

Quantum Computing

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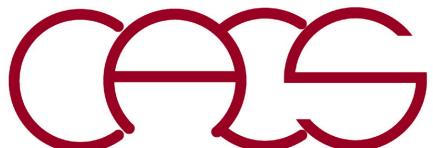
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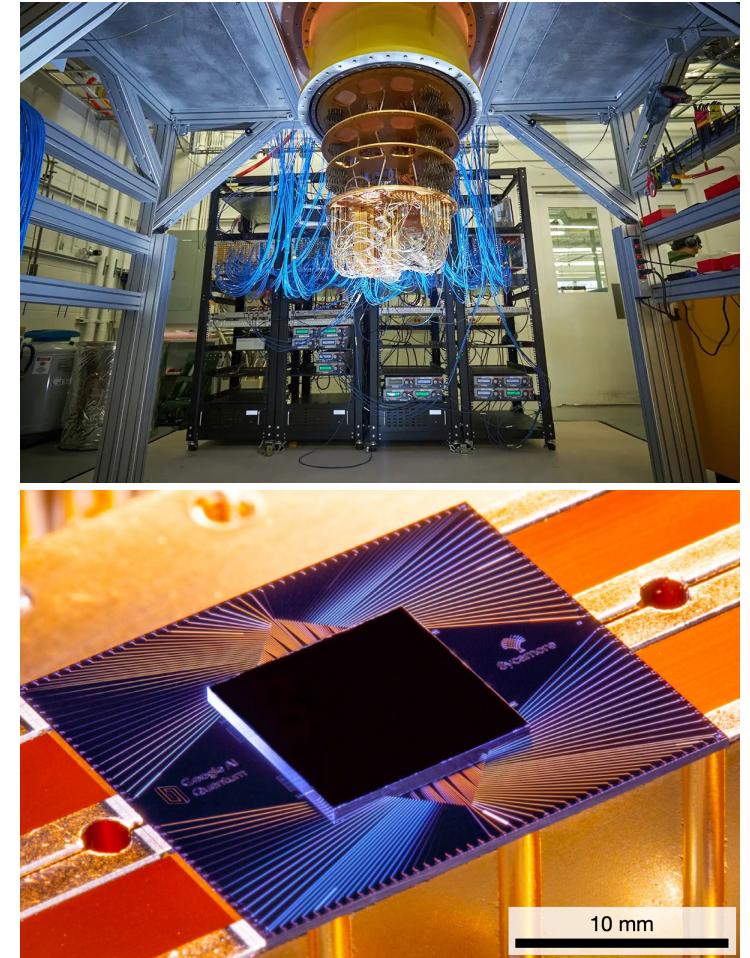
Goal: Quantum dynamics simulation on quantum circuits



Quantum Computing (QC) for Science

Quantum computing utilizes quantum properties such as superposition & entanglement for computation

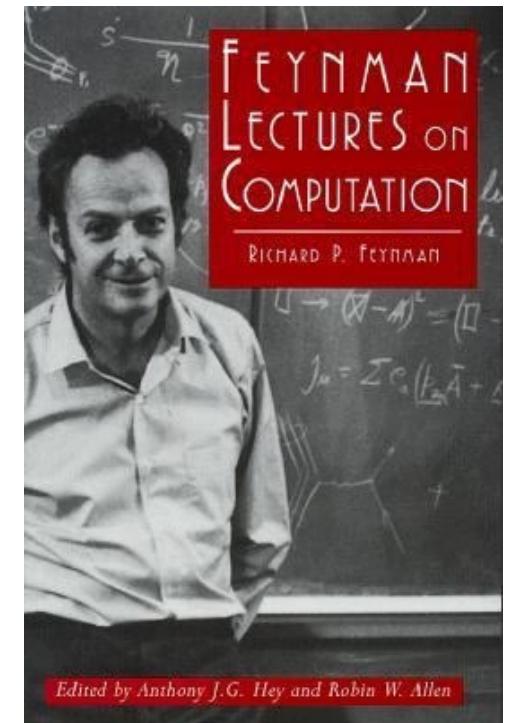
- U.S. Congress (Dec. 21, '18) signed National Quantum Initiative Act to ensure leadership in quantum computing & its applications
- Quantum supremacy demonstrated by Google
F. Arute, *Nature* **574**, 505 ('19)
- Quantum computing for science:
Universal simulator of quantum many-body systems
R. P. Feynman, *Int. J. Theo. Phys.* **21**, 467 ('82);
S. Lloyd, *Science* **273**, 1073 ('96)
- Success in simulating *static* properties of quantum systems (*i.e.*, ground-state energy of small molecules)
A. Aspuru-Guzik *et al.*, *Science* **309**, 1704 ('05)
- Challenge: Simulate quantum many-body *dynamics* on current-to-near-future noisy intermediate-scale quantum (NISQ) computers
J. Preskill, *Quantum* **2**, 79 ('18)



54-qubit Google Sycamore

Quantum Dynamics Simulations

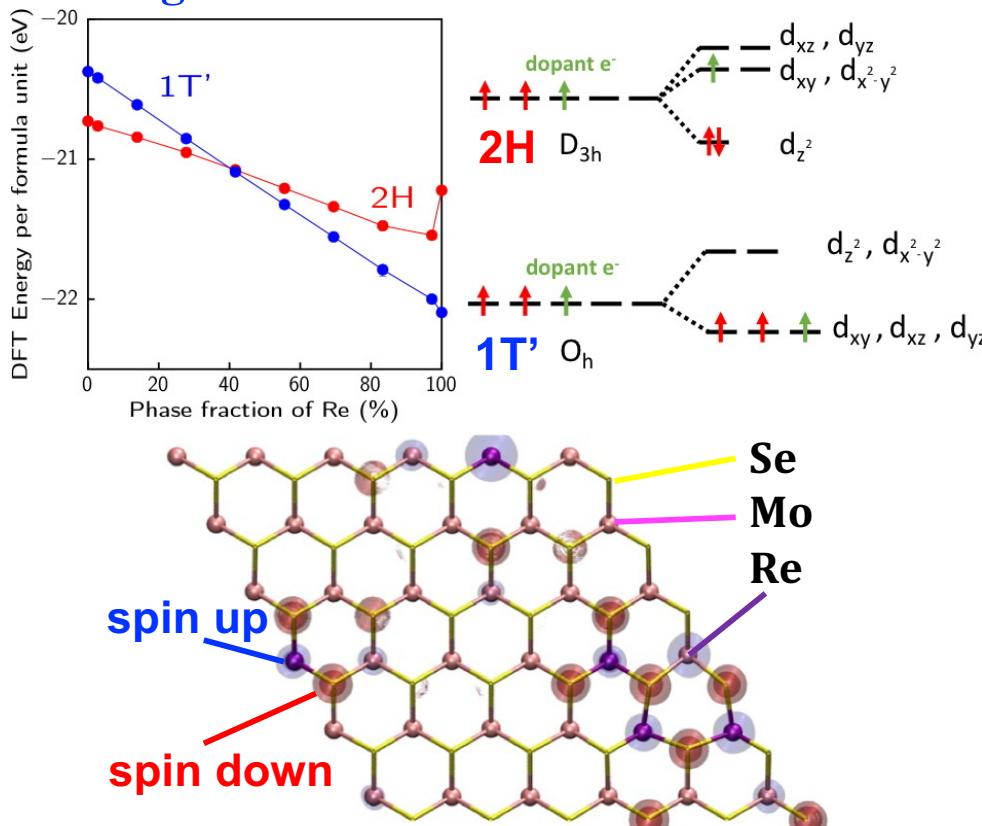
- An exciting scientific application of quantum computers is as a universal simulator of quantum many-body dynamics, as envisioned by Richard Feynman [*Int. J. Theor. Phys.* **21**, 467 ('82)]
- Seth Lloyd provided concrete algorithms and analysis [*Science* **273**, 1073 ('96)]
- Second edition of *Feynman Lectures on Computation* will add a section on “Simulating quantum dynamics” by John Preskill [[arXiv:2106.10522](https://arxiv.org/abs/2106.10522) ('21)]
- Simulated nontrivial quantum dynamics on publicly available IBM's Q16 Melbourne & Rigetti's Aspen NISQ computers, *i.e.*, ultrafast control of emergent magnetism by THz radiation in 2D material [[L. Bassman et al., Phys. Rev. B](https://arxiv.org/abs/2001.08505) **101**, 184305 ('20)]



