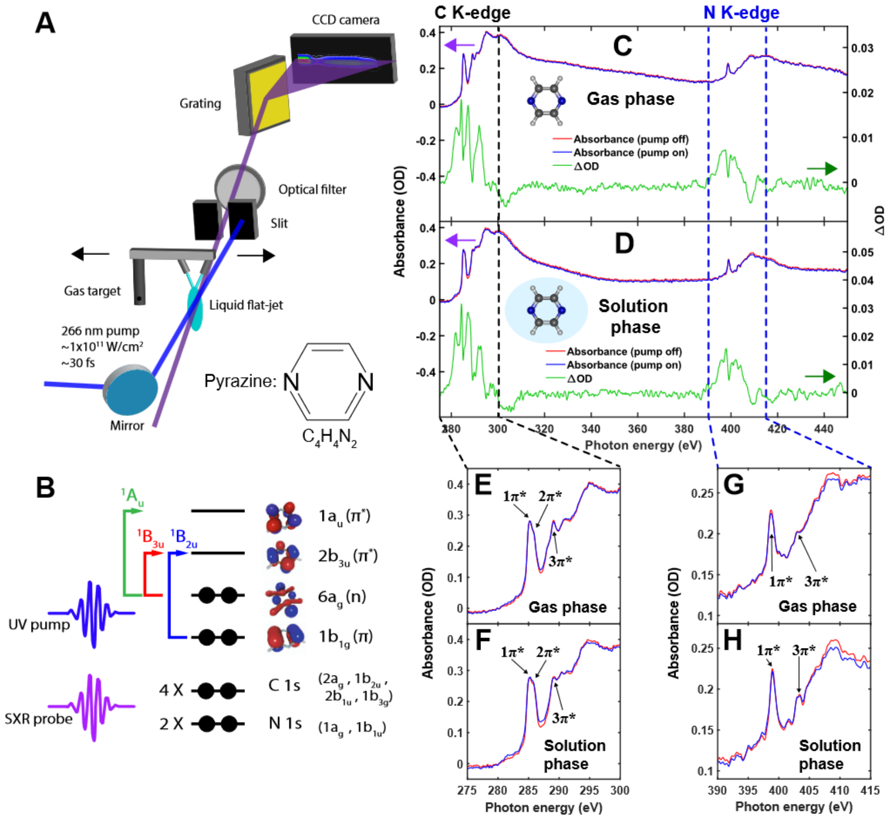
2022 nobel prize for entanglement



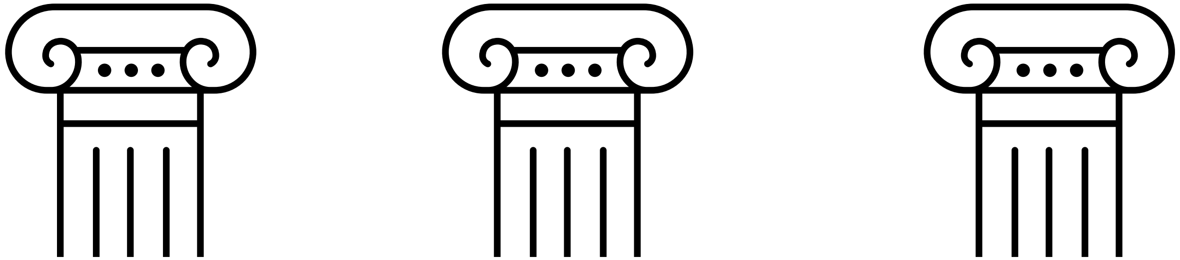
Atzori, Matteo, and Roberta Sessoli. "The Second Quantum Revolution: Role and Challenges of Molecular Chemistry." *Journal of the American Chemical Society* 141, no. 29 (July 24, 2019): 11339–52. https://doi.org/10.1021/jacs.9b00984.

Deutsch, Ivan H. "Harnessing the Power of the Second Quantum Revolution." *PRX Quantum* 1, no. 2 (November 13, 2020): 020101. https://doi.org/10.1103/PRXQuantum.1.020101.

Limits of current theoretical tools for describing nC in space



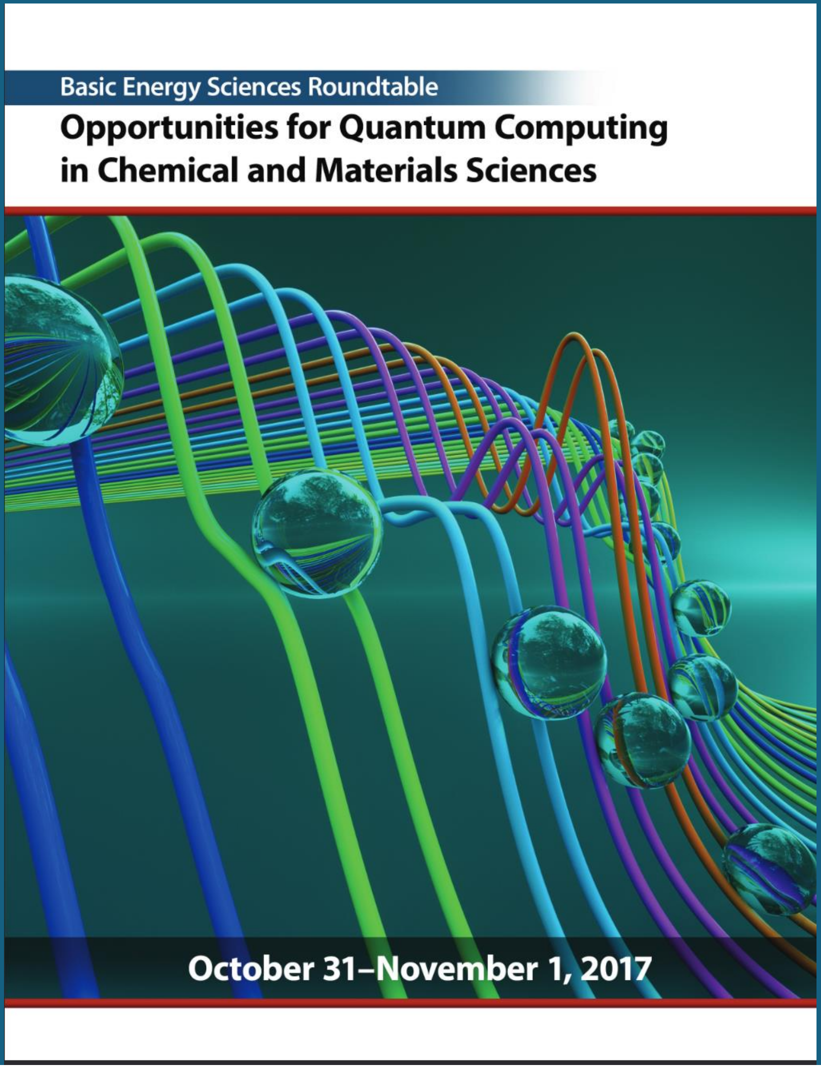
Scaling | Universality | Renormalisation



