Quantum Computing - Fundamentals, Hardware, and HPC/AI

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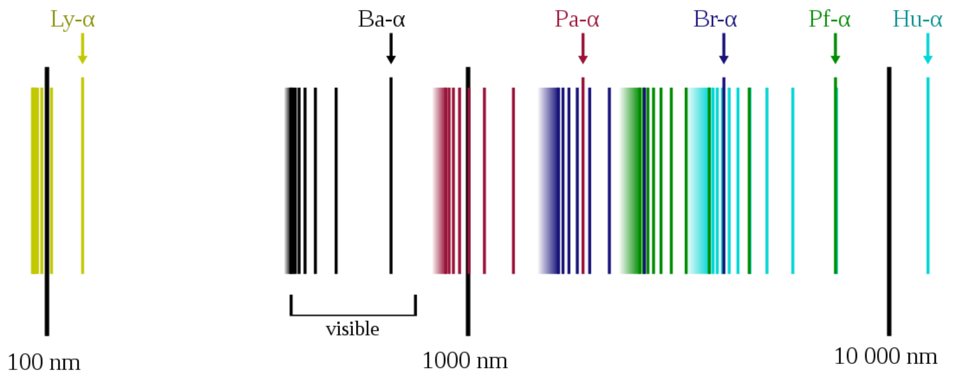
BRIEF HISTORICAL PEDAGOGY

- **Ultraviolet Catastrophe and Planck's Photon:**
  - Rayleigh-Jeans law based on classical thermodynamics and continuous wave mechanics predicted singular energy values.
  - Max Planck resolves issue with particle statistical mechanics **and** quantized energy values
- **Duality and de Broglie's Matter Wave:**
  - If light is a particle, then why can't particles be waves?
  - Using special relativity, de Broglie postulated matter waves.
- **Probability Wave's and Schrodinger's Equation:**
  - Differential equation for evolution of a matter wave
  - Time-independent version implies the existence of stationary, or eigenstates
  - Unitary Evolution, dictates all coherent quantum evolution
- **Bohr's Correspondence Principle**
  - Q: Why don't I see these quantum effects?
  - A: Because h is tiny and you are big.
  - When things get big (not necessarily length, could be e.g., energy), quantum mechanics washes out.
  - De Broglie Wavelength of a baseball ~10^-35 m

$$E = h\nu = hc/\lambda$$

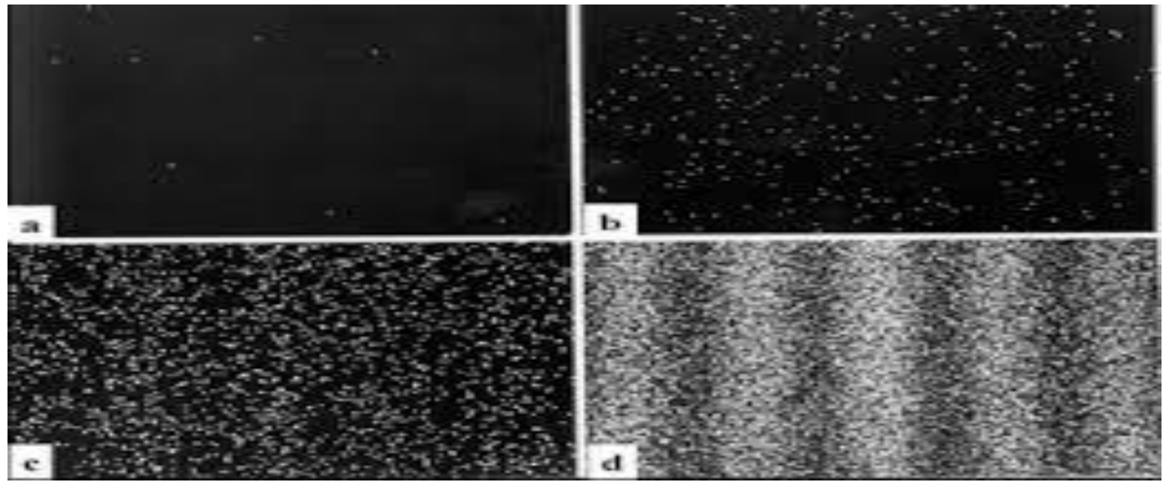


$$E^2 - |\hat{p}|^2 c^2 = m^2 c^4$$

$$|\hat{p}| = h\nu/c = h/\lambda \qquad \rightarrow \lambda_{dB} = h/p = h/mv$$

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \qquad \hat{H}|\psi(t)\rangle = E|\psi(t)\rangle$$

$$|\psi(t)\rangle = \sum_n a_n \exp(-iE_n t/\hbar)|\psi_n\rangle$$



POSTULATES OF QUANTUM MECHANICS

- **Postulate 1**
  - You can fully specify a system by its quantum wave function (state), whose absolute value squared is a probability distribution.
  - Probability distributions have mathematical rules

$$\int_{-\infty}^{\infty} \psi^*(r,t)\psi(r,t)dr = 1$$

$$\langle\psi|\psi\rangle = \sum_n \langle\psi_n|\psi_n\rangle = 1$$

$$\rho = |\psi\rangle\langle\psi|$$

$$\|\hat{\rho}\|_1 = \mathrm{Tr}|\hat{\rho}| = \textstyle\sum_i |\hat{\rho}_{ii}| = 1$$

$$\hat{\rho} = \hat{\rho}^\dagger$$

$$\vec{x}^\dagger\ \hat{\rho}\ \vec{x} \geq 0 \text{ for all } \vec{x}$$

- **Postulate 2:**
  - Quantum Observables are Hermitian
  - Specifies real eigenvalues (measurement outcomes)

$$A = \overline{A^T}$$

- **Postulates 3 and 4:**
  - Only the eigenvalues of an observable can be measured
  - If a state is not an eigenstate of the operator, more than one eigenvalue will be measured
  - The expectation value is the weighted sum of measurement outcomes

$$|0\rangle = \begin{bmatrix}1\\0\end{bmatrix}, \quad |+\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix} \qquad \hat{\sigma}^z = \begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$$

$$\langle 0|\sigma^z|0\rangle = 1, \quad \langle +|\sigma^z|+\rangle = 0$$

- **Postulate 5**
  - Schrodinger's Equation dictates state evolution (system dynamics)