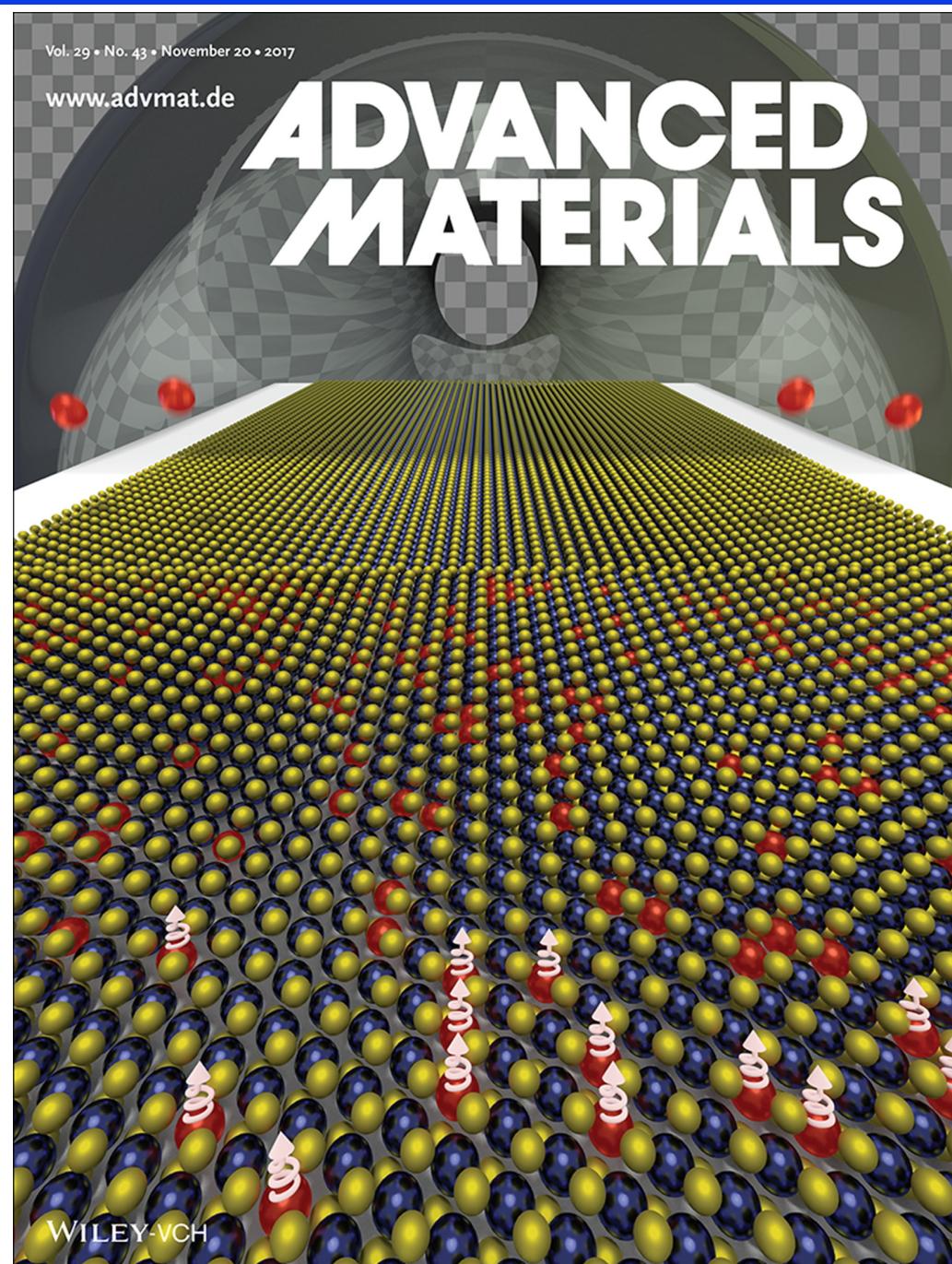
Do it yourself at <https://quantum-computing.ibm.com>

Emergent Magnetism: Structural Transition *via* Doping

- Experiment at Rice showed 2H-to-1T' phase transformation by alloying MoSe₂ with Re
- Simulations at USC elucidated its electronic origin
- Simulation & experiment showed novel magnetism centered at Re atoms



V. Kochat *et al.*, Adv. Mater. 29, 1703754 ('17)



Transverse Field Ising Model

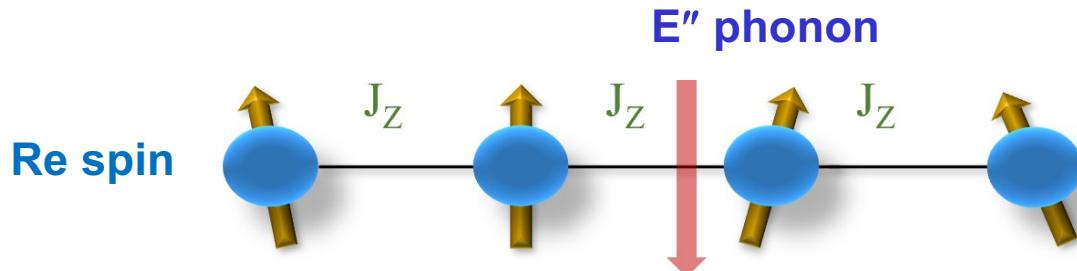
- Electromagnetic-field control of quantum states in a chain of rhenium-magnets in MoSe_2 monolayer to realize desired material properties on demand, thereby pushing the envelope of “quantum materials science”

$$H(t) = -J_z \sum_{j=1}^{N-1} \sigma_z^j \sigma_z^{j+1} - \varepsilon_{ph} \sin(\omega_{ph} t) \sum_{j=1}^N \sigma_x^j$$

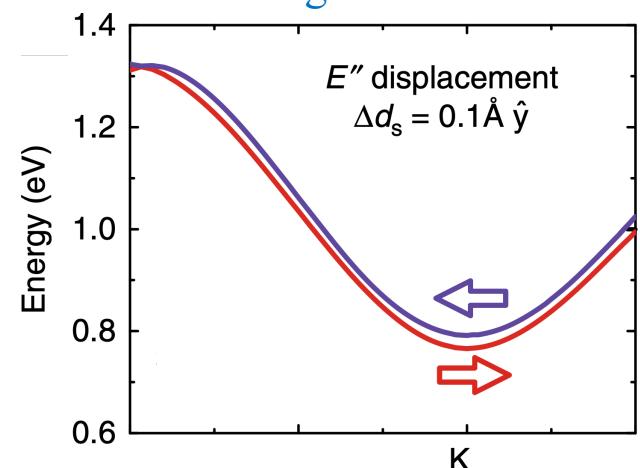
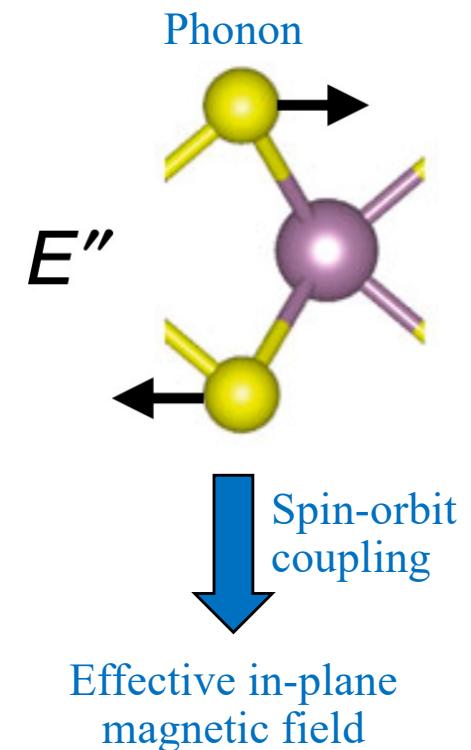
$= H_z + H_x(t)$

Phonon frequency
 Phonon-induced energy split

$$\sigma_z^j = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; \quad \sigma_x^j = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} // \text{Act on } j\text{-th qubit}$$



