Quantum Computational Science

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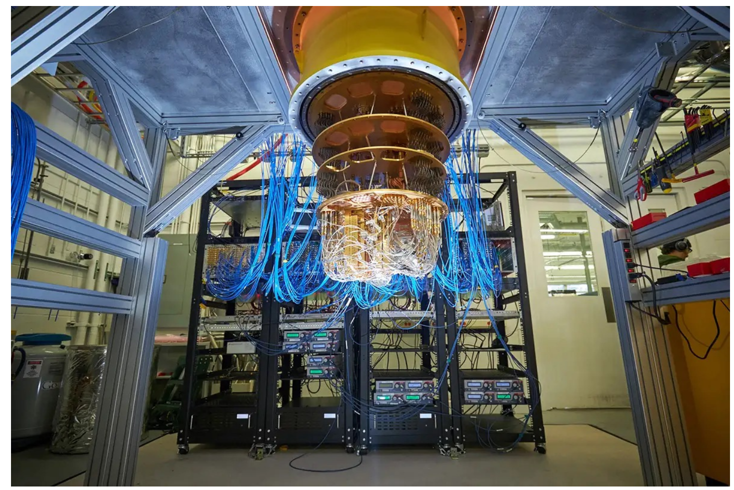
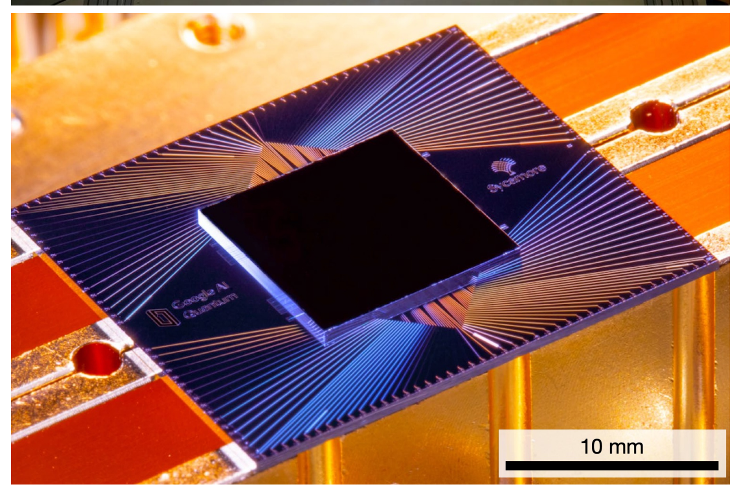
Goal: Quantum dynamics simulation on quantum circuits

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

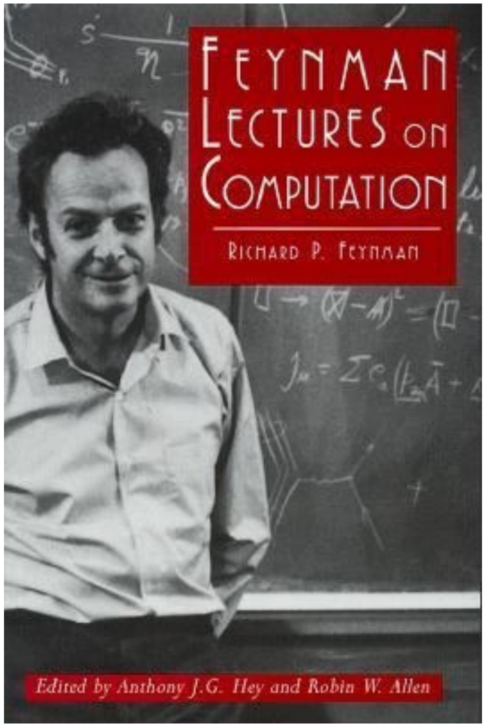
Quantum Dynamics Simulations

- **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 ('21)]

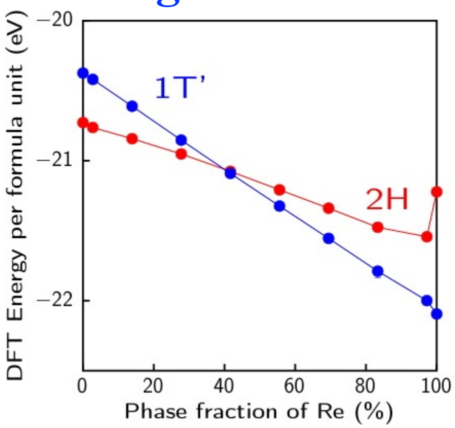
- **Simulated nontrivial quantum dynamics on publicly available IBM's Q16 Melbourne & Rigetti's Aspen NISQ computers, *i.e.*, ultrafast control of emergent magnetism by THz radiation in 2D material** [L. Bassman *et al., Phys. Rev. B* **101**, 184305 ('20)

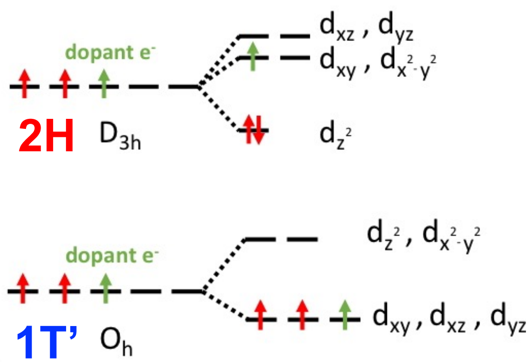


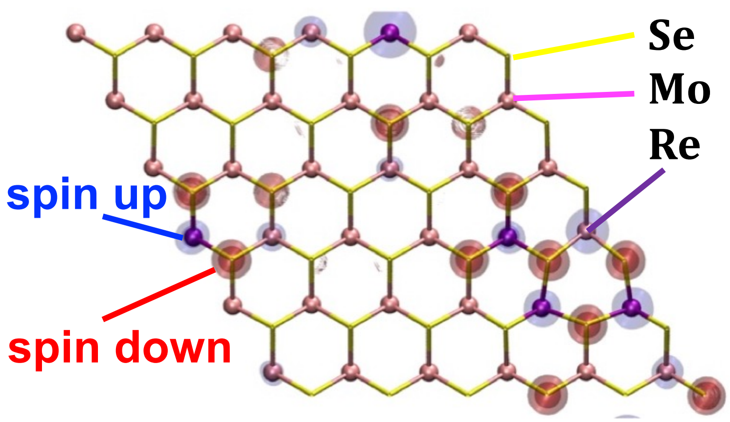
Do it yourself at https://quantum-computing.ibm.com