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$$

EXPONENTIAL GROWTH OF QUANTUM STATES

- **Multiple qubits can be represented with the Kronecker product**
  - States grow as 2^n for n qubits
  - Operators grow as 2^{2n}

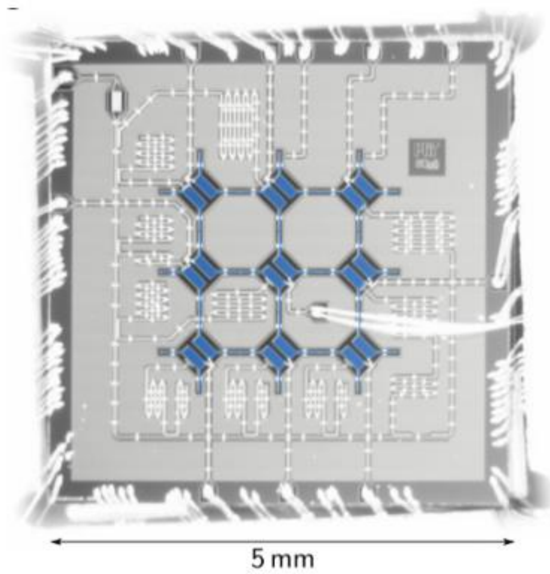
$$|0\rangle, |1\rangle = \begin{bmatrix}1\\0\end{bmatrix}, \begin{bmatrix}0\\1\end{bmatrix} \qquad |00\rangle, |01\rangle = \begin{bmatrix}1\\0\\0\\0\end{bmatrix}, \begin{bmatrix}0\\1\\0\\0\end{bmatrix} \qquad |101\rangle = \begin{bmatrix}0\\0\\0\\0\\0\\1\\0\\0\end{bmatrix} \qquad |0101\rangle = \begin{bmatrix}0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\1\\0\\0\end{bmatrix}$$

META QUANTUM: QUANTUM SIMULATION

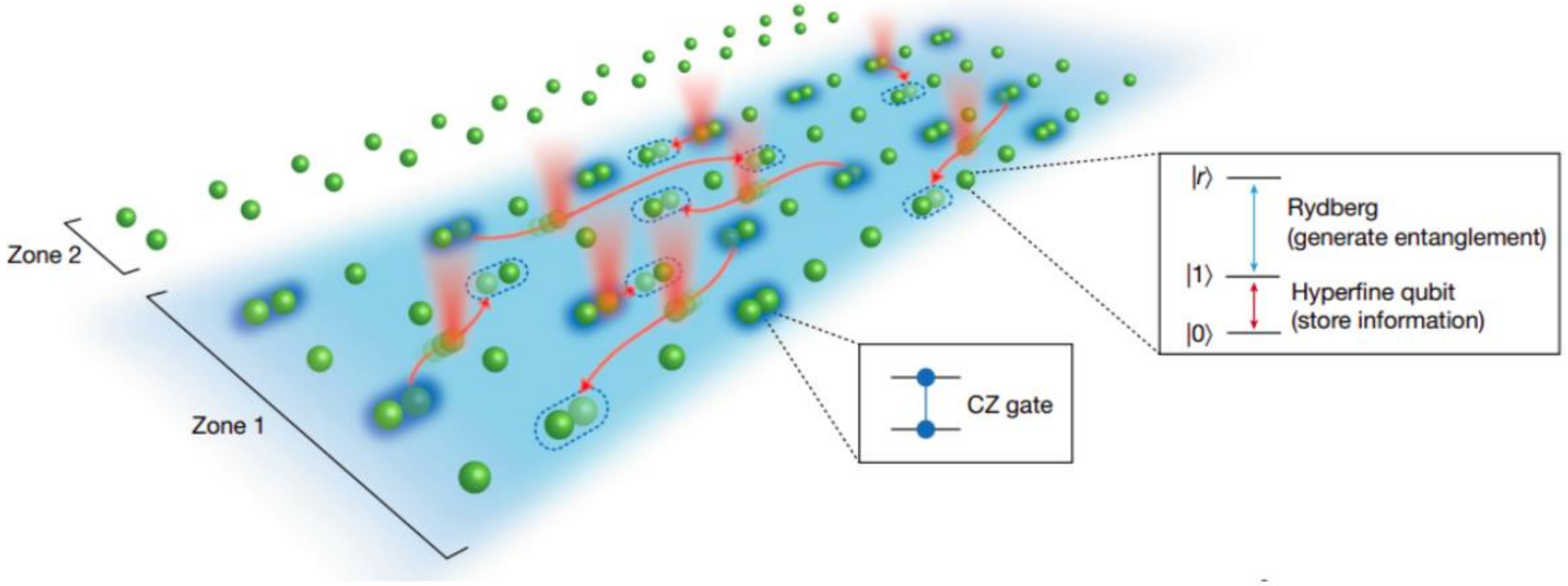
- More tractable quantum systems that impersonate less tractable quantum systems

- Can be accomplished with any platform
  - Superconducting
  - Rydberg arrays

- Pathway towards quantum *advantage*
  - Study interesting/useful quantum processes



Nat. Phys. **18**, 172–178 (2022). 10.1038/s41567-021-01430-w.



Nature 604, 451–456 (2022). 10.1038/s41586-022-04592-6.