The three pillars of most Quantum Theoretical tools rely on are from earth-bound observations!

Chang, Yi-Ping, Tadas Balciunas, Zhong Yin, Marin Sapunar, Bruno N. C. Tenorio, Alexander C. Paul, Shota Tsuru, et al. "Observation of Electronic Coherence Created at Conical Intersections and Its Decoherence in Aqueous Solution." arXiv, February 16, 2024. https://doi.org/10.48550/arXiv.2402.10508.

Stanley, H. Eugene. "Scaling, Universality, and Renormalization: Three Pillars of Modern Critical Phenomena." *Reviews of Modern Physics* 71, no. 2 (March 1, 1999): S358–66. https://doi.org/10.1103/RevModPhys.71.S358.



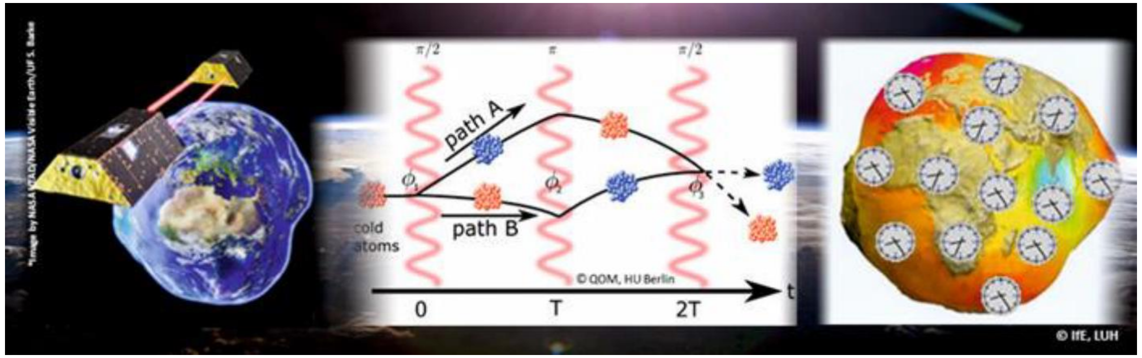
https://science.osti.gov/bes/Research/qis

Atzori, Matteo, and Roberta Sessoli. “The Second Quantum Revolution: Role and Challenges of Molecular Chemistry.” *Journal of the American Chemical Society* 141, no. 29 (July 24, 2019): 11339–52. https://doi.org/10.1021/jacs.9b00984.

Advanced measuerments at a distance

Quantum Astronomy / Entangled photon spectroscopy

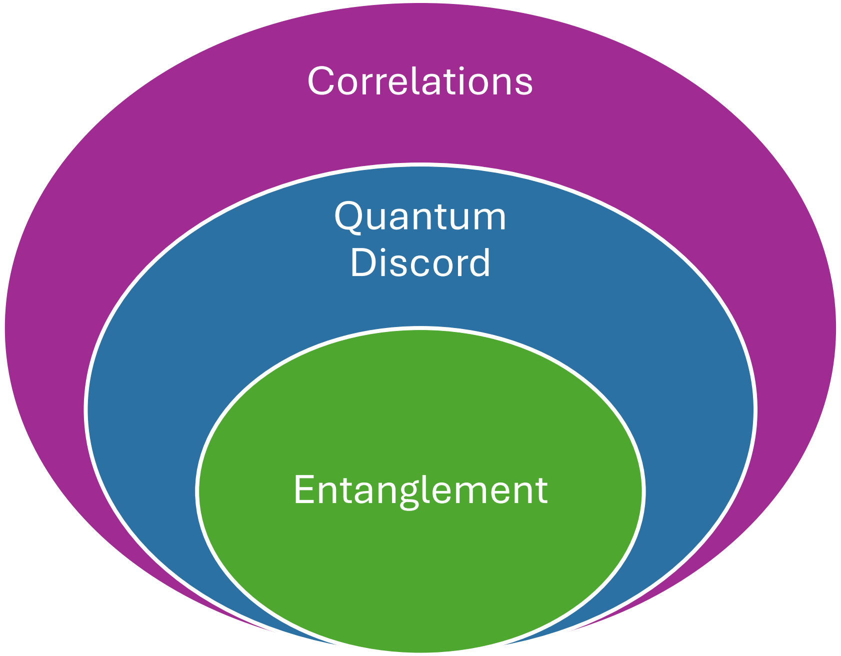
Barbieri, Cesare, Giampiero Naletto, and Luca Zampieri. “Quantum Astronomy at the University and INAF Astronomical Observatory of Padova, Italy.” *Astronomy* 2, no. 3 (September 2023): 180–92. https://doi.org/10.3390/astronomy2030013.