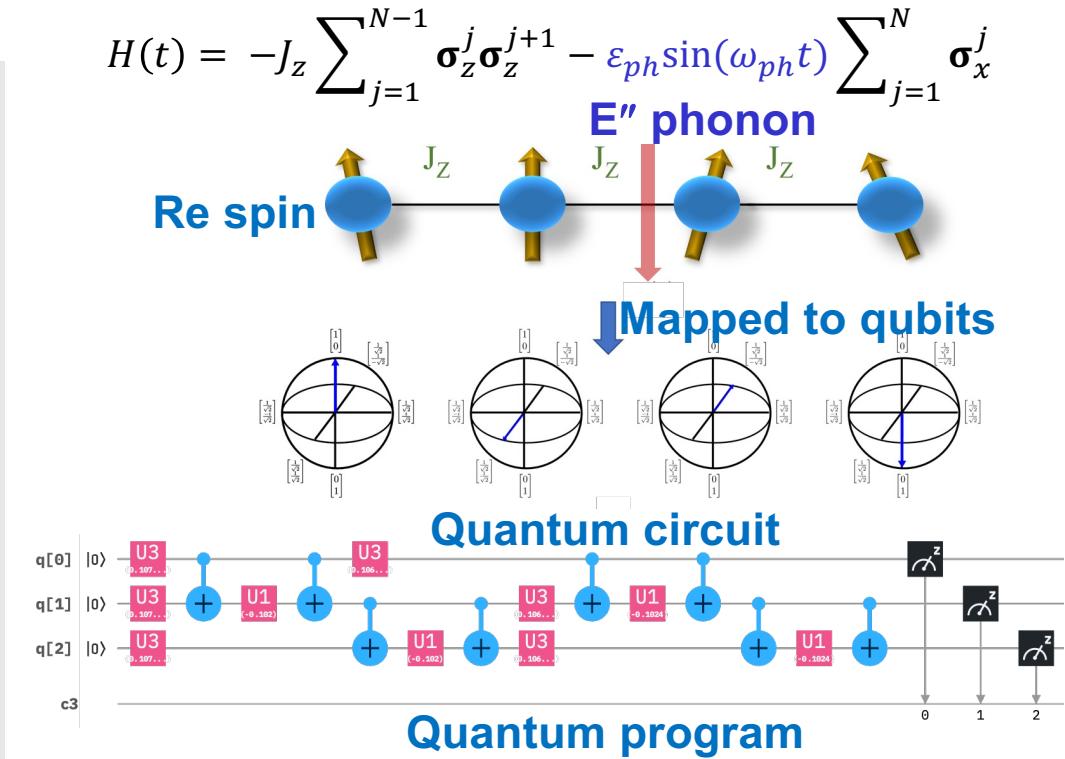
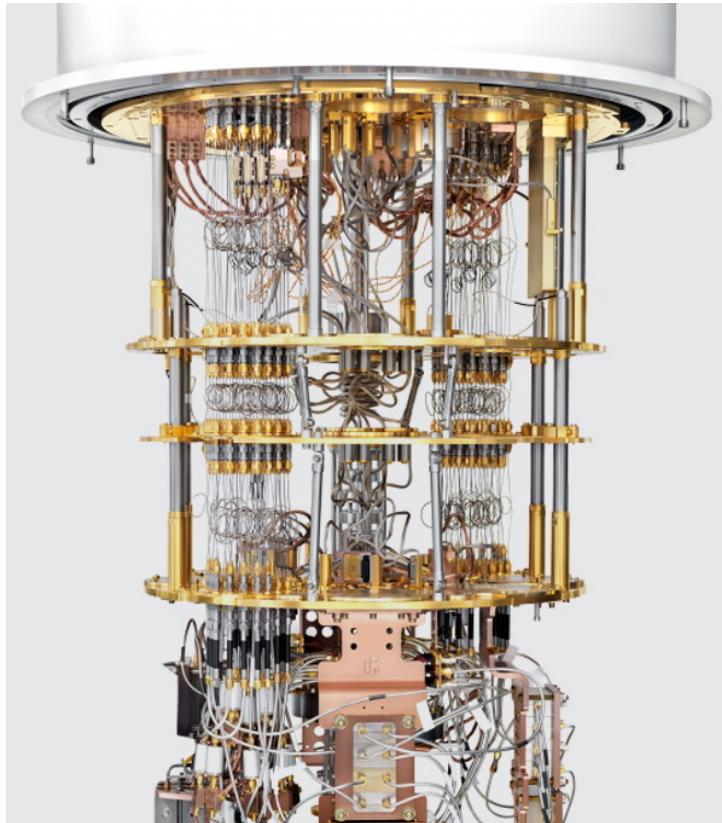
D. Shin et al., Nat. Commun. 9, 638 ('18)



Quantum Computing of Magnetism

- Simulated quantum many-body dynamics on IBM's Q16 Melbourne & Rigetti's Aspen quantum processors

L. Bassman et al., Phys. Rev. 101, 184305 ('20)



```
32  l... ....#define the two non-commuting terms that comprise the Hamiltonian-
33  l... Hz = PauliTerm("Z", 0, epsilon_0)-
34  l... Hy = PauliTerm("Y", 0, epsilon_ph*np.sin(w_ph*t))-#
35  l... #exponentiate the terms of the Hamiltonian for use in Trotter approx-
36  l... exp_Hz = exponential_map(Hz)(delta_t/(2.0*hbar))-#
37  l... exp_Hy = exponential_map(Hy)(delta_t/hbar)-
```

Will derive & implement the circuit in the hands-on session

Quantum Dynamics on NISQ Computers

- Time-evolution operator for wave function $|\Psi(t)\rangle$ for small time interval Δt (atomic unit, $\hbar = 1$)

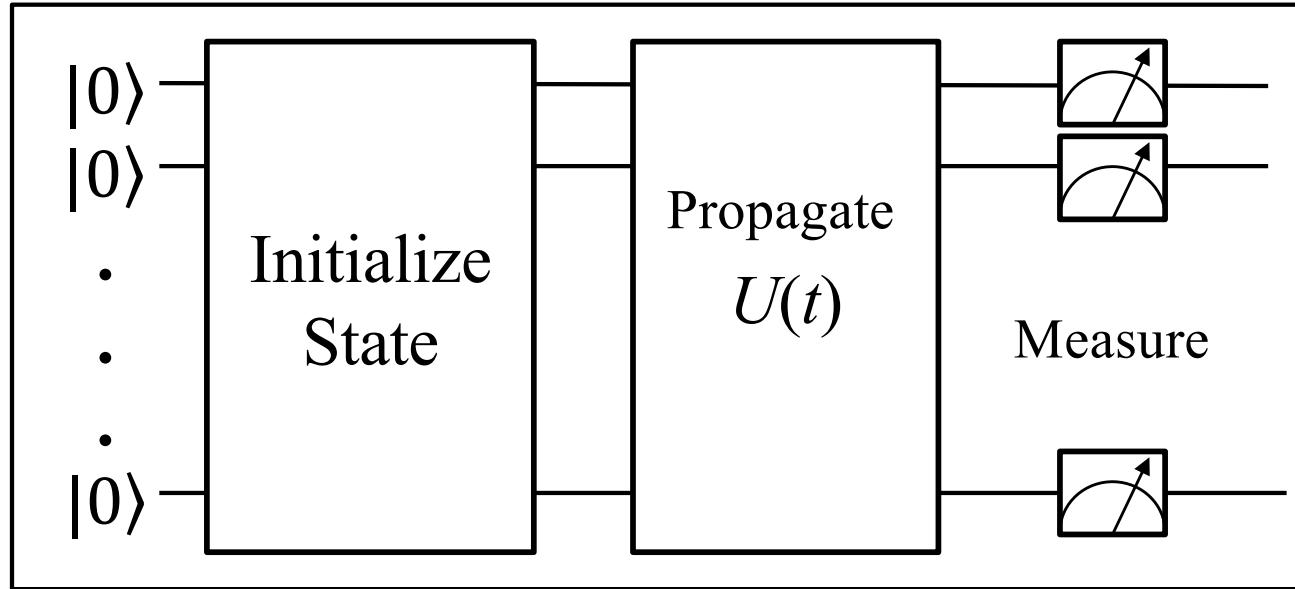
$$|\Psi(\Delta t)\rangle = U(\Delta t)|\Psi(t=0)\rangle$$
$$U(\Delta t) = \exp(-iH\Delta t)$$

- Time discretization with time-step Δt and Trotter expansion

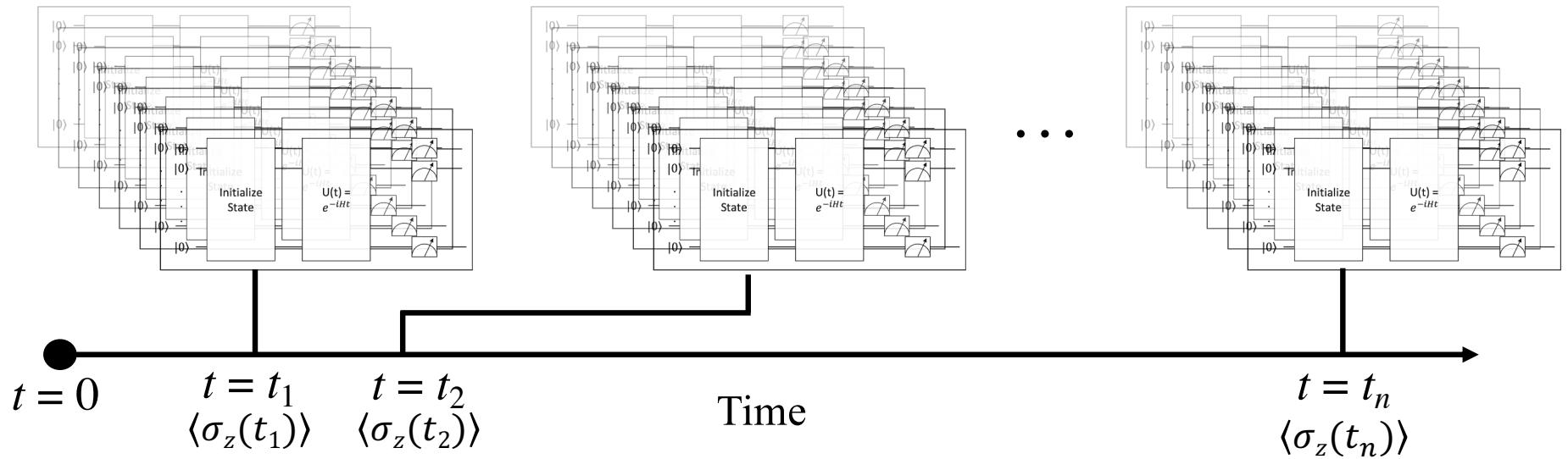
$$U(n\Delta t) \approx \prod_{k=0}^{n-1} \exp(-iH_z\Delta t) \exp(-iH_x(k + 1/2)\Delta t)$$