TRADITIONAL QUANTUM ALGORITHMS

- **Require Highly Coherent Quantum Computers**
- **Bernstein-Vazirani**
  - Calculates the dot product of unknown bitstring.
  - Classically requires n function calls, quantumly 1. Polynomial (linear) speedup.
  - Uses similar quantum techniques to more famous algorithms, but is significantly simpler.
- **Quantum Fourier Transform**
  - Fourier Transform for an exponentially large space. Exponential speedup.
- **Shor's Algorithm**
  - Factors large integers. Exponential speedup.
- **Grover's Algorithm**
  - Amplifies a specified state in the space. Polynomial speedup.

$$f_s(x) = s \cdot x \bmod 2$$

$$|0\rangle \xrightarrow{H^{\otimes n}} \frac{1}{\sqrt{2}} \sum_{x\in\{0,1\}^n} |x\rangle \xrightarrow{f_s} \frac{1}{\sqrt{2}} \sum_{x\in\{0,1\}^n} (-1)^{s\cdot x}|x\rangle$$

$$\xrightarrow{H^{\otimes n}} |s\rangle$$

QUANTUM NOISE

- **In a closed system, there is no noise**
  - In truth, the universe is one giant wave function
  - If we could track all of it, we would lose no information
  - Noise = information loss

$$|\psi_q\rangle \otimes |\psi_e\rangle = \frac{1}{\sqrt{2}}(|0_q\rangle + |1_q\rangle) \otimes |0_e\rangle$$

$$\rightarrow_{CNOT} \frac{1}{\sqrt{2}}(|0_q 0_e\rangle + |1_q 1_e\rangle)$$

- **Laboratory (Computer) Quantum Systems are Open**
  - If the environment interacts with system (or even if our system interacts with the environment, like here!) entanglement occurs
  - As we cannot measure the universe, only our experiment (or qubit), retrievable information is partial trace

$$\mathrm{Tr}_e[|\psi_q\rangle \otimes |\psi_e\rangle] = |\psi_q\rangle$$

$$\mathrm{Tr}_e[\frac{1}{\sqrt{2}}(|0_q 0_e\rangle + |1_q 1_e\rangle)] = \rho_q'$$

- **"Noise" is Information Loss**
  - Partial trace of original system, full density matrix, has coherences (off-diagonal elements), pure state
  - Partial trace of open system, reduced density matrix, incoherent, classical mixture (maximally mixed state)

$$\rho_q = |\psi_q\rangle\langle\psi_q| = \frac{1}{2}\left(|0_q\rangle\langle 0_q| + |1_q\rangle\langle 1_q| + |0_q\rangle\langle 1_q| + |1_q\rangle\langle 0_q|\right)$$

$$\rho_q' = |\psi_q\rangle\langle\psi_q| = \frac{1}{2}\left(|0_q\rangle\langle 0_q| + |1_q\rangle\langle 1_q|\right)$$

QC PLATFORMS (SINCE LAST I CHECKED)

- **Superconducting Qubits**
    - Google, IBM, Amazon, Rigetti
    - ~105 qubits
    - Josephson-junction
- **Neutral Atoms**
    - QuEra and Academic Labs
    - ~256 qubits
    - Rydberg atoms
- **Trapped Ion**
    - IonQ U Maryland
    - ~64-100 qubits
    - Ions interact through vibrations
- **Vacancy Centers**
    - Academic Labs
    - Impurities (e.g., Nitrogen) in diamond. Not often discussed for scalable QC, promising for sensing (e.g., Mitre)
- **Optical Quantum Computing**
    - PsiQuantum and Xanadu
    - Room temperature, but photons reticent to interact