Emergent Magnetism: Structural Transition *via* Doping

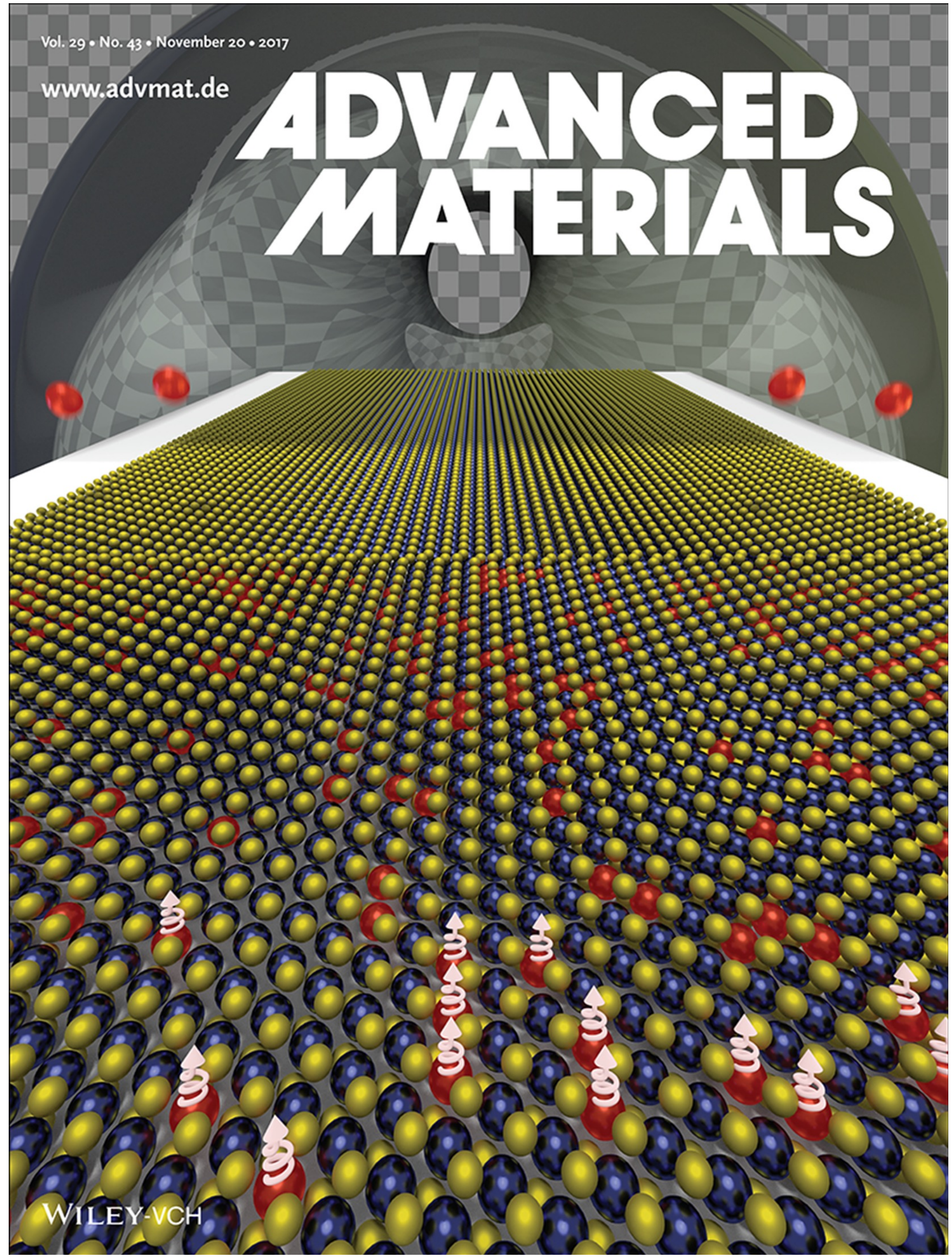
- Experiment at Rice showed 2H-to-1T' phase transformation by alloying $MoSe_2$ with Re
- Simulations at USC elucidated its electronic origin
- Simulation & experiment showed novel magnetism centered at Re atoms







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"**

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

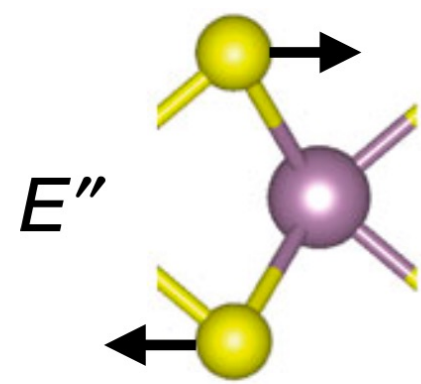
$$= H_z + H_x(t)$$

Phonon frequency

Phonon-induced energy split

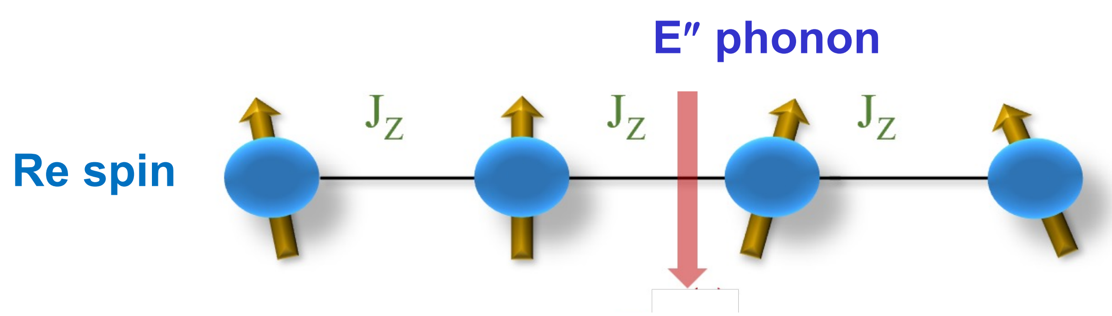
$$\sigma_z^j = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix};\ \sigma_x^j = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$ // Act on j-th qubit