- One simulation run provides measurement for only one time instance ($t = n\Delta t$) — if you can see intermediate time steps, it's not quantum computing

Quantum Computing Runs

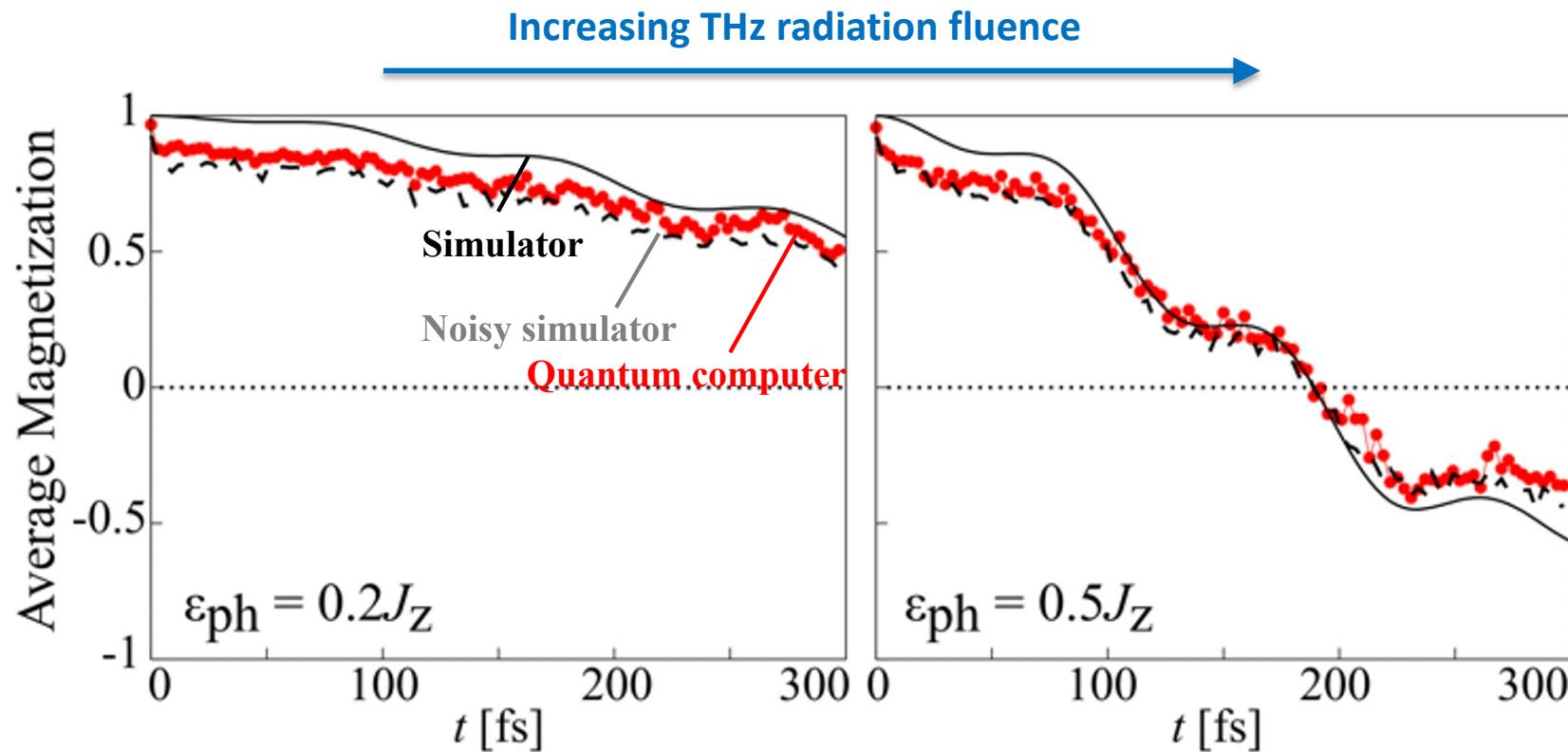


For each time instance, many runs to obtain statistics



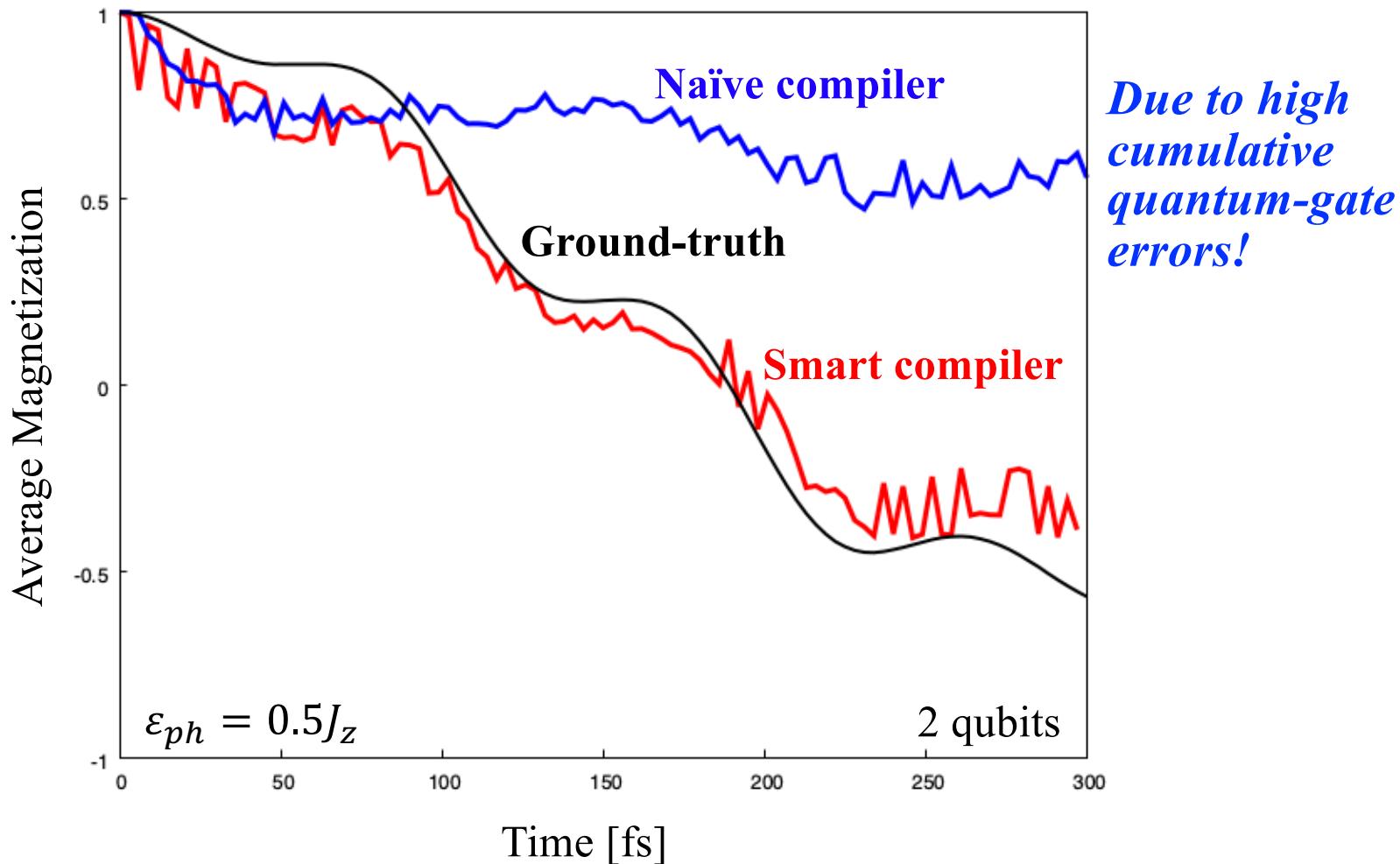
Quantum Computing Results

- Quantum-dynamics simulations on a NISQ computers show dynamic suppression of magnetization by THz radiation