TAYLOR'S RESEARCH AREAS

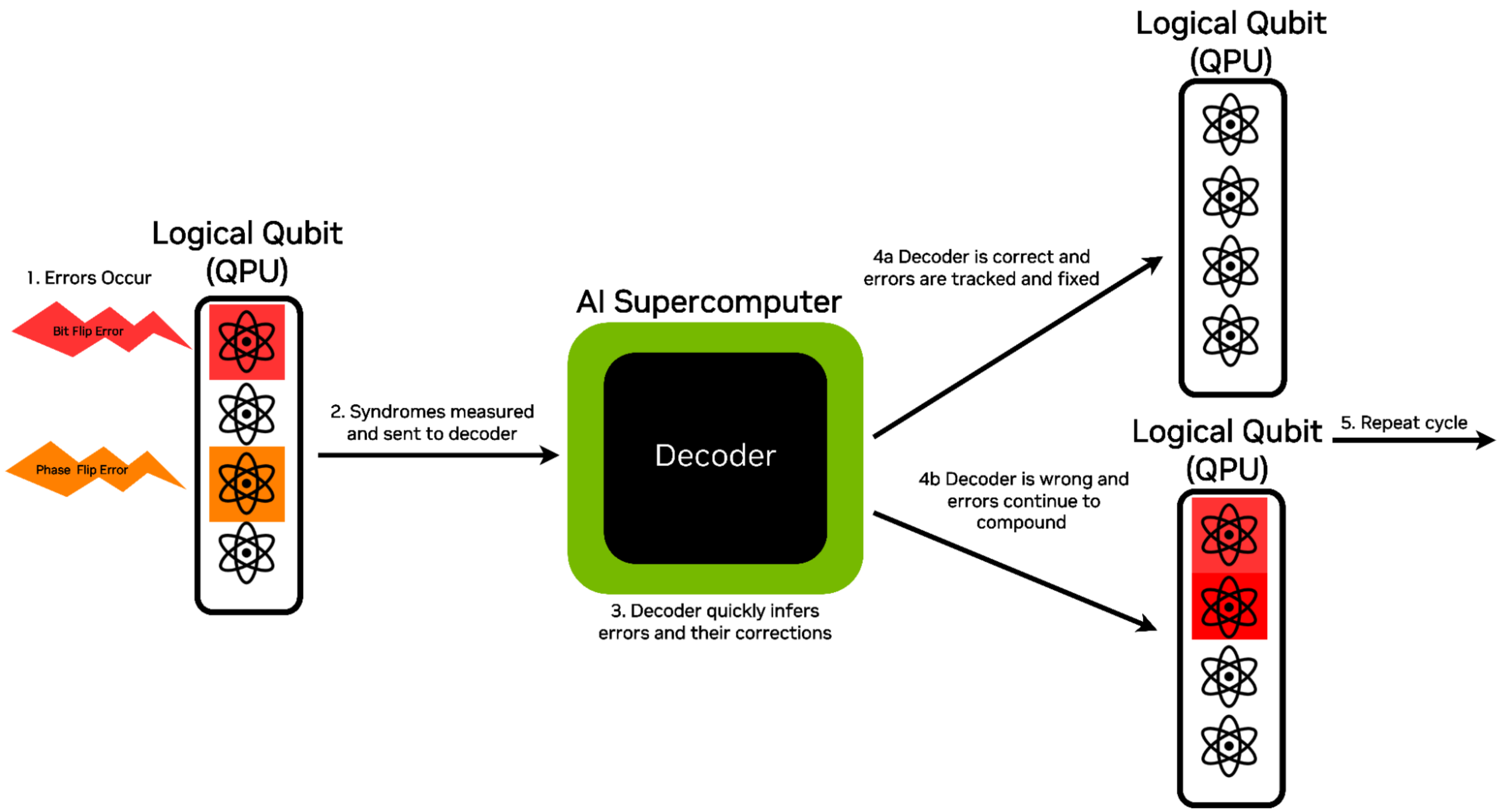
Grounded Quantum Algorithms

AI/ML for Quantum Systems

Efficient Computation for Quantum Systems

Quantum Architecture/Hardware

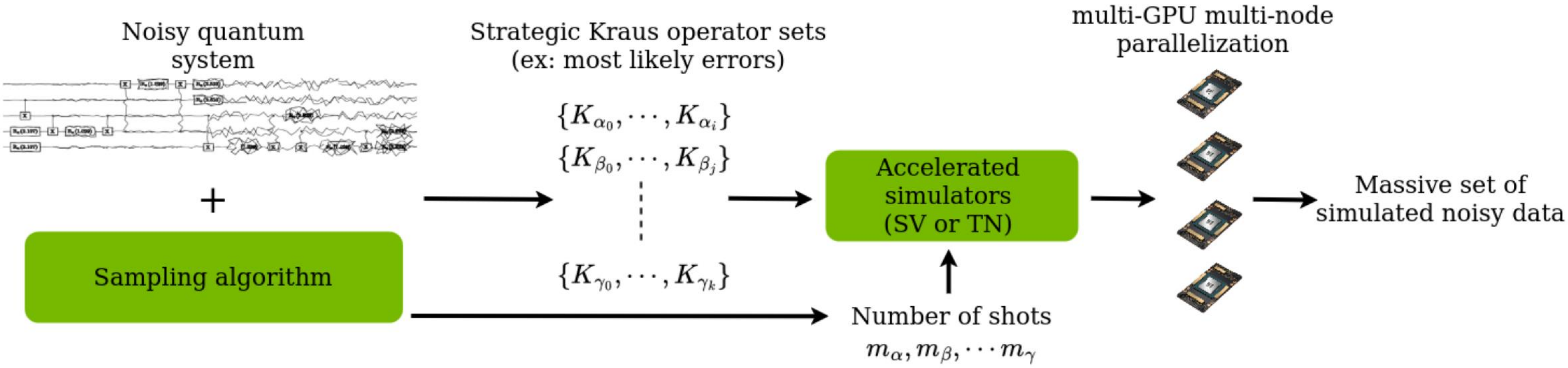
AI FOR QUANTUM: QEC DECODERS



- HPC for offline training data collection
- AI for online detection of errors
- Virtuous cycle for quantum hardware development

https://developer.nvidia.com/blog/nvidia-and-quera-decode-quantum-errors-with-ai/

HPC FOR DATA QUANTUM: DATA COLLECTION



Noisy quantum system

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Sampling algorithm

Strategic Kraus operator sets (ex: most likely errors)

$$\{K_{\alpha_0}, \cdots, K_{\alpha_i}\}$$

$$\{K_{\beta_0}, \cdots, K_{\beta_j}\}$$

$$\vdots$$

$$\{K_{\gamma_0}, \cdots, K_{\gamma_k}\}$$

Accelerated simulators (SV or TN)