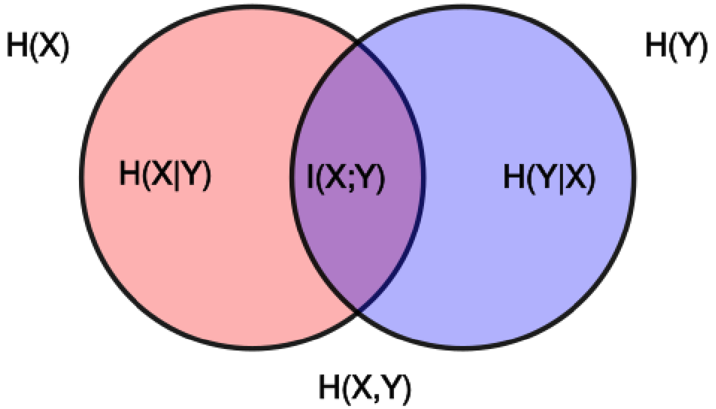


Carraz, Olivier, Aaron Strangfeld, Luca Massotti, Guenther March, Arnaud Heliere, Ilias Daras, and Pierluigi Silvestrin. “ESA Activities and Perspectives on Quantum Space Gravimetry.” Copernicus Meetings, February 22, 2023. https://doi.org/10.5194/egusphere-egu23-14485.

- Using Unruh effect in nC clouds to calculate whether the universe is expanding at the same pace at distant galaxies
- Using Fabbri and Navarro-Salas effect to see if nC are in the vicinity of a black hole (the case of HR 6819)
- Using nC clouds as Unruh–DeWitt detectors to see if something accelerate non-uniformly inside them.
- Shift in plasma frequency in interstellar environments due to Moore / Dynamic Casimir effect (i.e. van-Allen band like protective structures)

Quantum Discord as a tool for chemistry of nC





- Can quantify aromaticity
- Can be used to quantify charge transfer and resonant energy transfer
- Can be used in total energy methods beyond current limitations of rate theories
- Can suggest protocols for experimentally measuring quantum correlations

Ding, Lexin, Stefan Knecht, Zoltán Zimborás, and Christian Schilling. “Quantum Correlations in Molecules: From Quantum Resourcing to Chemical Bonding,” 2022. https://doi.org/10.48550/ARXIV.2205.15881.

Yeşiller, Mahir H., and Onur Pusuluk. “Electron Delocalization in Aromaticity as a Superposition Phenomenon.” arXiv, July 2, 2023. https://doi.org/10.48550/arXiv.2307.00672.

Calculating Quantum Discord is NP complete!

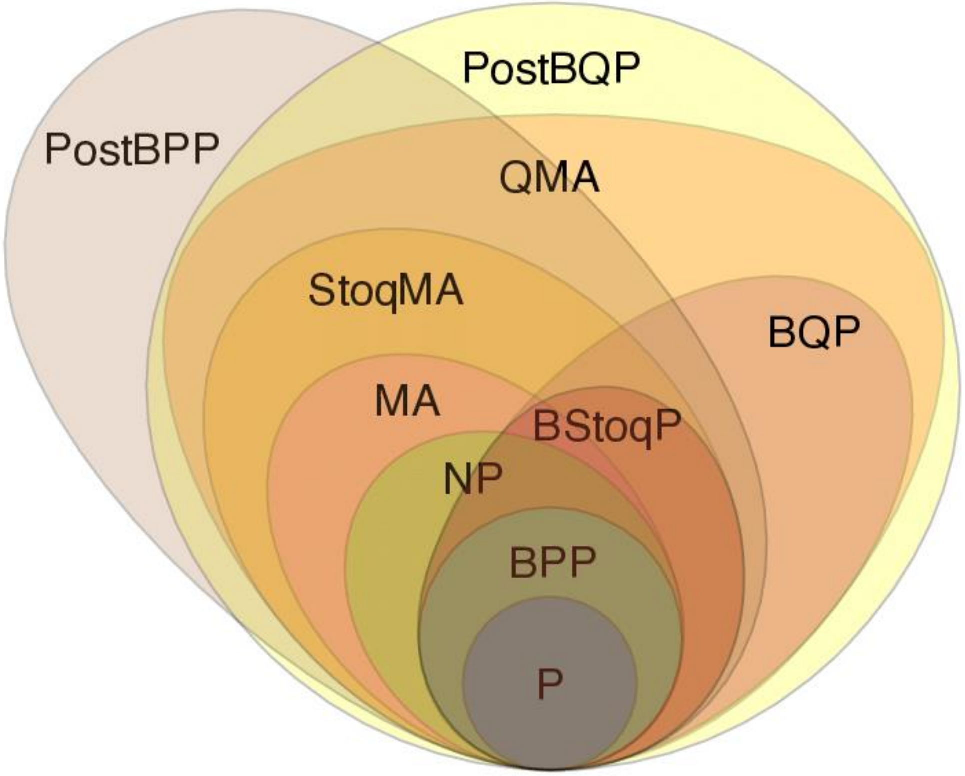
Resource	**Determinism**	**Complexity class**	**Resource constraint**
Space	Non-Deterministic	NSPACE(f(n))	**O(f(n))**
		NL	**O(log n)**
		NPSPACE	**O(poly(n))**
		NEXPSPACE	**O($2^{poly(n)}$)**
	Deterministic	DSPACE(f(n))	**O(f(n))**
		L	**O(log n)**
		PSPACE	**O(poly(n))**
		EXPSPACE	**O($2^{poly(n)}$)**
Time	Non-Deterministic	NTIME(f(n))	**O(f(n))**
		NP	**O(poly(n))**
		NEXPTIME	**O($2^{poly(n)}$)**
	Deterministic	DTIME(f(n))	**O(f(n))**
		P	**O(poly(n))**
		EXPTIME	**O($2^{poly(n)}$)**