Circuit Size vs. Simulation Fidelity

- Reduced circuit size improves the fidelity of simulation



Naïve compiler: circuit size \propto time

Smart compile: Constant circuit size w.r.t. time

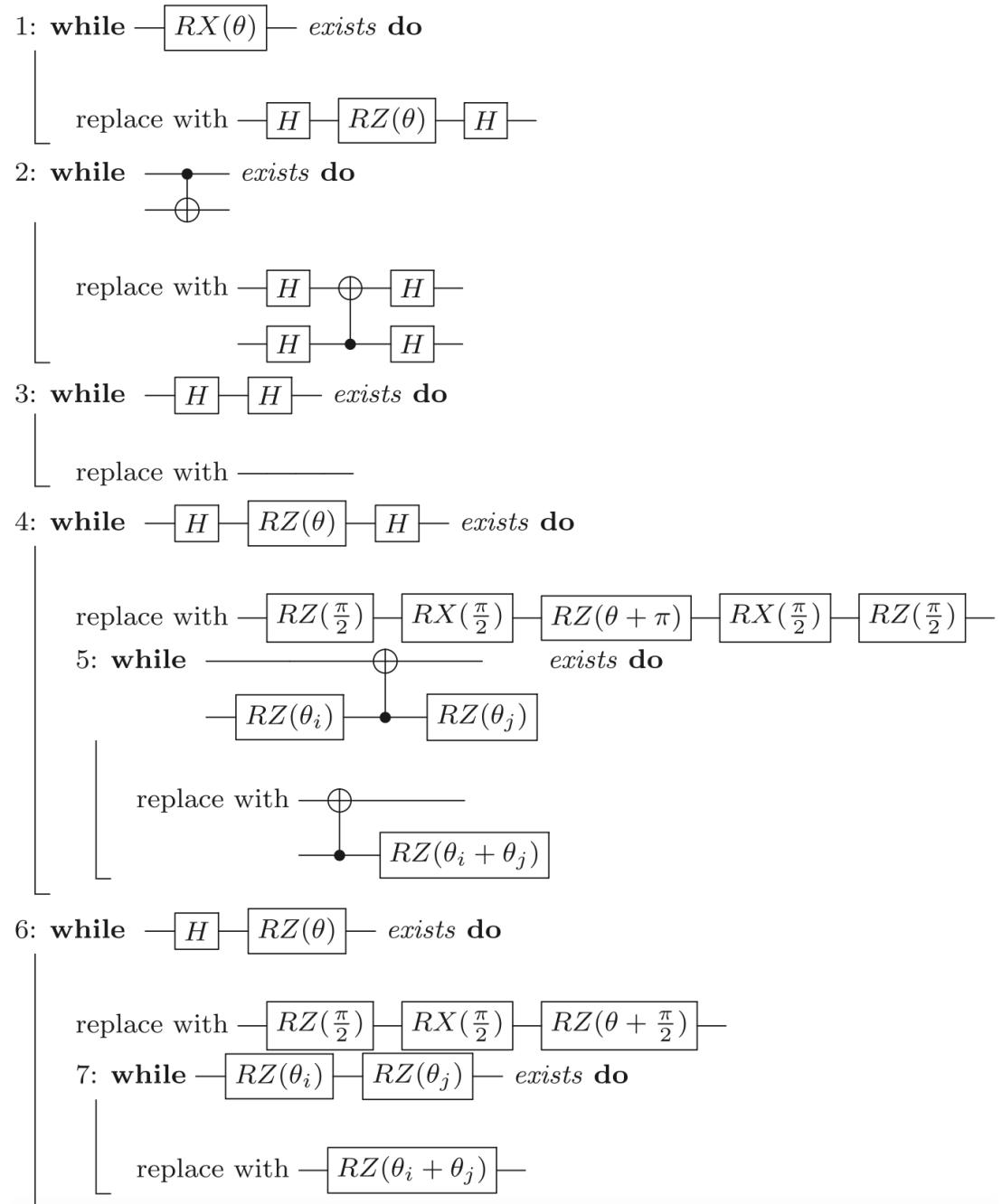
Quantum Compiler: Math

- **Problem:** High gate errors make long-time simulations impractical
- **Solution:** Domain-specific compiler = use algebraic identities to derive an equivalent circuit with reduced circuit size

No.	Common gate set in TFIM circuits	Equivalent
1	$\text{---} \boxed{RX(\theta)} \text{---}$	$\text{---} \boxed{H} \text{---} \boxed{RZ(\theta)} \text{---} \boxed{H} \text{---}$
2	$\text{---} \boxed{H} \text{---}$	$\text{---} \boxed{RZ(\frac{\pi}{2})} \text{---} \boxed{RX(\frac{\pi}{2})} \text{---} \boxed{RZ(\frac{\pi}{2})} \text{---}$
3	$\text{---} \bullet \text{---} \oplus \text{---}$	$\text{---} Z \text{---}$ $\text{---} \boxed{H} \text{---} \bullet \text{---} \boxed{H} \text{---}$
4	$\text{---} \bullet \text{---} \oplus \text{---}$	$\text{---} \boxed{H} \text{---} \bullet \text{---} \oplus \text{---} \boxed{H} \text{---} \bullet \text{---} \boxed{H} \text{---}$
5	$\text{---} \boxed{RX(\theta_i)} \text{---} \boxed{RZ(\pi)} \text{---}$	$\text{---} \boxed{RZ(-\pi)} \text{---} \boxed{RX(-\theta_i)} \text{---}$
6	$\text{---} \bullet \text{---} \boxed{Z} \text{---} \boxed{RX(\frac{\pi}{2})} \text{---} \boxed{RZ(\theta_i)} \text{---} \boxed{RX(-\frac{\pi}{2})} \text{---} \bullet \text{---} \boxed{RX(\frac{\pi}{2})} \text{---}$	$\text{---} \boxed{RX(-\frac{\pi}{2})} \text{---} \bullet \text{---} \boxed{Z} \text{---} \boxed{RX(\frac{\pi}{2})} \text{---} \boxed{RZ(\theta_i)} \text{---} \boxed{RX(-\frac{\pi}{2})} \text{---} \bullet \text{---} \boxed{Z} \text{---}$
7	$\text{---} \boxed{H} \text{---} \boxed{H} \text{---}$	—
8	$\text{---} \boxed{RX(\theta_i)} \text{---} \boxed{RX(\theta_j)} \text{---}$	$\text{---} \boxed{RX(\theta_i + \theta_j)} \text{---}$
9	$\text{---} \boxed{RZ(\theta_i)} \text{---} \boxed{RZ(\theta_j)} \text{---}$	$\text{---} \boxed{RZ(\theta_i + \theta_j)} \text{---}$
10	$\text{---} \boxed{RZ(\theta_i)} \text{---} \bullet \text{---} \boxed{RZ(\theta_j)} \text{---}$ $\text{---} \bullet \text{---} \boxed{Z} \text{---}$	$\text{---} \bullet \text{---} \boxed{RZ(\theta_i + \theta_j)} \text{---}$ $\text{---} \bullet \text{---} \boxed{Z} \text{---}$
11	$\text{---} \boxed{RZ(\theta_i)} \text{---} \bullet \text{---} \boxed{RZ(\theta_j)} \text{---}$ $\text{---} \bullet \text{---} \oplus \text{---}$	$\text{---} \bullet \text{---} \boxed{RZ(\theta_i + \theta_j)} \text{---}$ $\text{---} \bullet \text{---} \oplus \text{---}$

Algorithm for IBM Native Gates

- Heuristic algorithm similar to unit propagation in artificial intelligence (AI)
- The heuristic order & types of identities applied are specific to the particular quantum dynamics we simulated

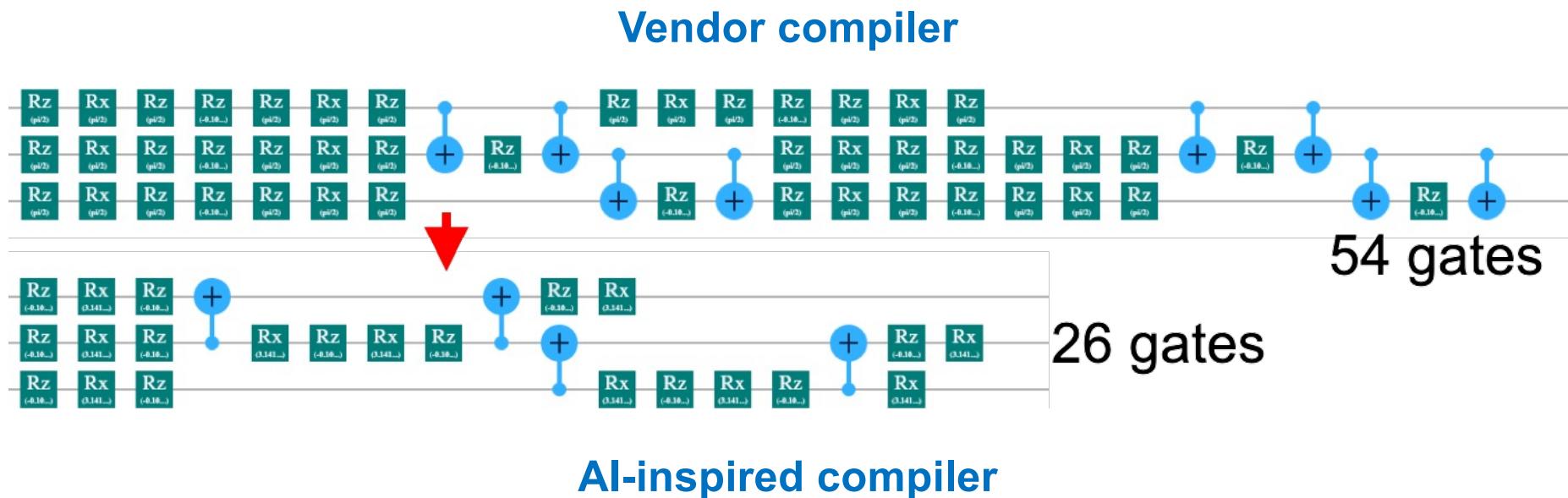


L. Bassman et al.,

Quantum Sci. Tech. 6, 014007 ('21)