Number of shots $m_\alpha, m_\beta, \cdots m_\gamma$

multi-GPU multi-node parallelization

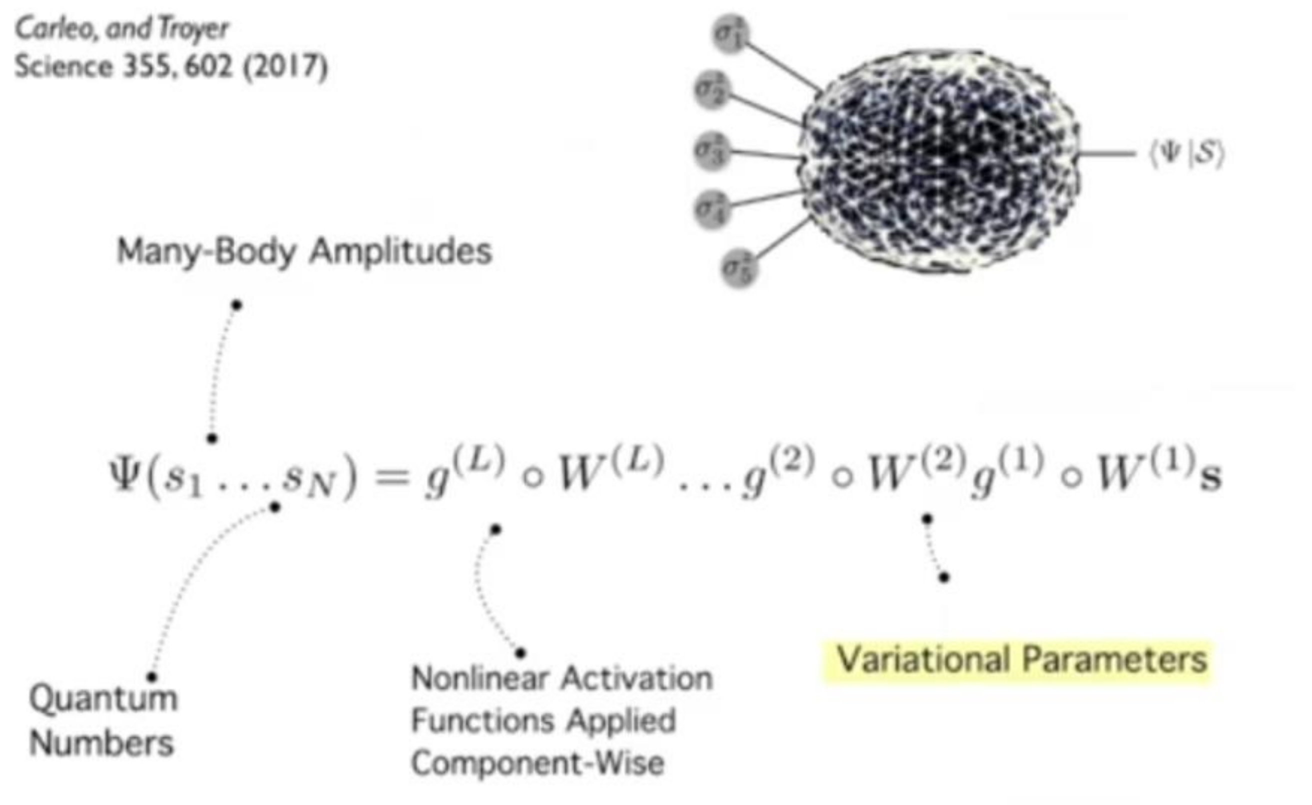
Massive set of simulated noisy data

- Greatly reduce complexity of data collection from simulated noisy quantum systems
- Generate data corpus that is sufficient for large model training
- HPC supporting quantum hardware development

TLP, J. Lietz, T. Nguyen, A.J. McCaskey, B. Khailany. *Augmenting Simulated Noisy Quantum Data Collection by Orders of Magnitude Using Pre-Trajectory Sampling with Batched Execution.* Supercomputing 2025.

AI LEARNING QUANTUM: NEURAL QUANTUM STATES

- Sample state from a DNN
  - Compression of high-dimensional function
- Use sampled state to estimate
  - Full quantum state
  - Physical quantities of interest
- ML solution to quantum questions
  - Condensed matter and materials science
  - Quantum chemistry

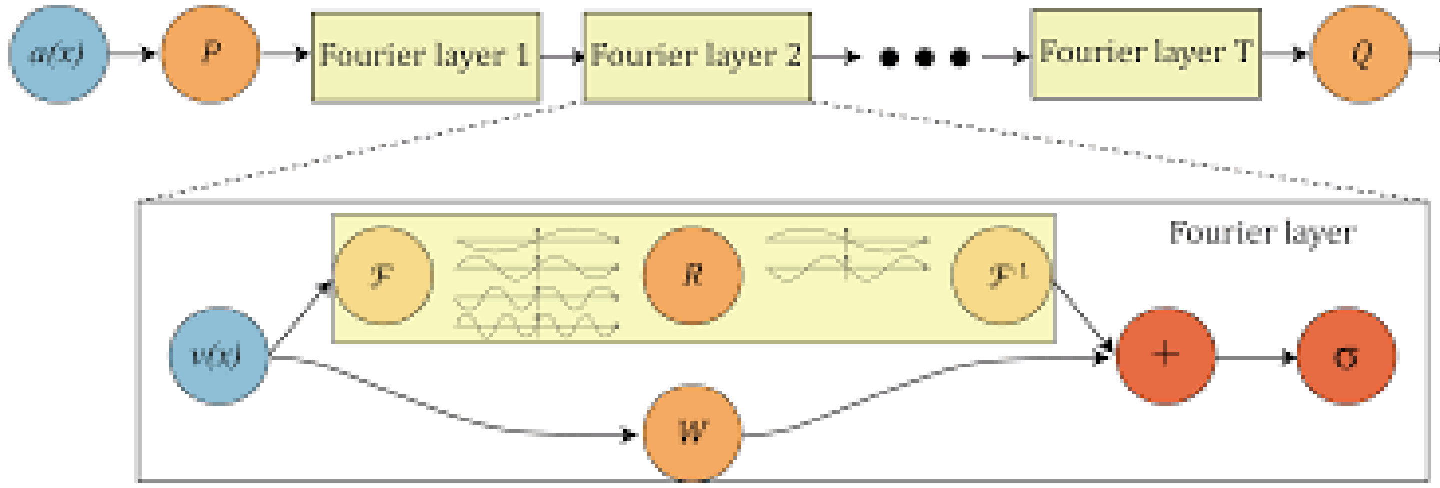

Carleo, and Troyer
Science 355, 602 (2017)