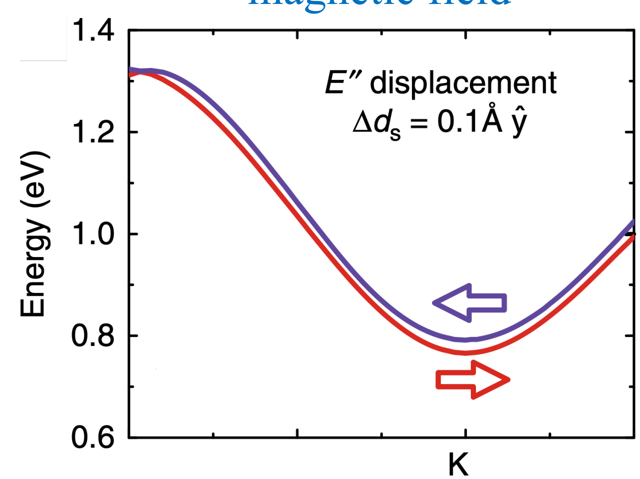
Phonon



Spin-orbit coupling

Effective in-plane magnetic field



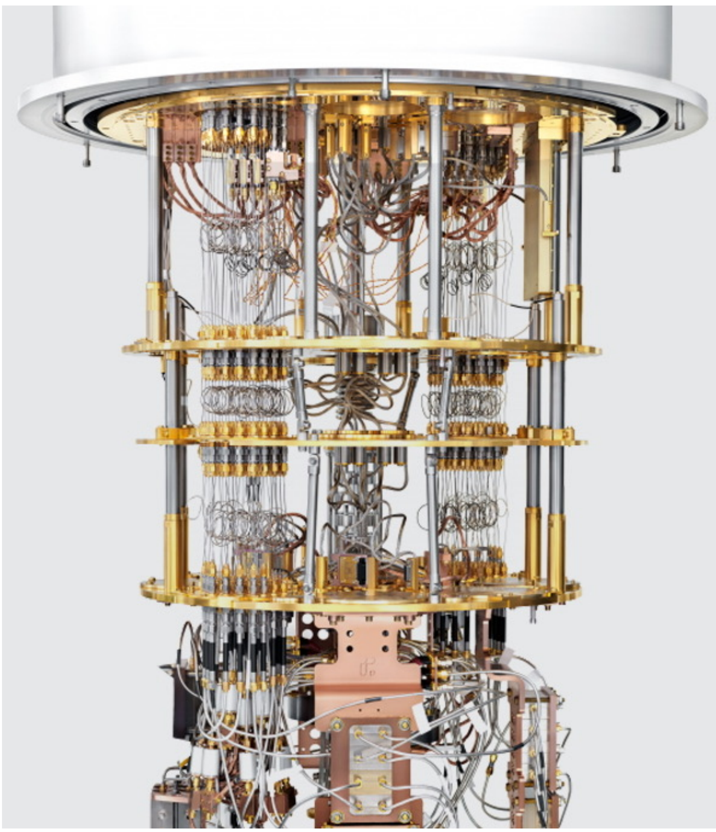


D. Shin *et al.*, *Nat. Commun.* **9**, 638 ('18)

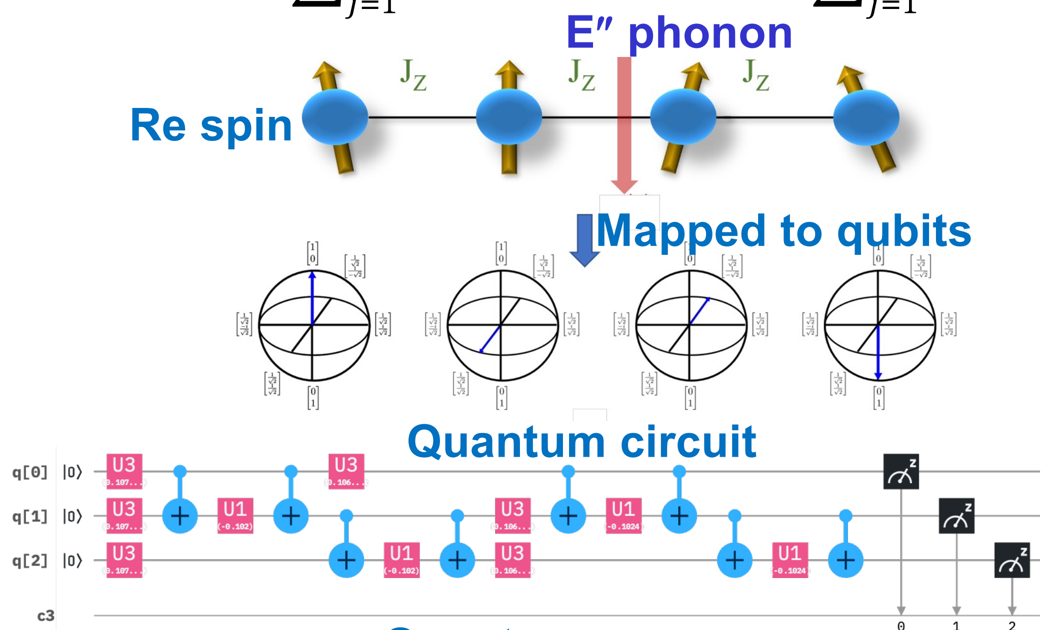
Quantum Computing of Magnetism

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

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



$$H(t) = -J_z \sum_{j=1}^{N-1} \boldsymbol{\sigma}_z^j \boldsymbol{\sigma}_z^{j+1} - \varepsilon_{ph} \sin(\omega_{ph} t) \sum_{j=1}^{N} \boldsymbol{\sigma}_x^j$$