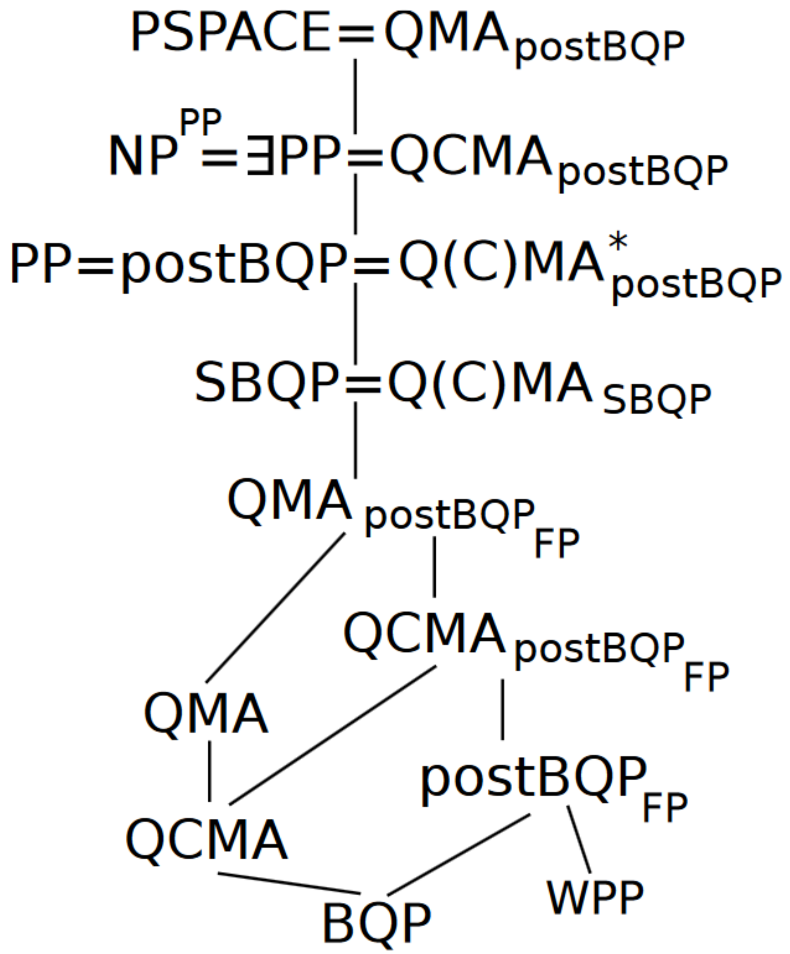
Limits	Engineering	Design and Validation	Energy, time	Space, time	Information, Complexity
Funda-mental	Abbe (diffraction) Amdahl Gustafson	Error-corr. & dense codes Fault-tolerance thresholds	Einstein $E=mc^2$ Heisenberg $\Delta E \Delta t$ Landauer kT ln2 Bremermann Adiabatic thrms	Speed of light Planck scale Bekenstein Fisher T(n)$^{1/(d+1)}$	Shannon Holevo NC, NP, #P Turing (decidability)
Mate-rial	Dielectric constant Carrier mobility Surface morphology Fabrication-related	Analytical & numerical modeling	Conductivity Permittivity Bandgap Heat flow	Propagation speed Atomic spacing No gravitational collapse	Information transfer between carriers
Device	Gate dielectric Channel charge ctrl Leakage, Latency Crosstalk, Aging	Compact modeling Parameter selection	CMOS, quantum Charge-centric Signal to noise Energy conversion	Entropy density Entropy flow Interfaces & contacts Size & delay variation	Universality
Circuit	Delay, Inductance Thermal-related Yield, Reliability, IO	Interconnect Test Validation	Dark, darker, dim and gray silicon Cooling efficiency Power density/supply	Interconnect 2D or 3D	Circuit complexity bounds
System +SW	Specification, Implementation Validation, Cost		Synchronization, Physical integration Parallelism, *Ab initio* limits (Lloyd)		The CAP theorem