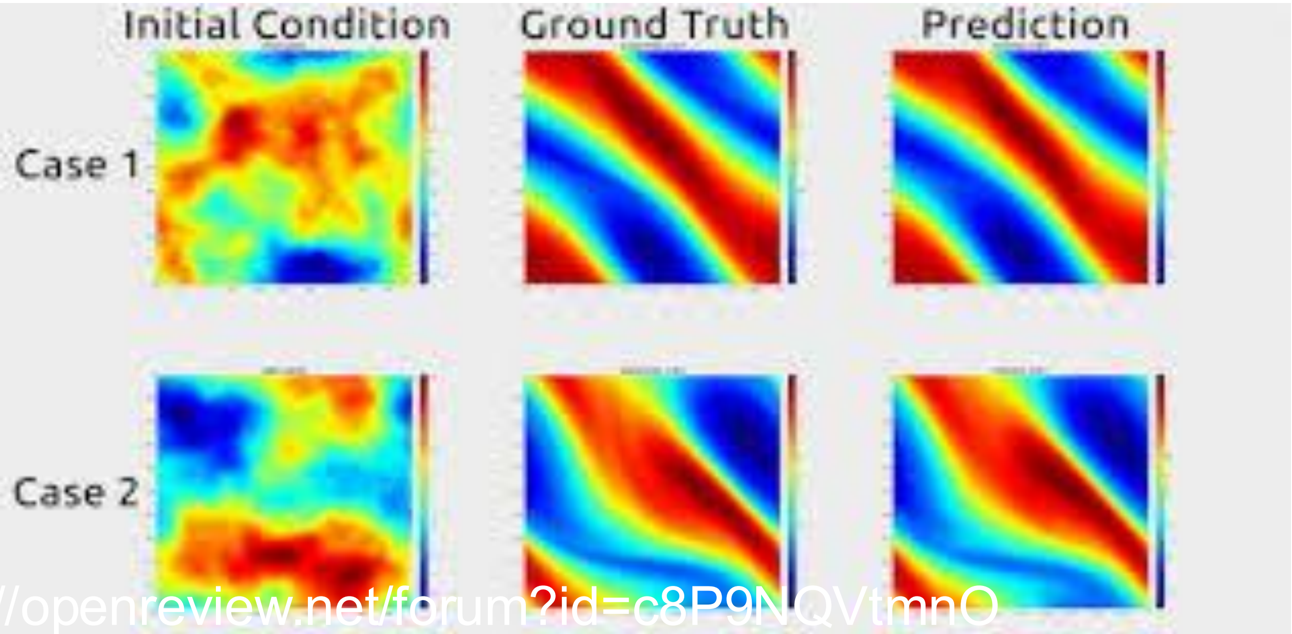
$$\Psi(s_1 \ldots s_N) = g^{(L)} \circ W^{(L)} \ldots g^{(2)} \circ W^{(2)} g^{(1)} \circ W^{(1)} \mathbf{s}$$

Giuseppe Carleo Workshop on Quantum Science and Quantum Technologies. *Neural quantum states*. ICTP Condensed Matter and Statistical Physics, 2017.

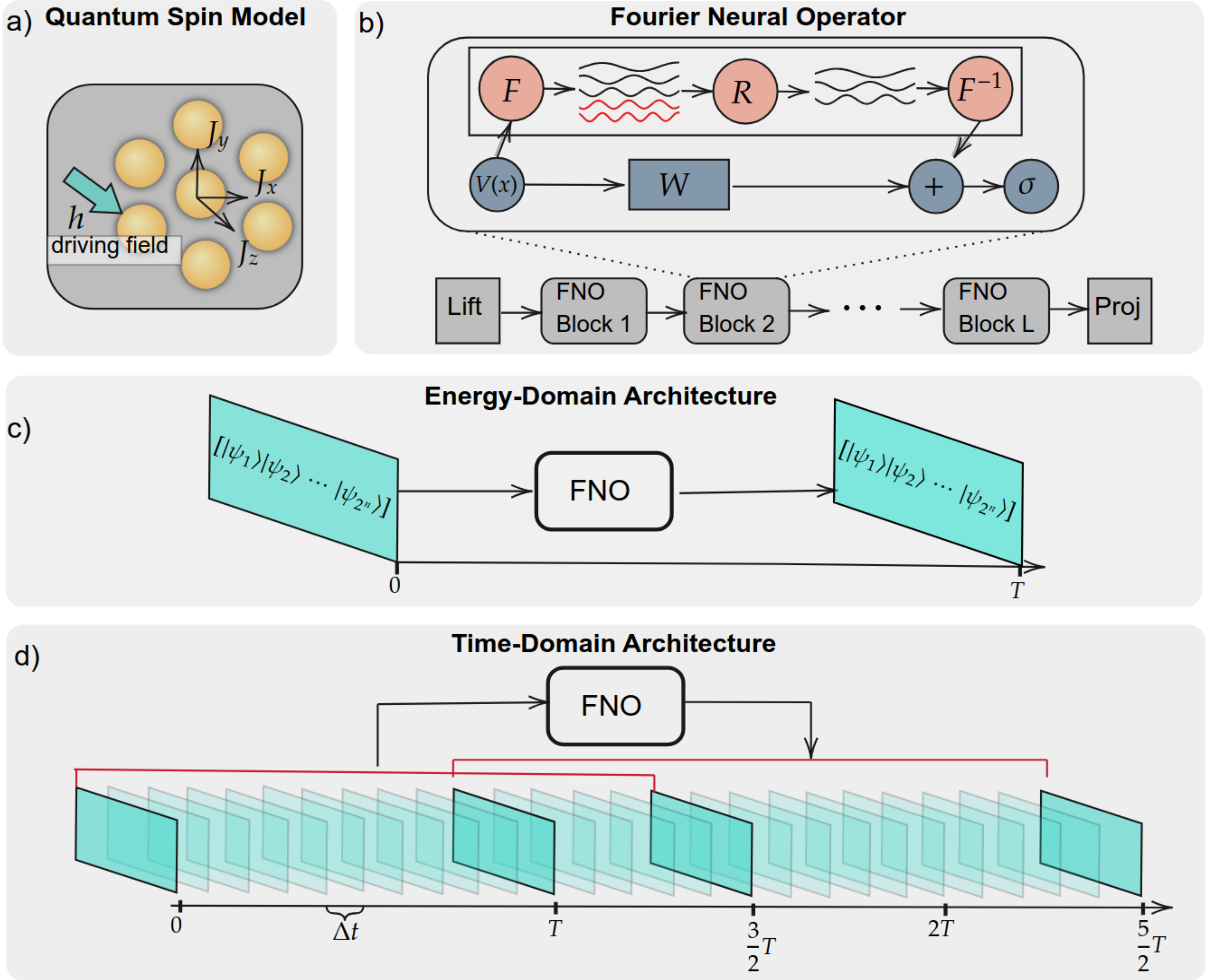
Extending techniques with the Carrasquilla Group ETH Zurich