Quantum program

```
    #define the two non-commuting terms that comprise the Hamiltonian
    Hz = PauliTerm("Z", 0, epsilon_0)
    Hy = PauliTerm("Y", 0, epsilon_ph*np.sin(w_ph*t))
    #exponentiate the terms of the Hamiltonian for use in Trotter approx
    exp_Hz = exponential_map(Hz)(delta_t/(2.0*hbar))
    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 $|\boldsymbol{\Psi}(\boldsymbol{t})\rangle$ for small time interval $\boldsymbol{\Delta t}$ (atomic unit, $\hbar = 1$)**

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

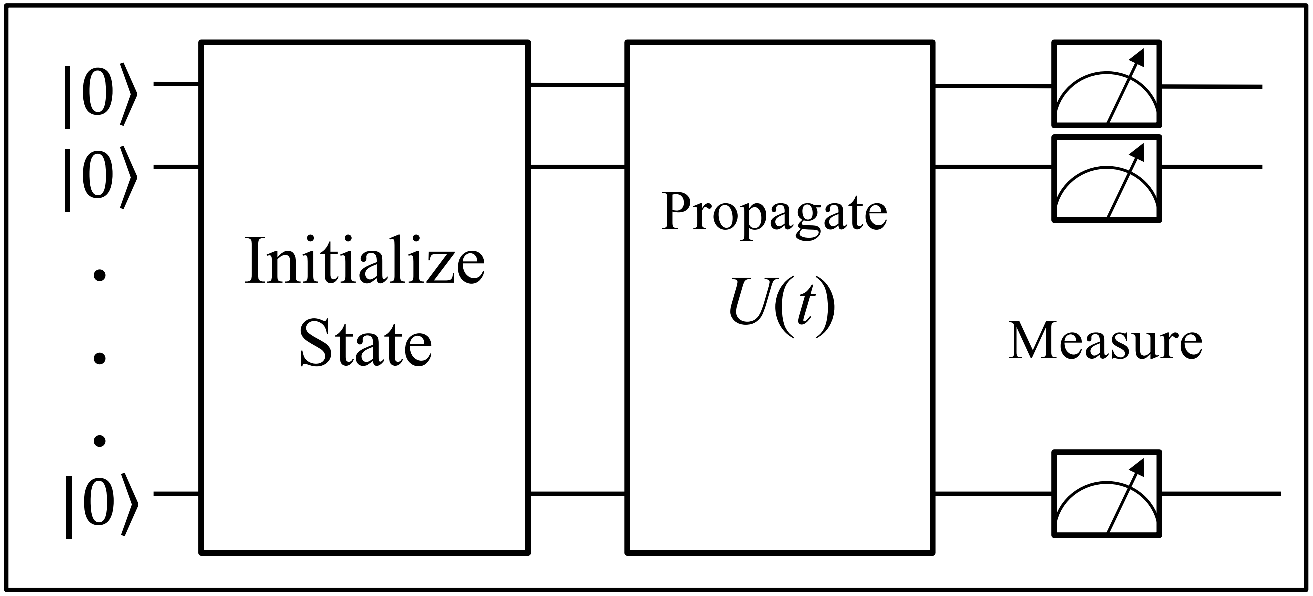
$$U(\Delta t) = \exp(-iH\Delta t)$$

- **Time discretization with time-step $\boldsymbol{\Delta t}$ and Trotter expansion**