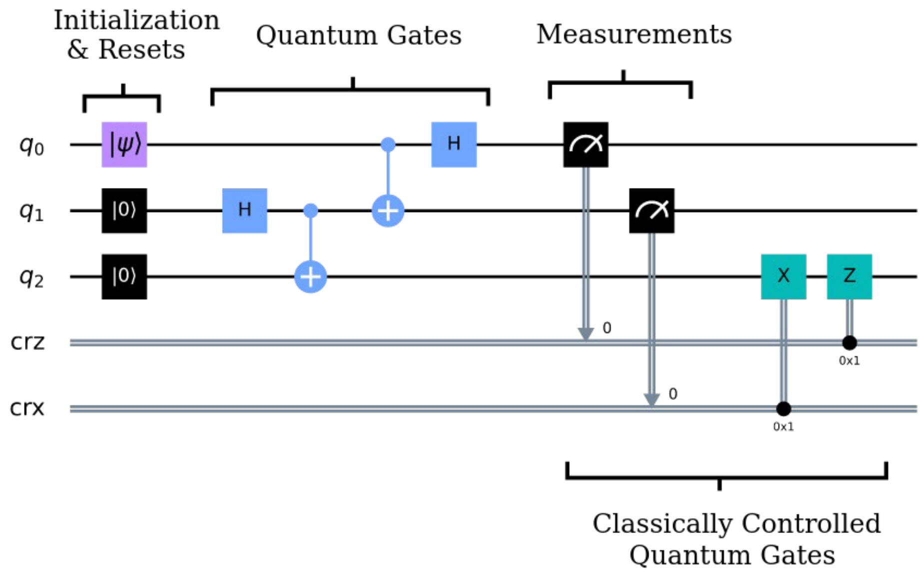
Quantum complexity classes are an active field of research, however it is widely believed that **quantum computers and traditional computers will complement each other in solving problems that are not possible in either by itself**

Example research:

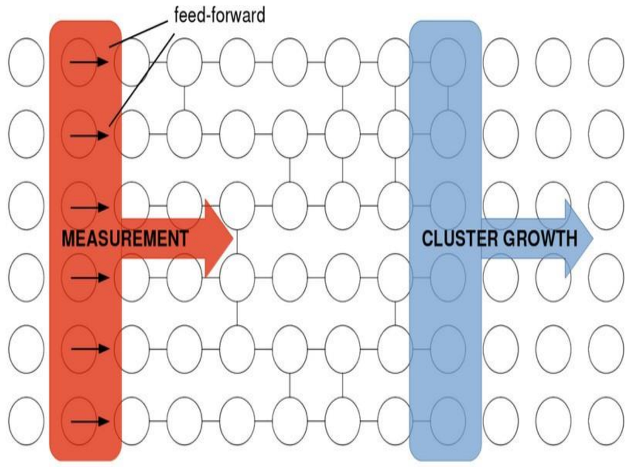
+ https://journals.aps.org/rmp/abstract/10.1103/RevModPhys.90.015002
+ https://arxiv.org/pdf/1704.01514.pdf

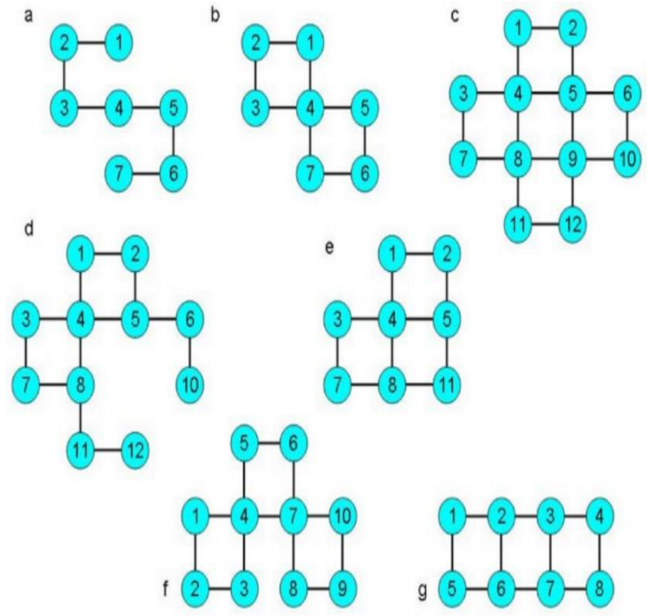






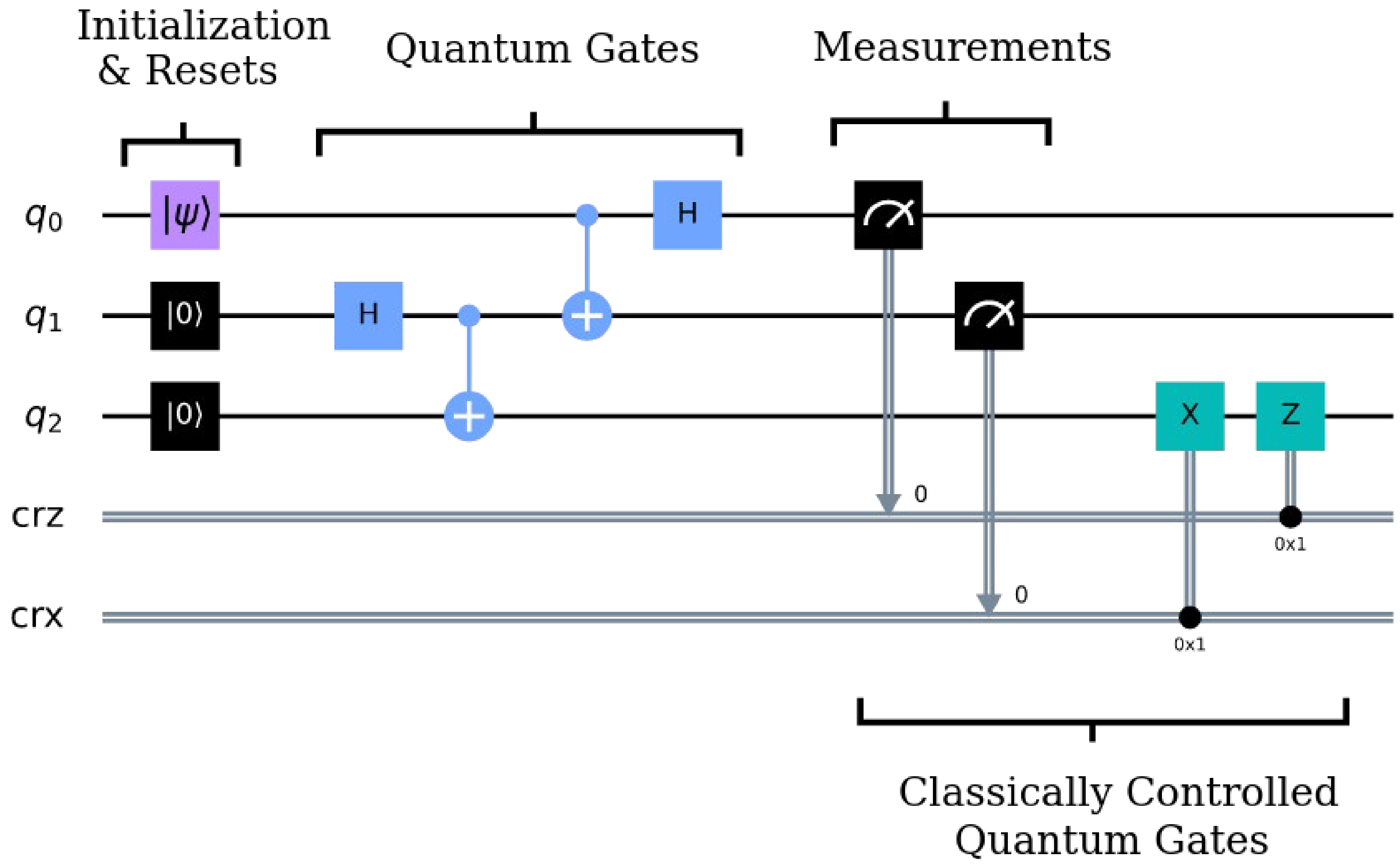
Circuit Model: D. Deutsch, Proc. R. Soc. A 425, 73 (1989).