AI FOR QUBIT DESIGN: FNOS



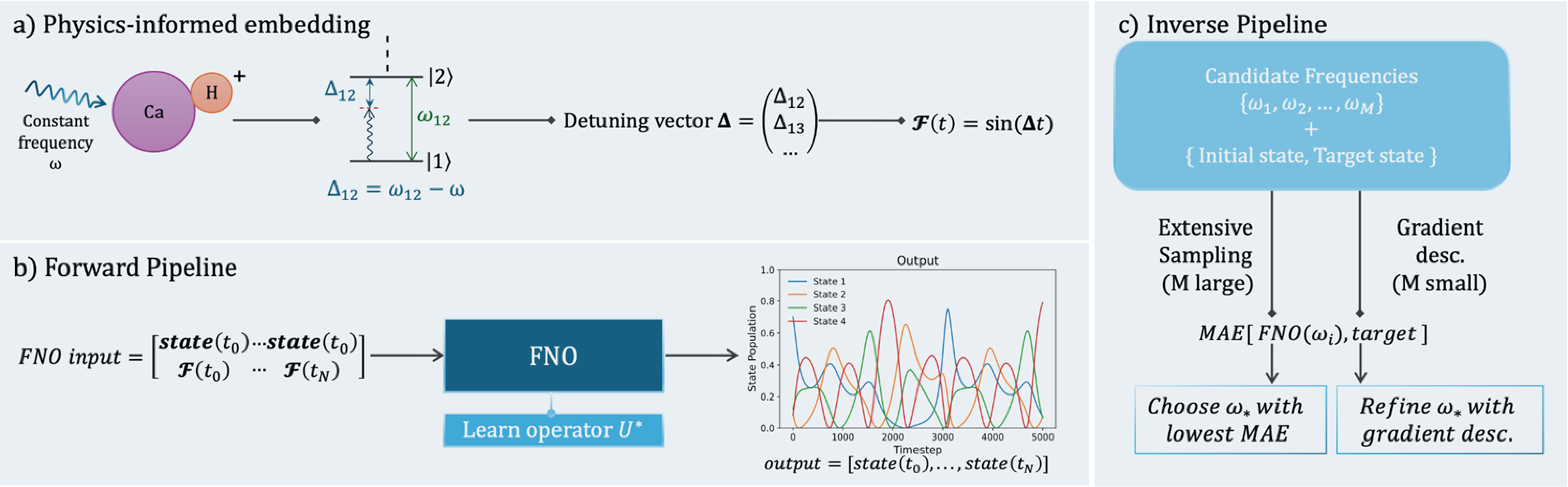


/openreview.net/forum?id=c8P9NQVtmnO



F. Shah, **TLP**, J. Berner, B. Tolooshams, J. Kossaifi, A. Anandkumar. arXiv:2409.03302.

AI FOR QUBIT DESIGN: FNOS



a) Physics-informed embedding

$\Delta_{12} = \omega_{12} - \omega$

Detuning vector $\mathbf{\Delta} = \begin{pmatrix} \Delta_{12} \\ \Delta_{13} \\ \cdots \end{pmatrix} \longrightarrow \boldsymbol{\mathcal{F}}(t) = \sin(\mathbf{\Delta} t)$

b) Forward Pipeline

$FNO\ input = \begin{bmatrix} \mathbf{state}(t_0) \cdots \mathbf{state}(t_0) \\ \boldsymbol{\mathcal{F}}(t_0) \quad \cdots \quad \boldsymbol{\mathcal{F}}(t_N) \end{bmatrix} \longrightarrow$ FNO $\longrightarrow$

Learn operator U^*

$output = [state(t_0), \dots, state(t_N)]$

c) Inverse Pipeline

Candidate Frequencies
$\{\omega_1, \omega_2, \dots, \omega_M\}$
+
{ Initial state, Target state }

Extensive Sampling (M large)

Gradient desc. (M small)

$MAE[\,FNO(\omega_i), target\,]$

Choose ω_* with lowest MAE

Refine ω_* with gradient desc.

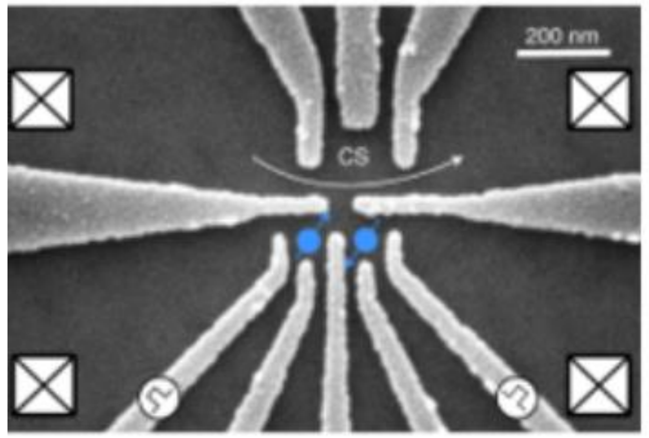
On small systems, we achieved speedups of >10^6x!
Imagine the impact on larger systems…