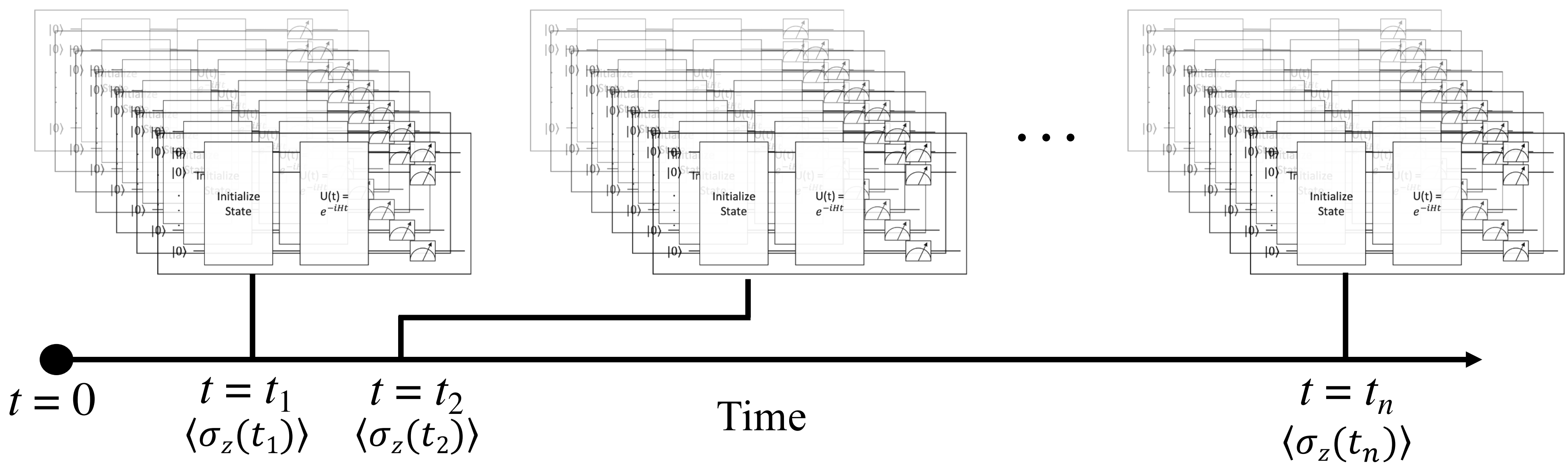
$$U(n\Delta t) \cong \prod_{k=0}^{n-1} \exp(-iH_z\Delta t)\exp(-iH_x(k+1/2)\Delta t)$$

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

Quantum Computing Runs

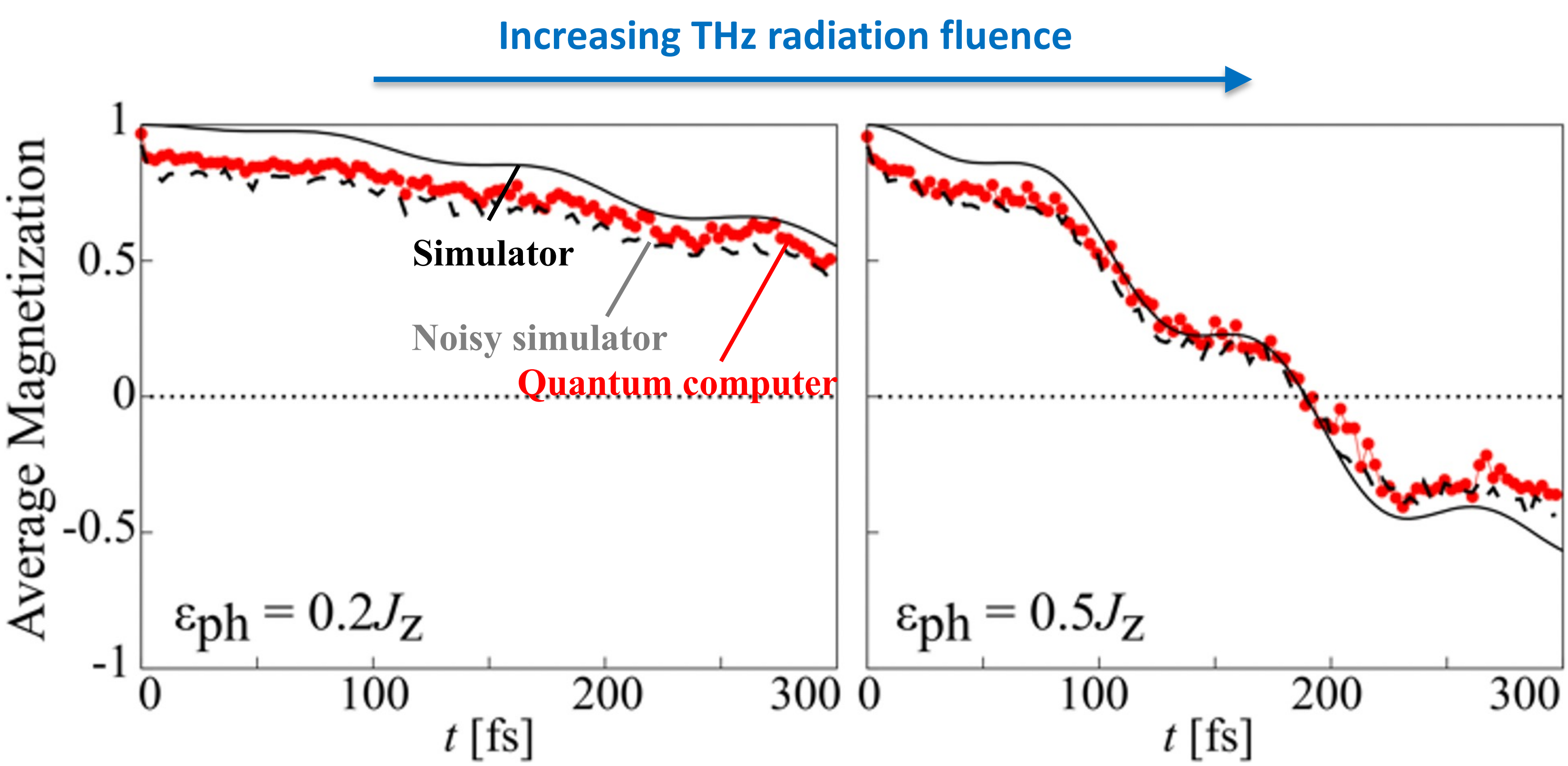


For each time instance, many runs to obtain statistics



Quantum Computing Results

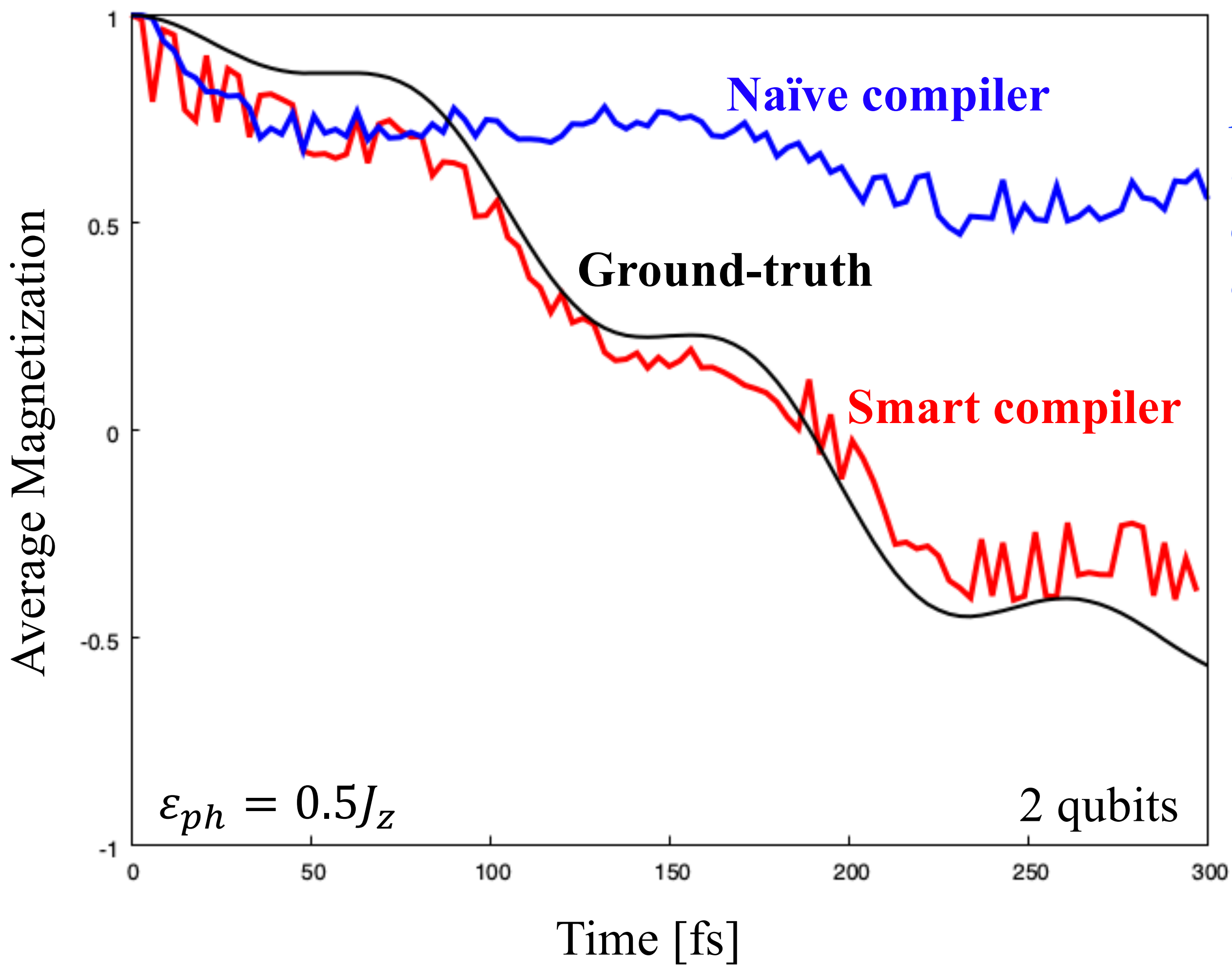
- **Quantum-dynamics simulations on a NISQ computers show dynamic suppression of magnetization by THz radiation**



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

Circuit Size *vs.* Simulation Fidelity

- **Reduced circuit size improves the fidelity of simulation**



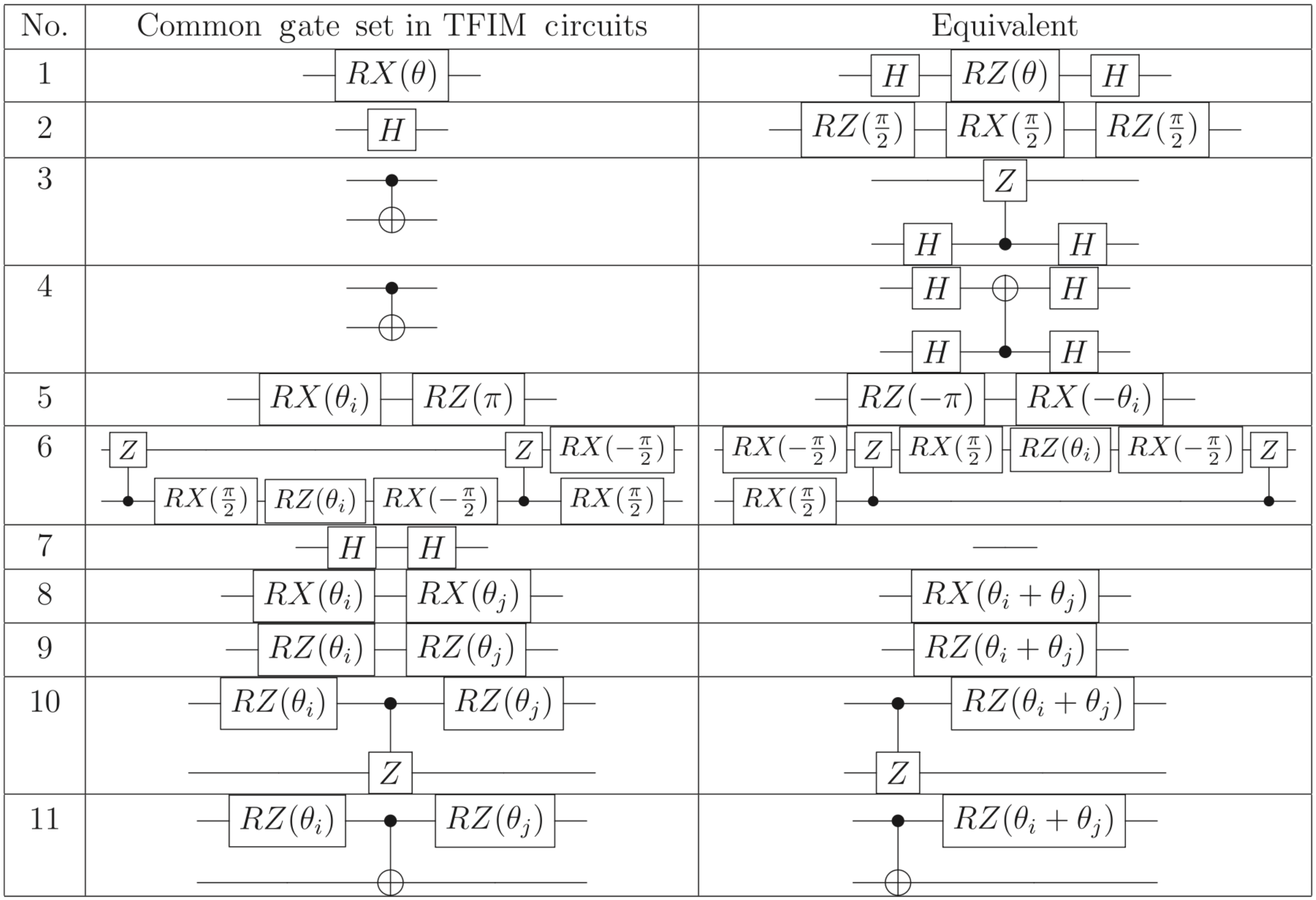
Due to high cumulative quantum-gate errors!