Cluster-state quantum computation
https://doi.org/10.1016/S0034-4877(06)80014-5

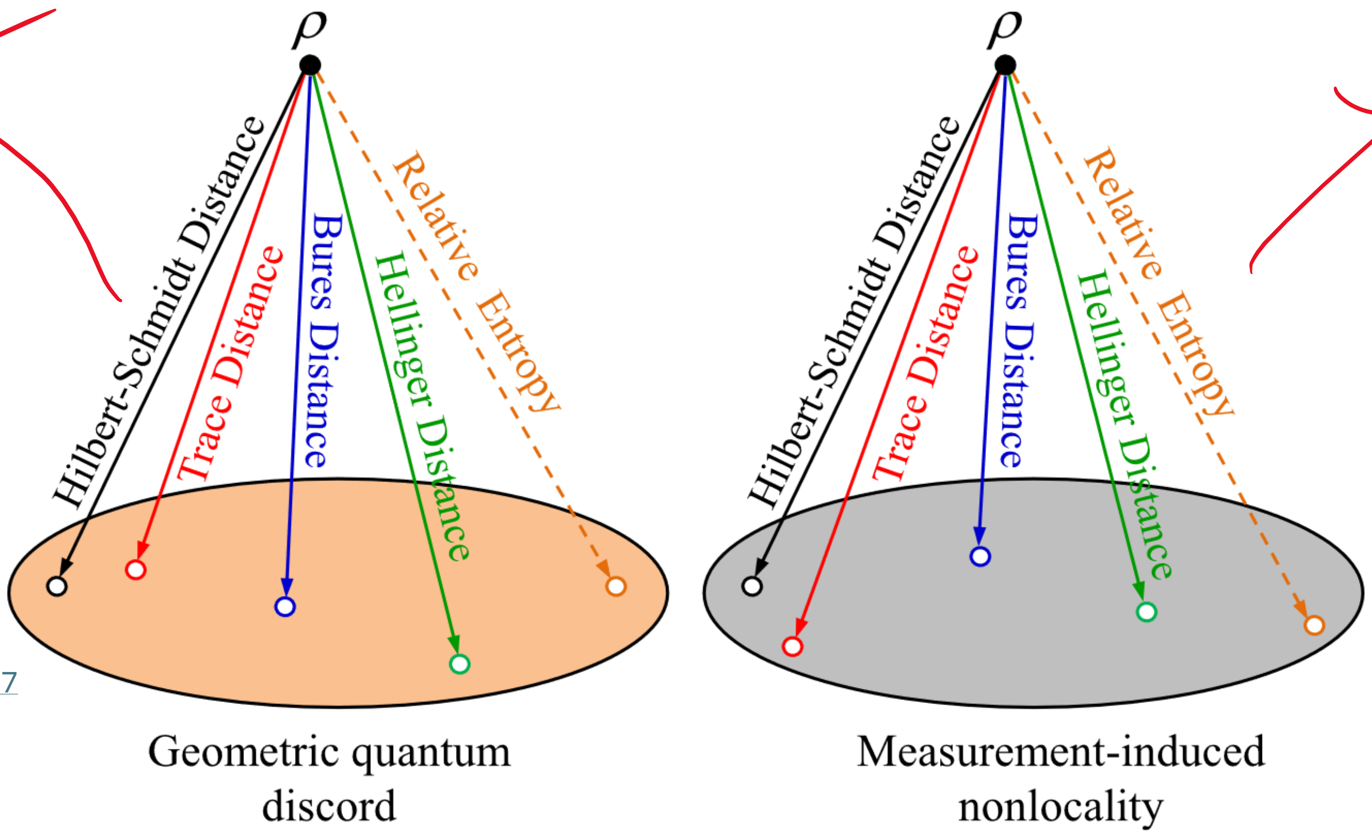
Model Name	Reference
Adiabatic	Albert Messiah. Quantum Mechanics. Dover, Mineola, 1961.
Topological	Nayak, et al. arxiv:0707.1889, 2007
Quantum Walks	Childs et al. arXiv:quant-ph/0209131.
Measurement-based	Raussendorf and Briegel. PRL 86(22):5188-5191, 2001.
Quantum Turing Machines	David Deutsch. Proceedings of the Royal Society, 400:97–117,1985.