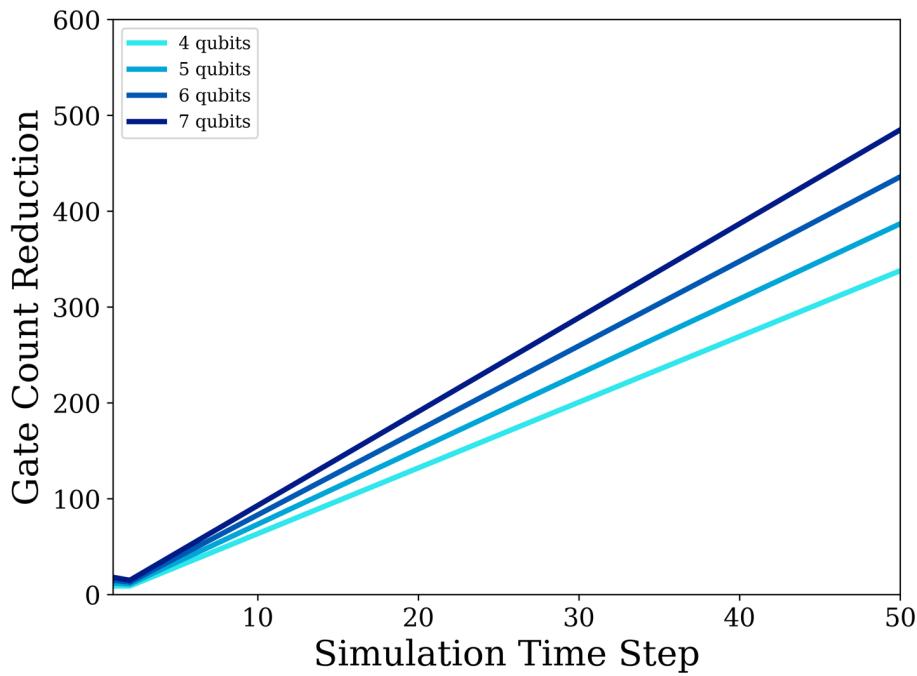
Domain-Specific Quantum Compiler

- Take advantage of specific problem structure
- AI-inspired quantum compiler reduced the circuit size by 30% to mitigate environmental noise

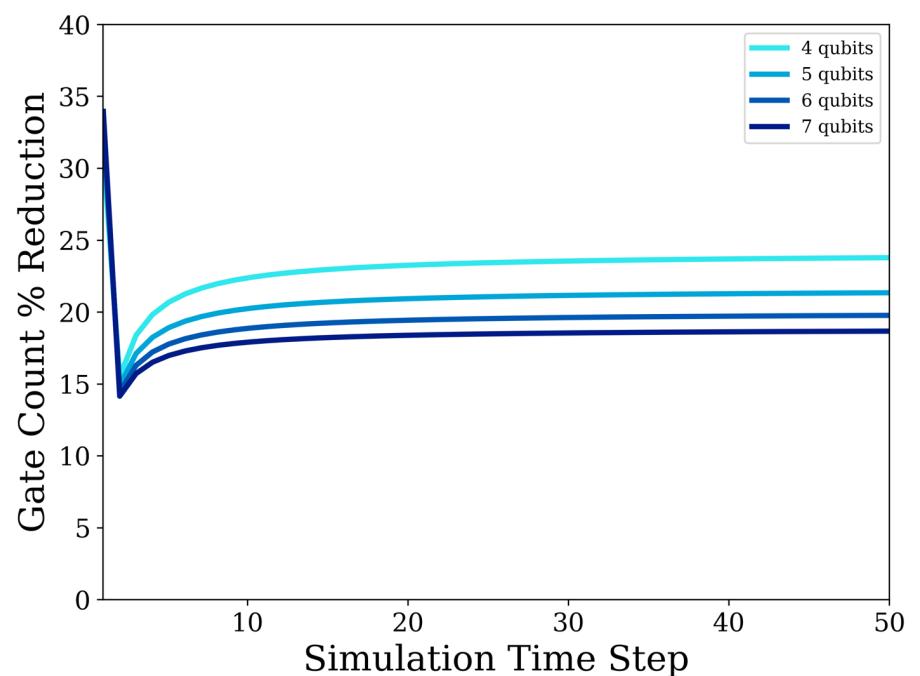


Performance of Domain-Specific Compiler

Absolute gate count difference
(IBM Compiler - DS Compiler)

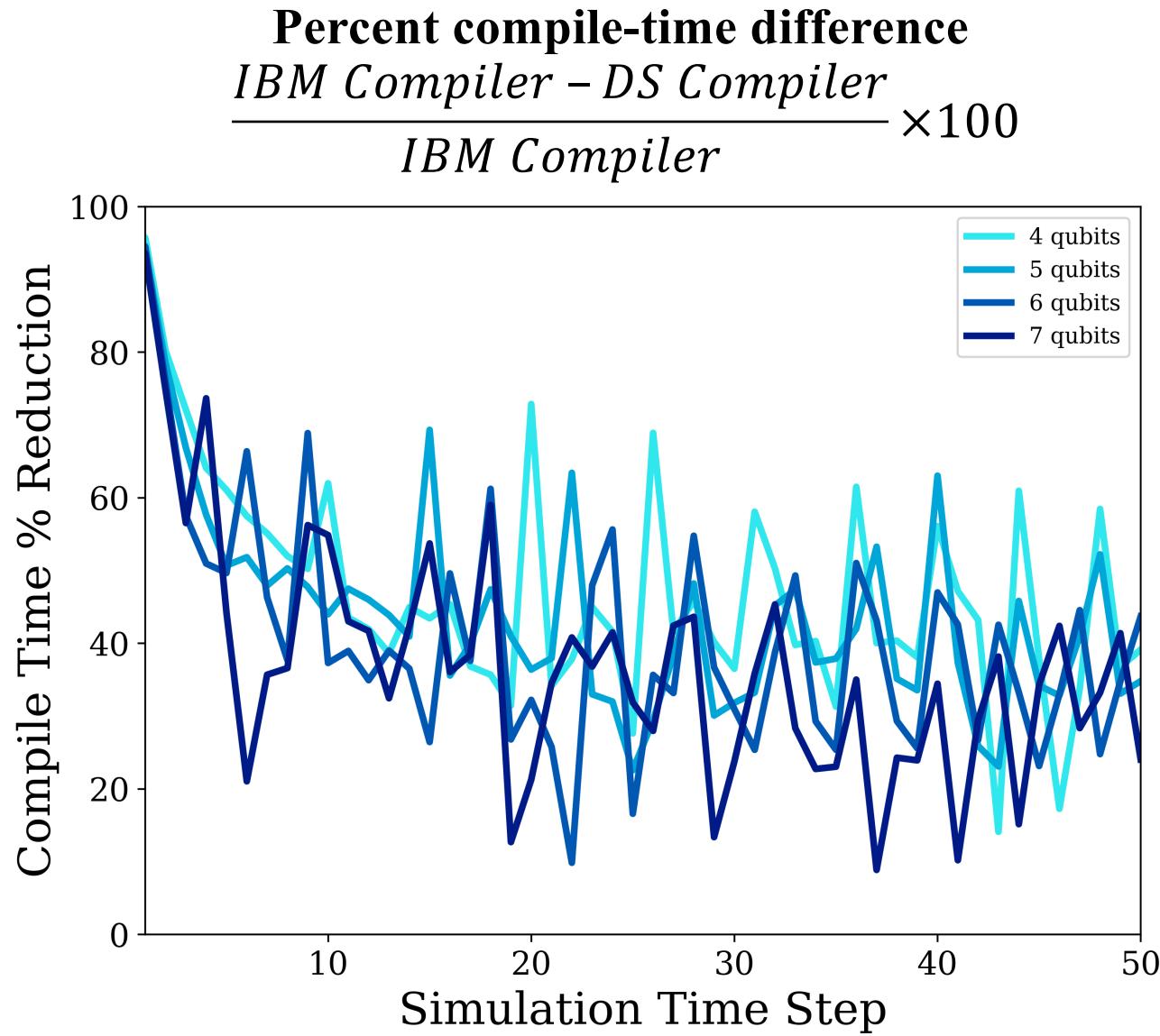


Percent gate count difference
 $\frac{IBM\ Compiler - DS\ Compiler}{IBM\ Compiler} \times 100$