Naïve compiler: circuit size ∝ 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**

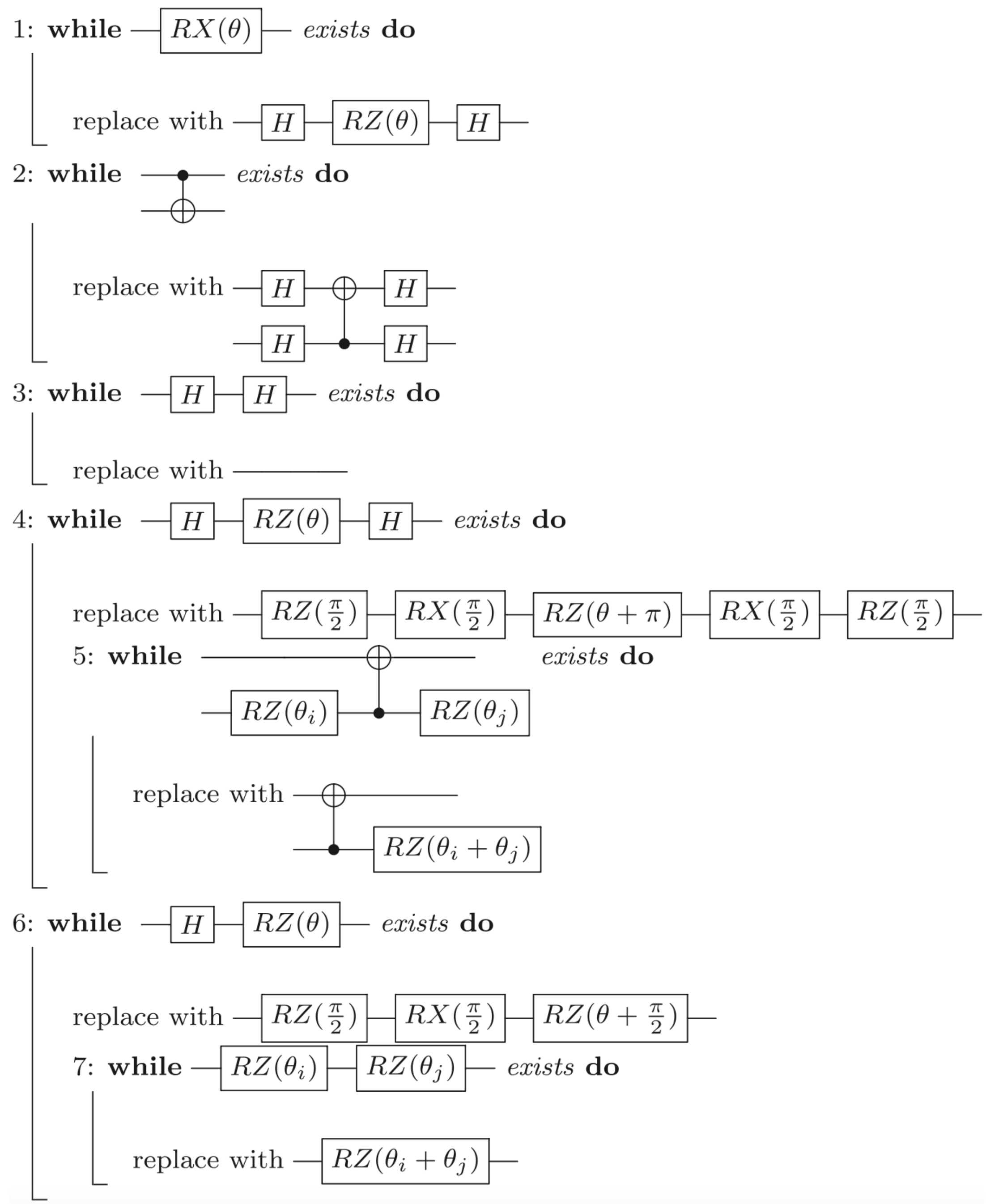


L. Bassman *et al.*, *Quantum Sci. Tech.* **6**, 014007 ('21)

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**

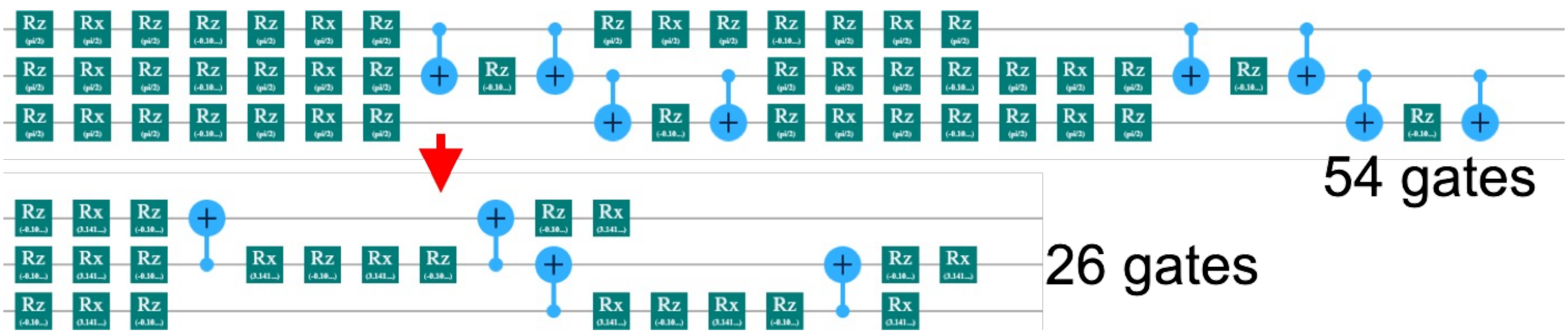


L. Bassman *et al.*,
Quantum Sci. Tech. **6**, 014007 ('21)

Domain-Specific Quantum Compiler

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

Vendor compiler



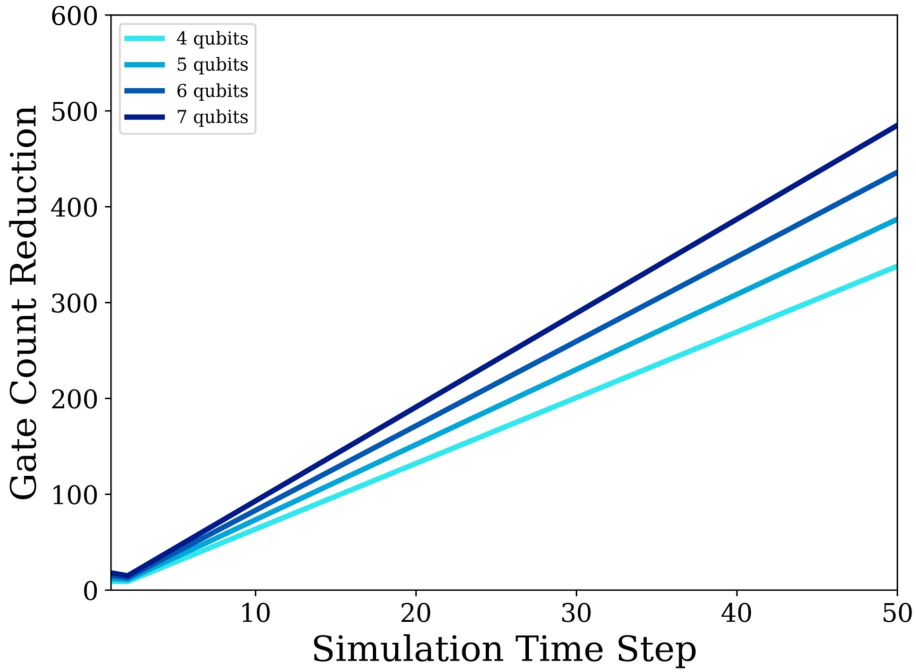
AI-inspired compiler

L. Bassman *et al.*, *Quantum Sci. Tech.* **6**, 014007 ('21)

Performance of Domain-Specific Compiler

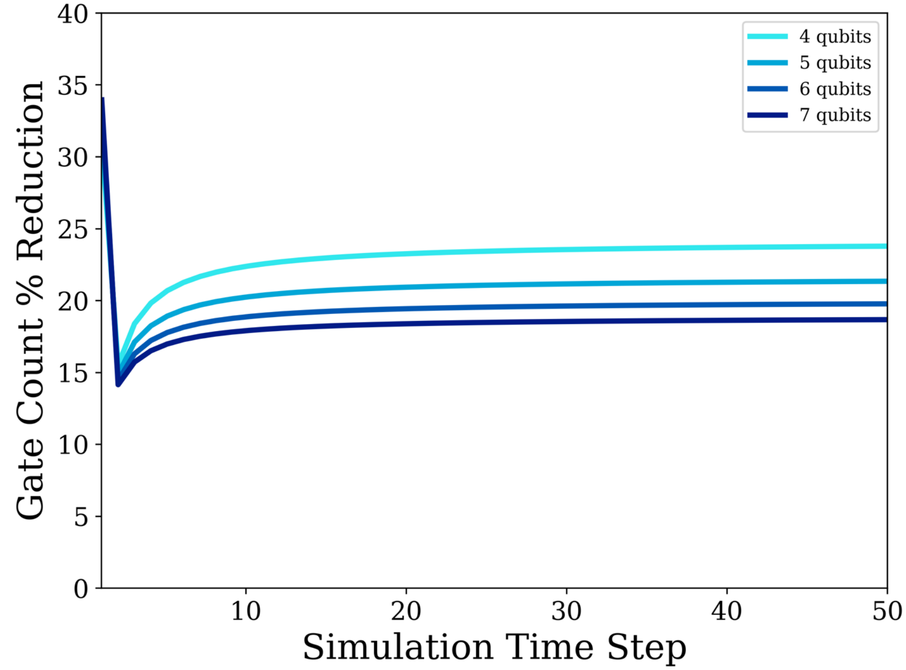
Absolute gate count difference

$(IBM\ Compiler - DS\ Compiler)$