Initialization
& Resets
Quantum Gates
Measurements
q0
q1
q2
crz
crx
|ψ⟩
|0⟩
|0⟩
H
H
X
Z
0
0
0x1
0x1
Classically Controlled
Quantum Gates

Calculation of quantum discord boils down to calculating a distance

- Make sure that you are in the same Hilbert space
- Make sure you are slicing in the right direction
- Make sure that electrons are still electrons

Good for TC



Better for QC?

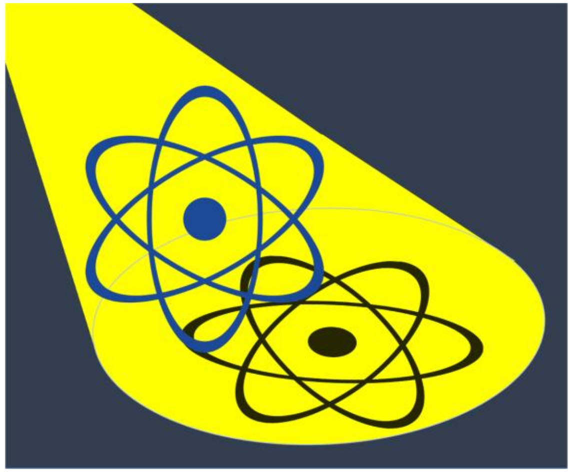
Yeşiller, Mahir H., and Onur Pusuluk. "Electron Delocalization in Aromaticity as a Superposition Phenomenon." arXiv, July 2, 2023. https://doi.org/10.48550/arXiv.2307.00672.

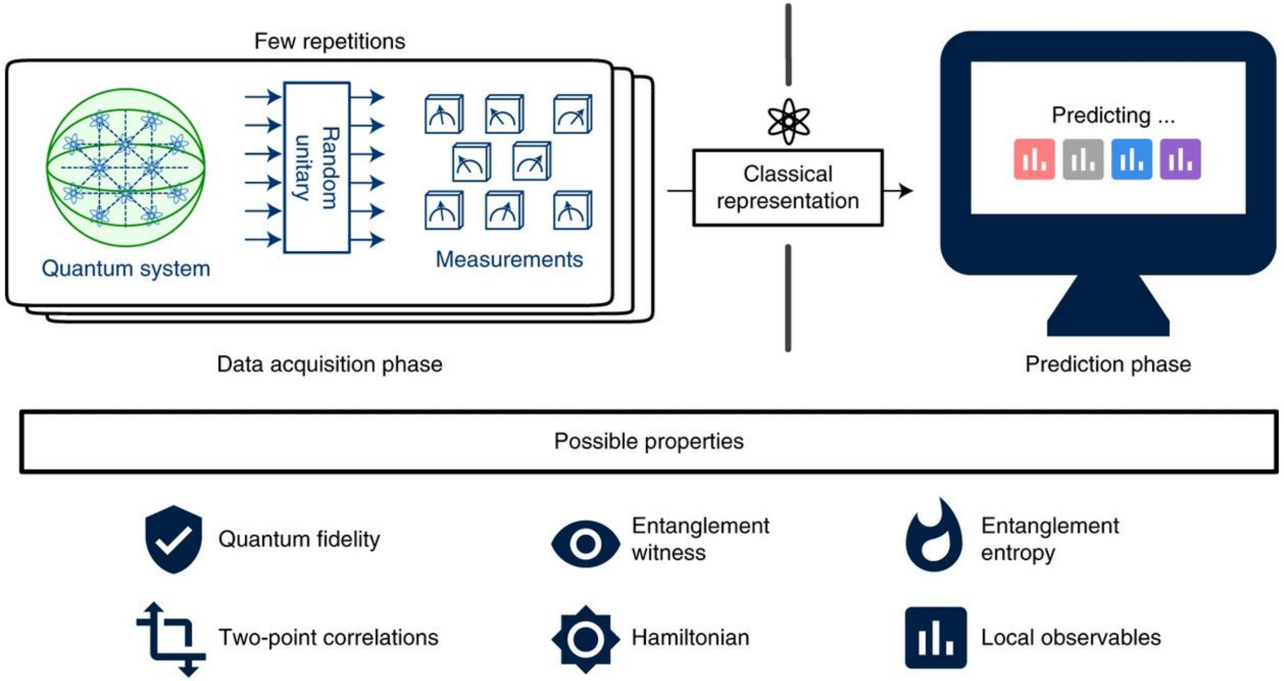
Hu, Ming-Liang, Xueyuan Hu, Jieci Wang, Yi Peng, Yu-Ran Zhang, and Heng Fan. "Quantum Coherence and Geometric Quantum Discord." *Physics Reports*, Quantum coherence and geometric quantum discord, 762–764 (November 6, 2018): 1–100. https://doi.org/10.1016/j.physrep.2018.07.004.

Classical shadow tomography

Tomography: In principle, any unknown quantum state can be fully characterized by quantum state tomography However, this procedure requires accurate expectation values for a set of observables whose size grows exponentially with the number of qubits.