Quantum Device Lab

AI FOR QUBIT DESIGN: FNOS

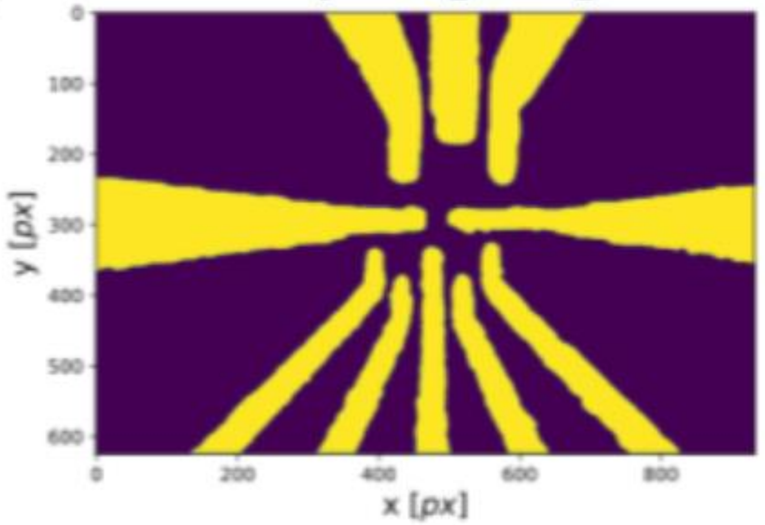
Oxford

SEM image of gates

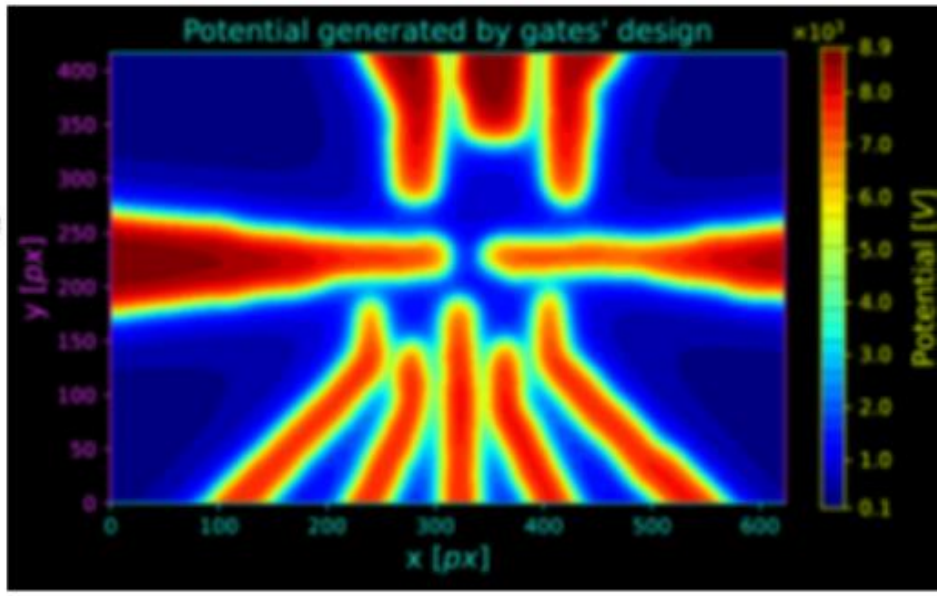


Transfer to binary image

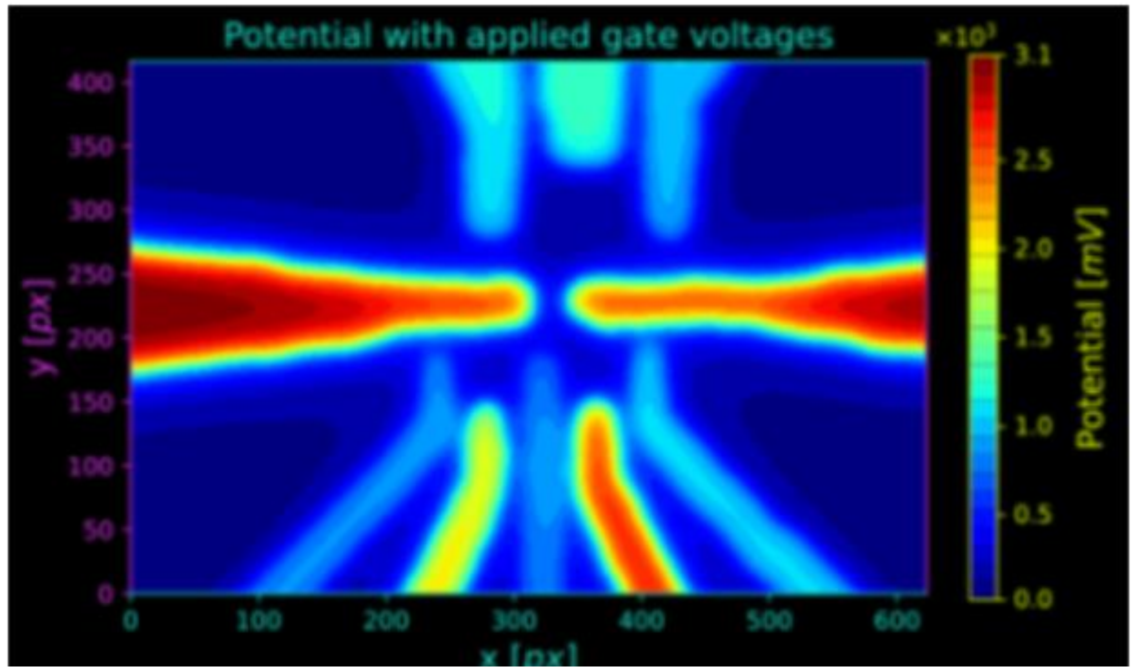
Binary image of gates



Calculate potential of each gate



Apply gate voltages



Thomas-Fermi approximation