Percent gate count difference

$$\frac{IBM\ Compiler - DS\ Compiler}{IBM\ Compiler} \times 100$$

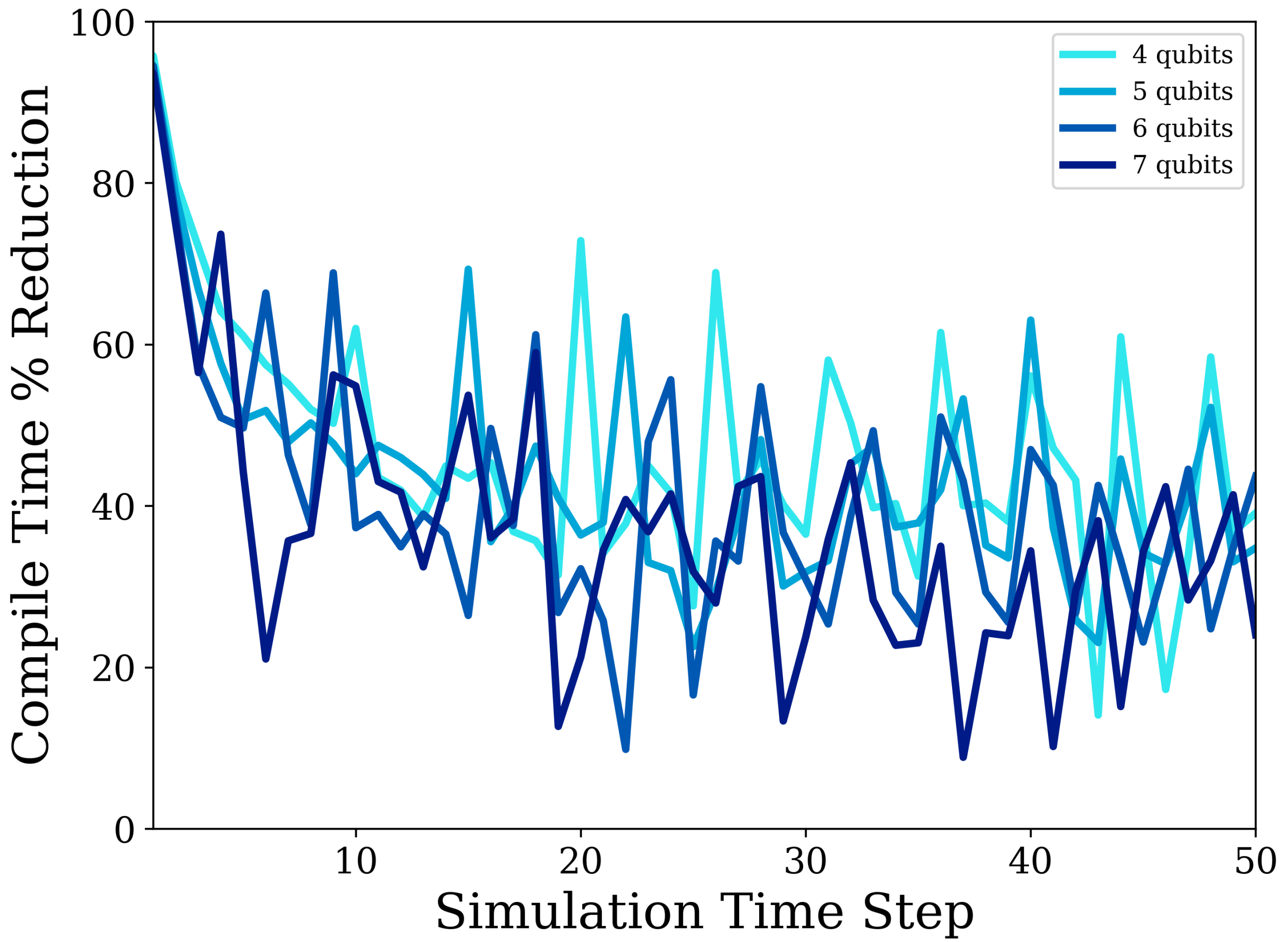


Domain-specific compiler reduces gate count compared to IBM compiler

Speed of Domain-Specific Compiler

Percent compile-time difference

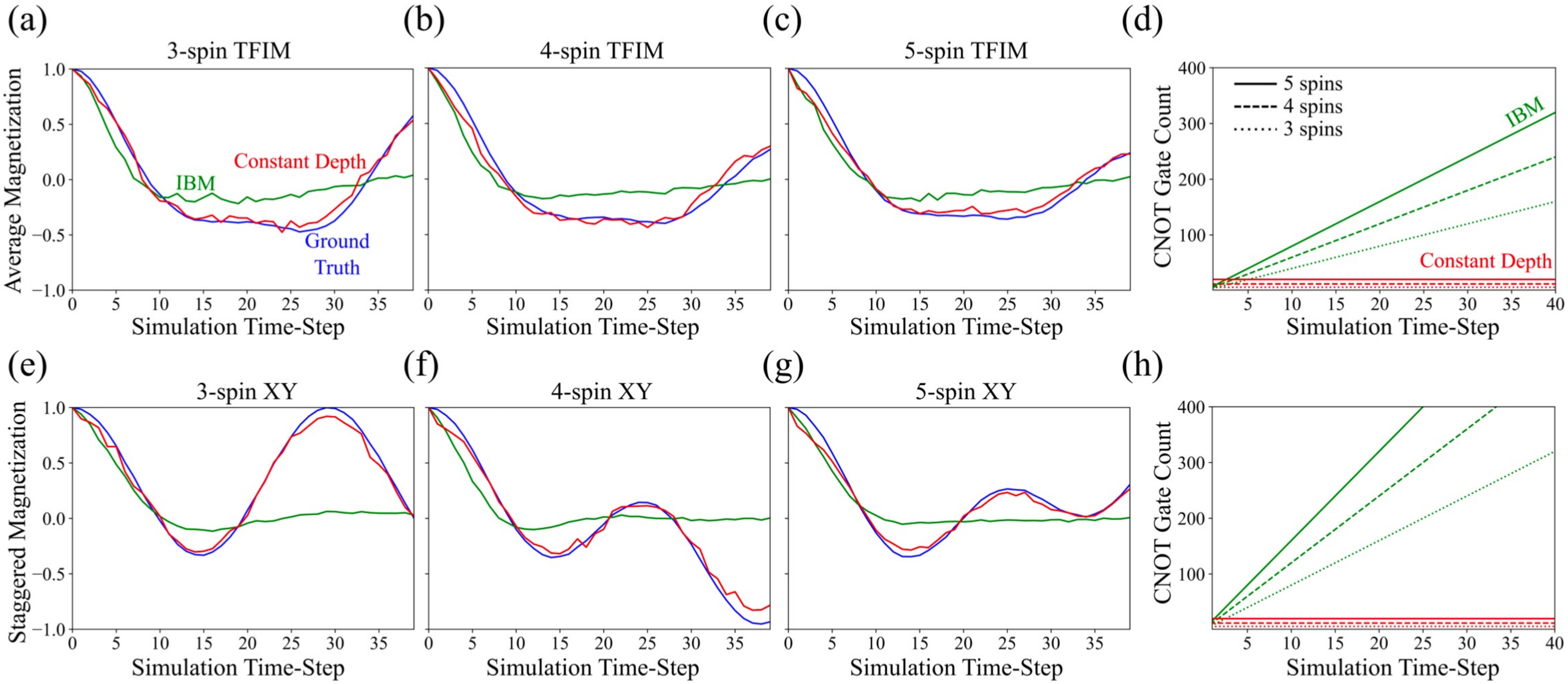
$$\frac{IBM\ Compiler - DS\ Compiler}{IBM\ Compiler} \times 100$$



… 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**



L. Bassman *et al.*, *arXiv*: 2103.07429v4 ('21)

Richer Physics: Heisenberg Model

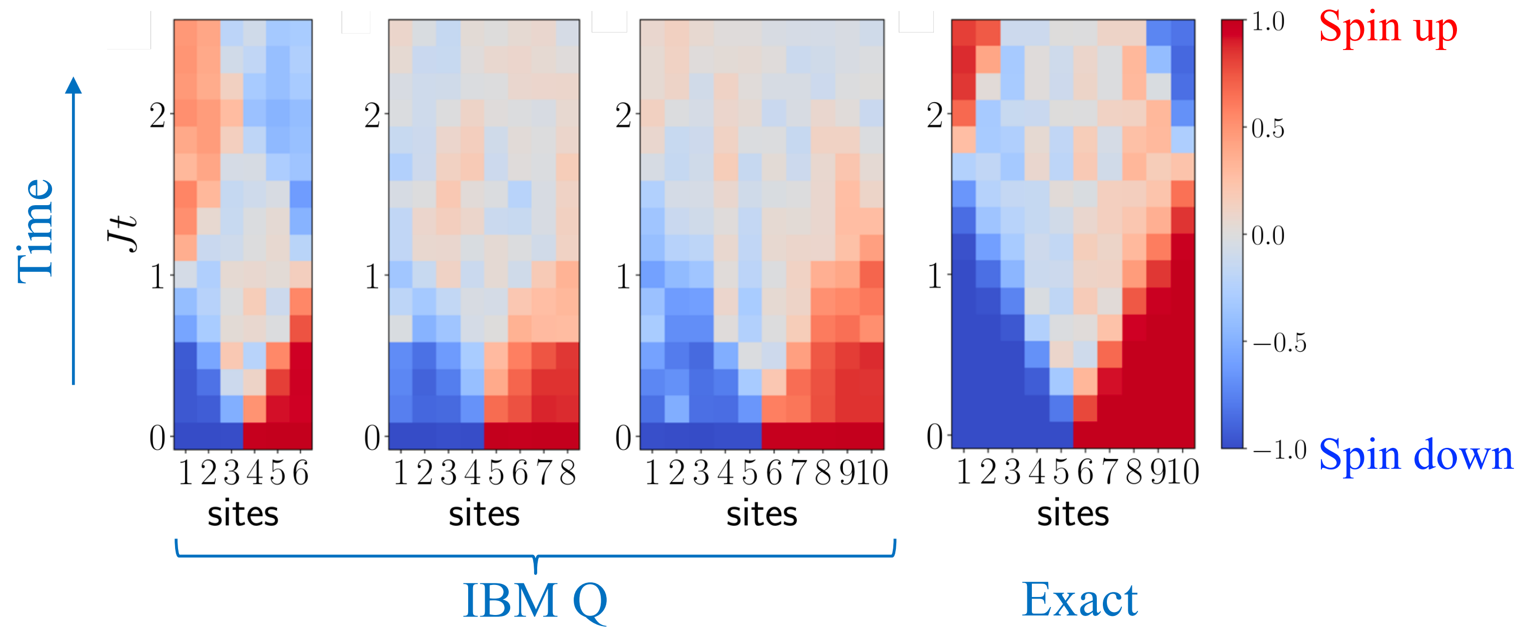
$$H = -\sum_{j=1}^{N-1}\underbrace{\left(J_x\sigma_x^j\sigma_x^{j+1} + J_y\sigma_y^j\sigma_y^{j+1} + J_z\sigma_z^j\sigma_z^{j+1}\right)}_{\text{Exchange coupling}} - h\sum_{j=1}^{N}\sigma_z^j$$