Domain-specific compiler reduces gate count compared to IBM compiler

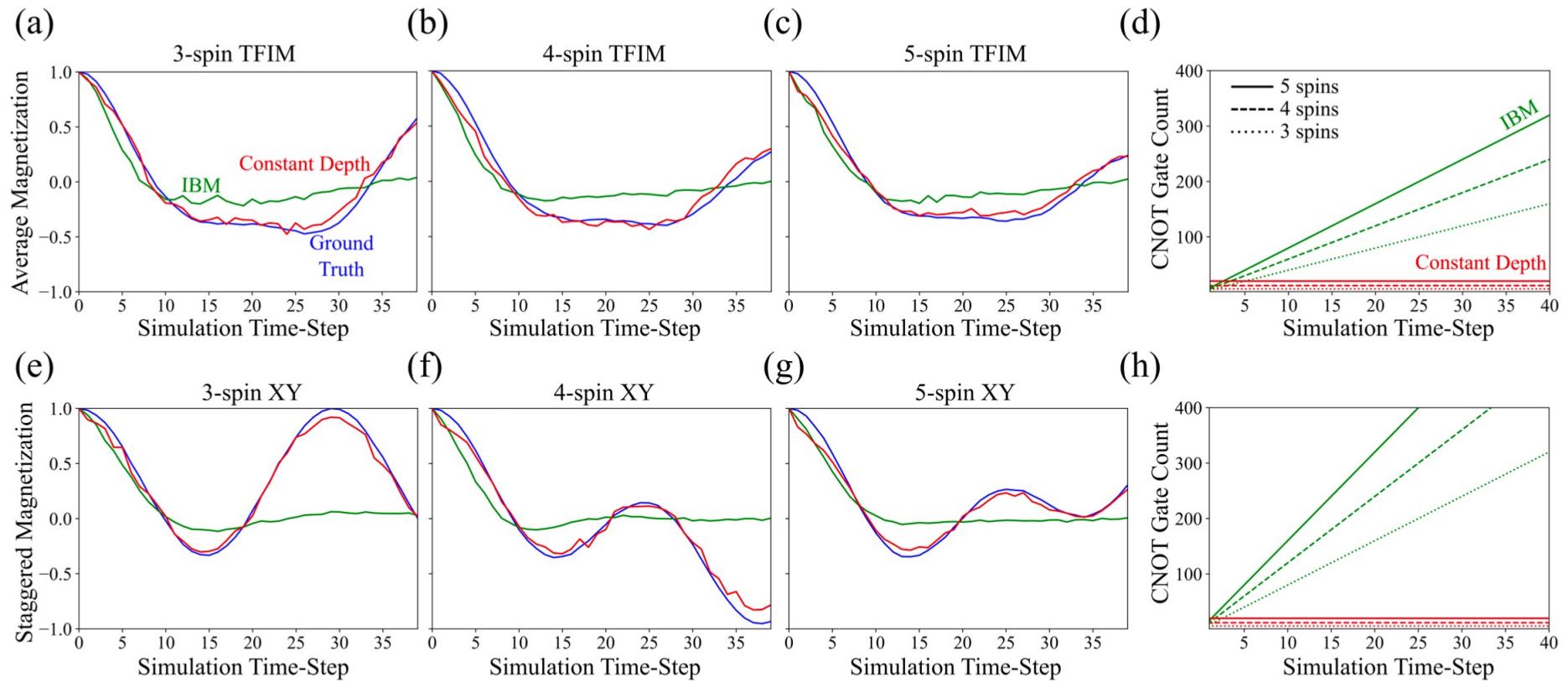
Speed of Domain-Specific Compiler



... and does it faster

Extension: Constant Circuit-Depth Algorithm

- Mathematical identities allow constant circuit depth independent of the number of time steps n for arbitrary number of spins N in a linear spin chain



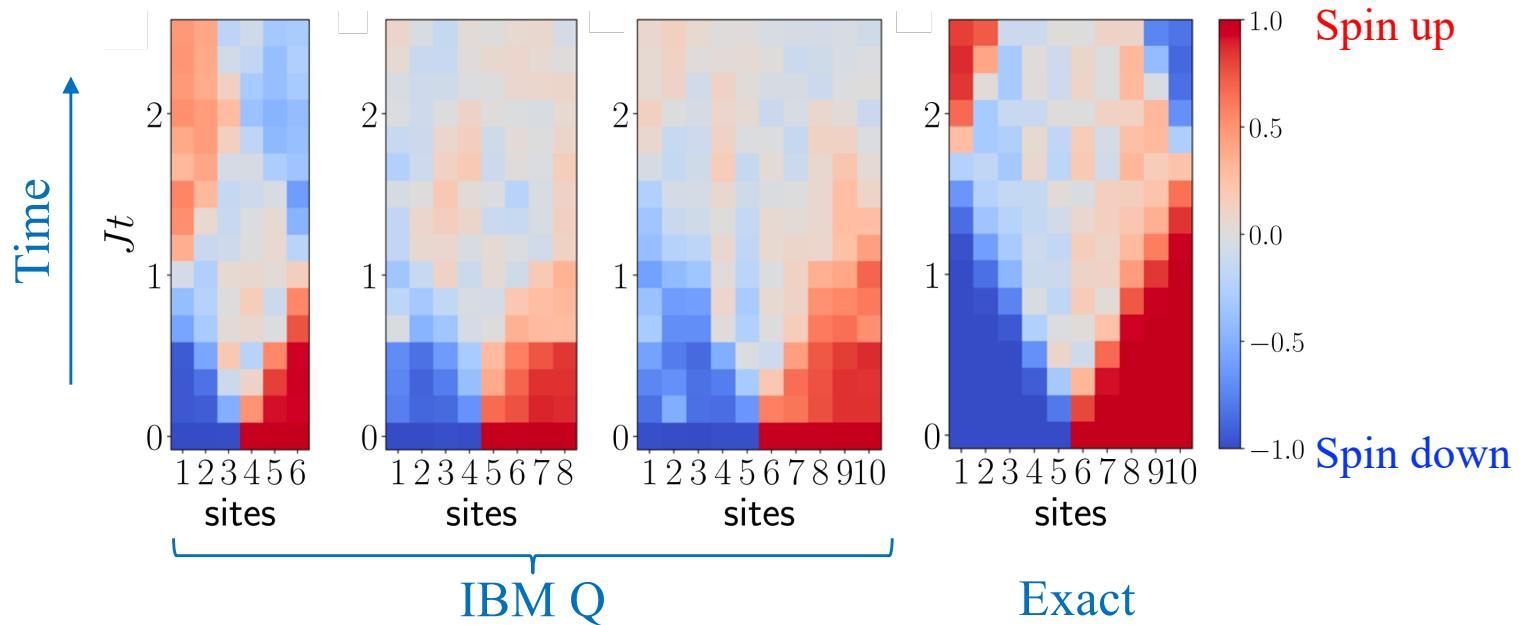
Richer Physics: Heisenberg Model

$$H = - \underbrace{\sum_{j=1}^{N-1} (J_x \sigma_x^j \sigma_x^{j+1} + J_y \sigma_y^j \sigma_y^{j+1} + J_z \sigma_z^j \sigma_z^{j+1})}_{\text{Exchange coupling}} - h \underbrace{\sum_{j=1}^N \sigma_z^j}_{\text{Magnetic field}}$$

Pauli spin-1/2 matrices

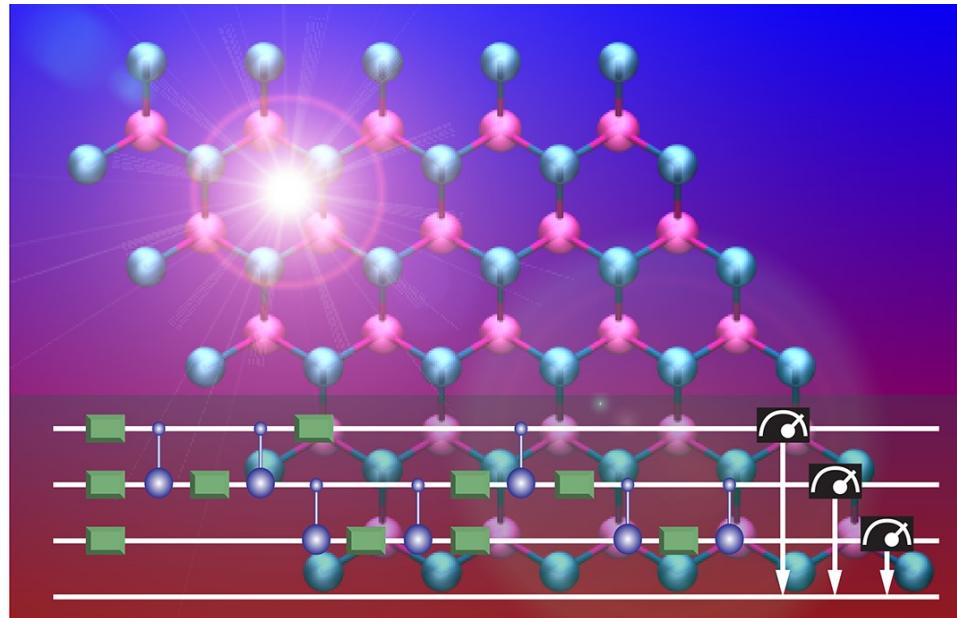
$$\sigma_x^j = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \sigma_y^j = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \sigma_z^j = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} // \text{Act on } j\text{-th qubit}$$