Shadow tomography: Predict target functions, not the full state (For MIN: the distance to locally invariant states)



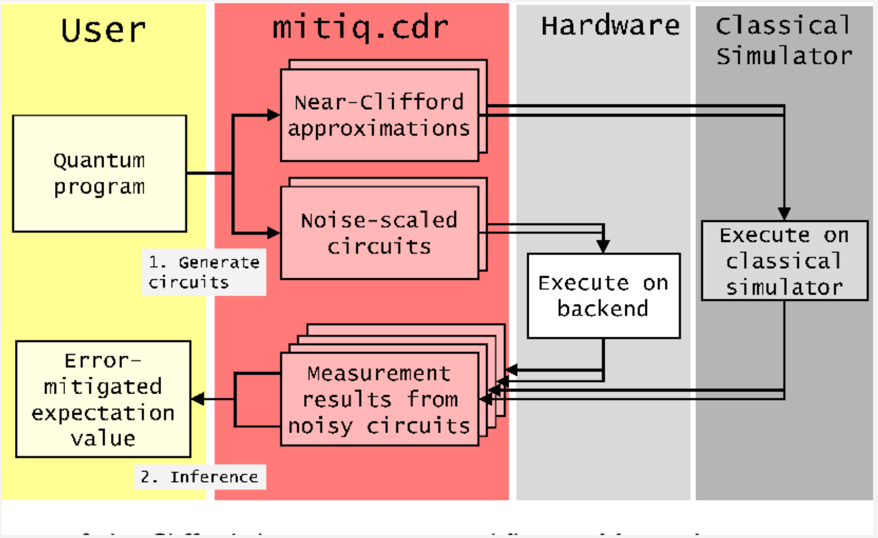


In the data acquisition phase, we perform a random unitary evolution and measurements on independent copies of an n-qubit system to obtain a classical representation of the quantum system—the classical shadow. Such classical shadows facilitate accurate prediction of a large number of different properties using a simple median-of-means protocol.

Huang, HY., Kueng, R. & Preskill, J. Predicting many properties of a quantum system from very few measurements. *Nat. Phys.* **16**, 1050–1057 (2020). https://doi.org/10.1038/s41567-020-0932-7

How to deal with the noise in NISQ era QC?

HPC+QPU method

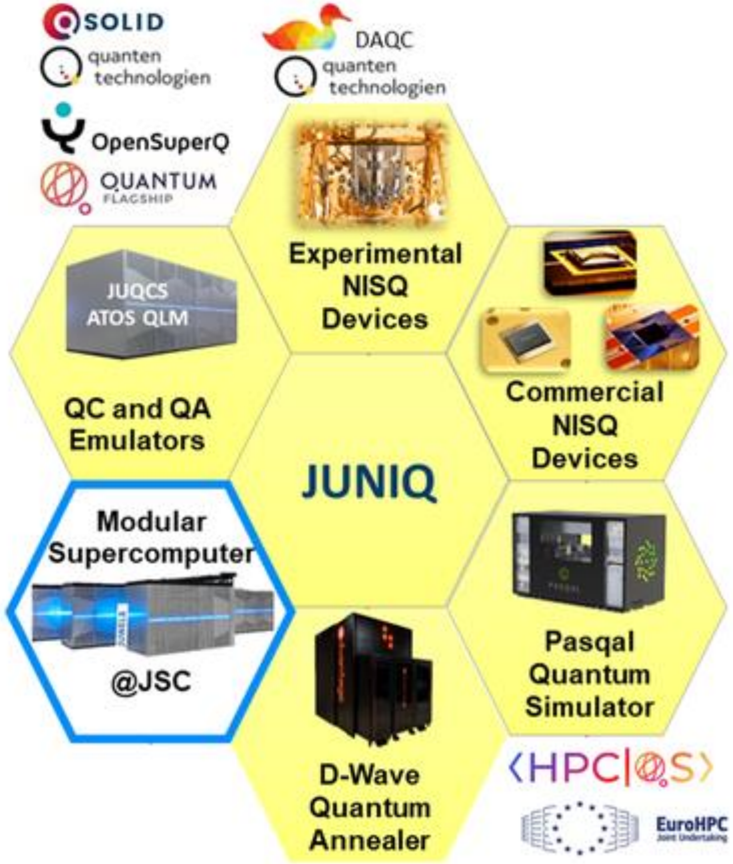


LaRose, Ryan, Andrea Mari, Sarah Kaiser, Peter J. Karalekas, Andre A. Alves, Piotr Czarnik, Mohamed El Mandouh, et al. “Mitiq: A Software Package for Error Mitigation on Noisy Quantum Computers.” *Quantum* 6 (August 11, 2022): 774. https://doi.org/10.22331/q-2022-08-11-774.

More qubits and topology method

Silva, M. P. da, C. Ryan-Anderson, J. M. Bello-Rivas, A. Chernoguzov, J. M. Dreiling, C. Foltz, F. Frachon, et al. “Demonstration of Logical Qubits and Repeated Error Correction with Better-than-Physical Error Rates.” arXiv, April 4, 2024. https://doi.org/10.48550/arXiv.2404.02280.

JUNIQ (EU) HPC+QPU



Spanish / Turkish Quantum excellence center is coming!

QTEdu: (https://qtedu.eu/)

- Another project submitted under DIGITAL-2023-SKILLS-05-SPECIALISED-EDU
- Training of specialized professionals on quantum technologies (such as astronomers, chemists, engineers)
- Take lectures anywhere/online (many universities are abroad)
- Certification + International diploma when all modules are completed.
- ECTS compatible