Domain-wall dynamics (6-, 8- & 10-site spin chains)



Open-Source Quantum Software

- Full-stack, cross-platform software for quantum dynamics simulations on NISQ computers was made available open-source



MISTIQS

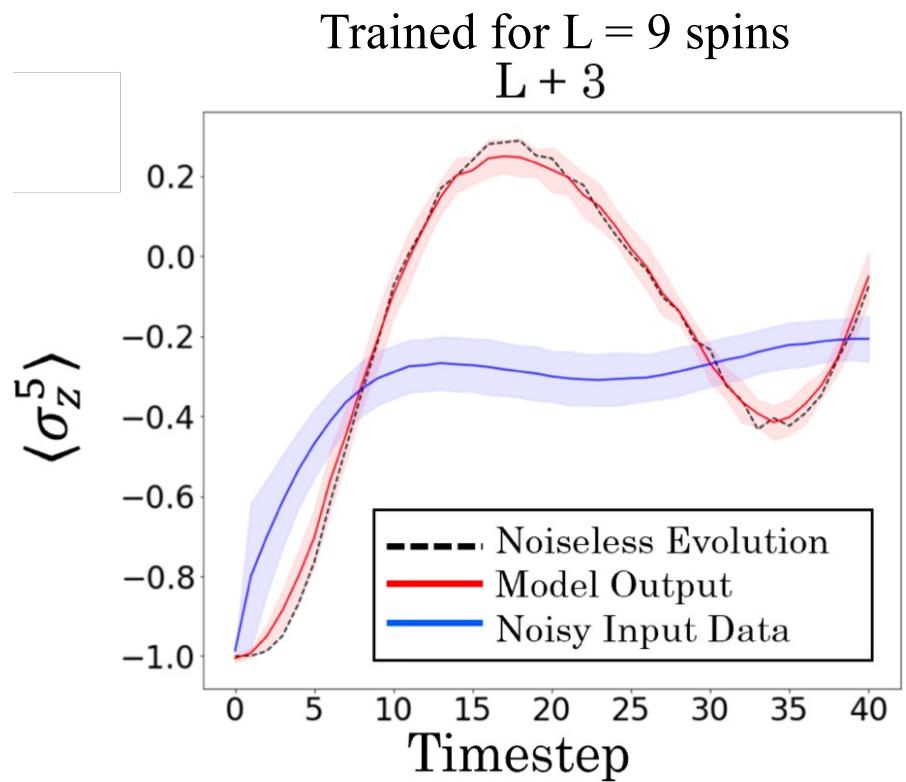
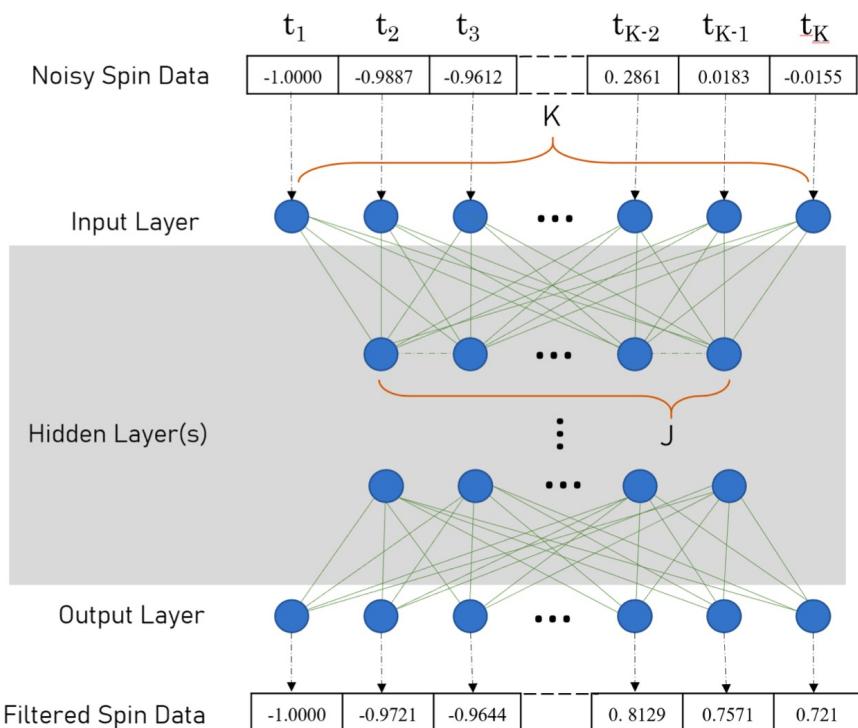
Multiplatform
Software for
Time-dependent
Quantum
Simulation

Paper: [C. Powers et al., SoftwareX 14, 100696 \('21\)](#)

Software: <https://github.com/USCCACS/MISTIQS>

Extension: Machine Learning

- Alternative noise mitigation using machine learning:
Autoencoder, trained with quantum simulations of small systems, is capable of filtering noise from dynamic simulations of larger systems run on quantum computers



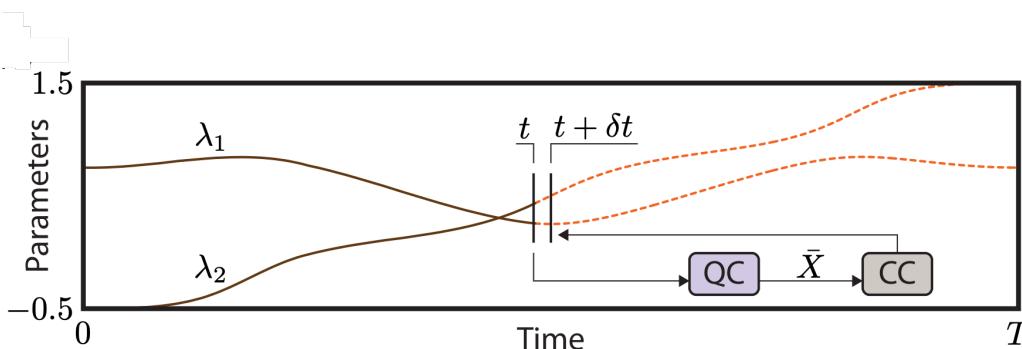
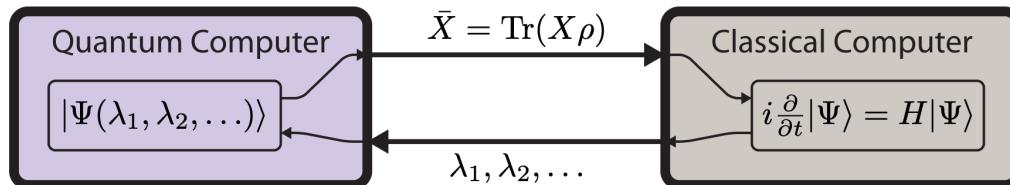
Variational Quantum Simulator

Hybrid quantum/classical approach: Boost the power of a classical supercomputer using a quantum co-processor

- A variational approach similar to variational quantum eigensolver (VQE) can be applied to quantum dynamics

$$\delta \int_{t_i}^{t_f} dt \left\langle \psi(t) \right| \left(i \frac{\partial}{\partial t} - H \right) \left| \psi(t) \right\rangle = 0$$

- Short-time propagation of a many-body wave function on a quantum computer is mapped back to a parameterized variational wave function, $|\Psi(\lambda_1(t), \dots, \lambda_p(t))\rangle$, which is tractable on a classical computer



Where to Go from Here

- New MS degree in Quantum Information Science ([MSQIS](#)) started in 2021
- Required foundational courses
 1. EE 520: Introduction to Quantum Information Processing
 2. EE 514: Quantum Error Correction
 3. Phys 513: Applications of Quantum Computing
- Core — at least two courses from
 1. EE 589: Quantum Information Theory
 2. Phys 550: Open Quantum Systems
 3. Phys 559: Quantum Devices
 4. Phys 660: Quantum Information Science & Many-Body Physics
- Phys 513: Application of Quantum Computing (co-taught with Prof. Rosa Di Felice) — quantum simulations on quantum circuits & adiabatic quantum annealer ([syllabus](#))
- Phys 516 (this course): Core elective for MSQIS