Magnetic field

Pauli spin-1/2 matrices

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

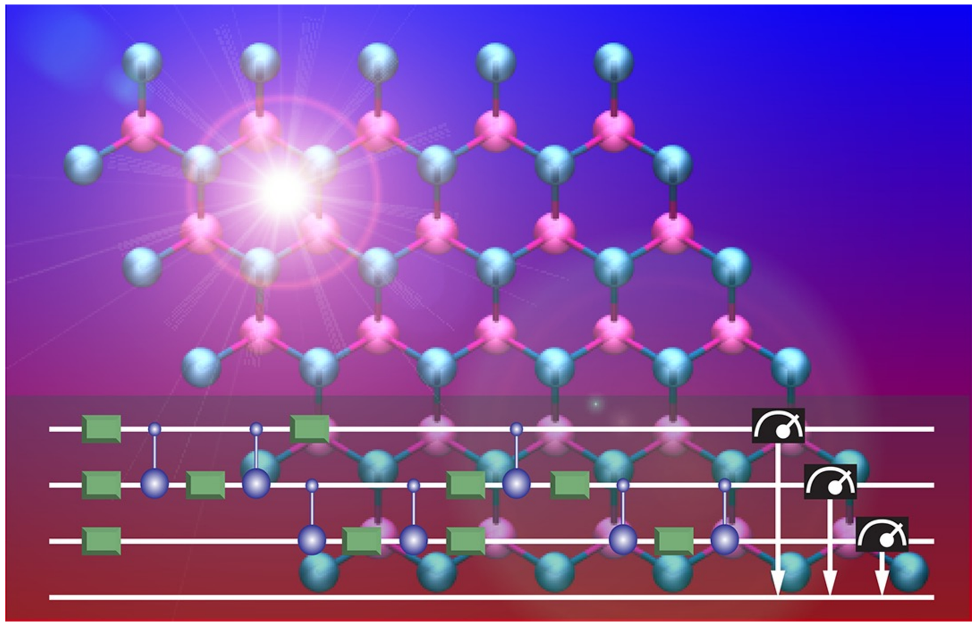
Domain-wall dynamics (6-, 8- & 10-site spin chains)



A. Smith *et al.*, *npJ Quantum Info.* **5**, 106 ('19)

Open-Source Quantum Software

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



MISTIQS

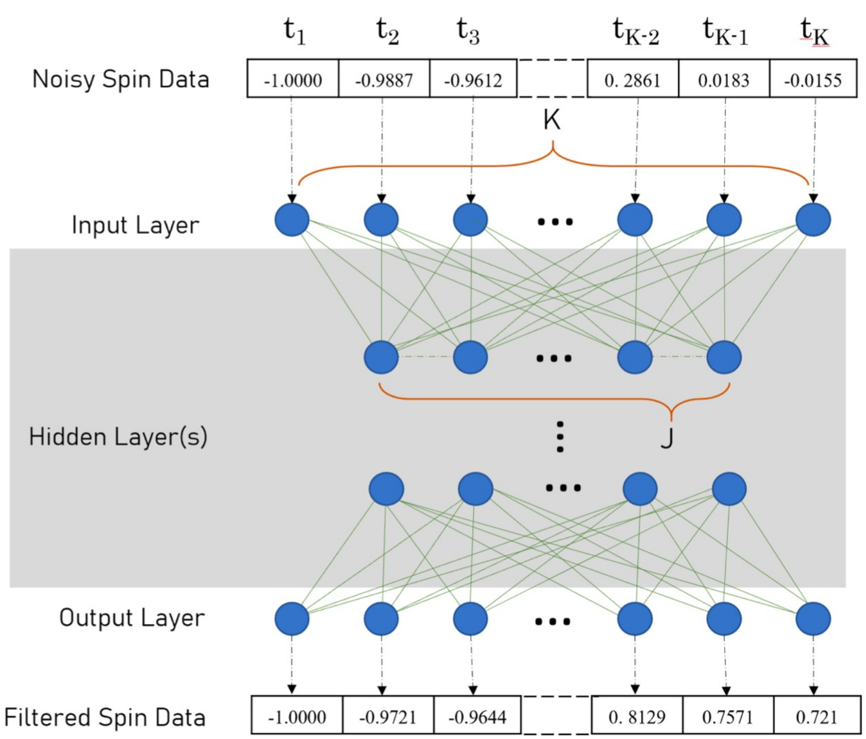
Mult**I**platform
Software for
TIme-dependent
Quantum
Simulation

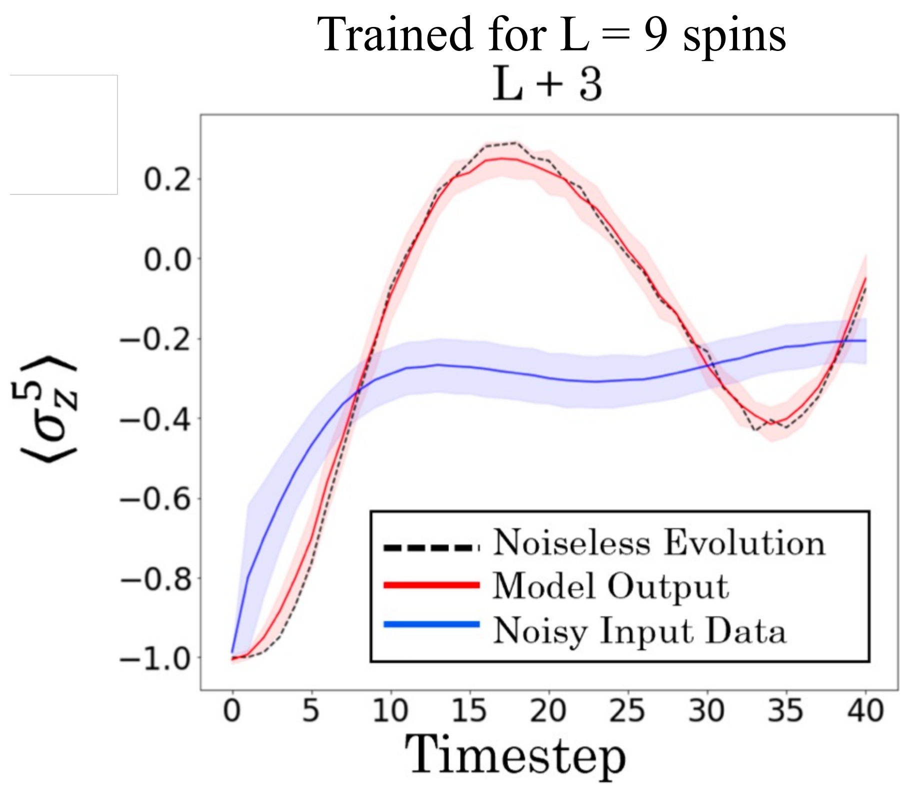
Paper: C. Powers *et al.*, *SoftwareX* **14**, 100696 ('21)

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**





[C. Powers *et al.*, *NeurIPS workshop* ('21)]

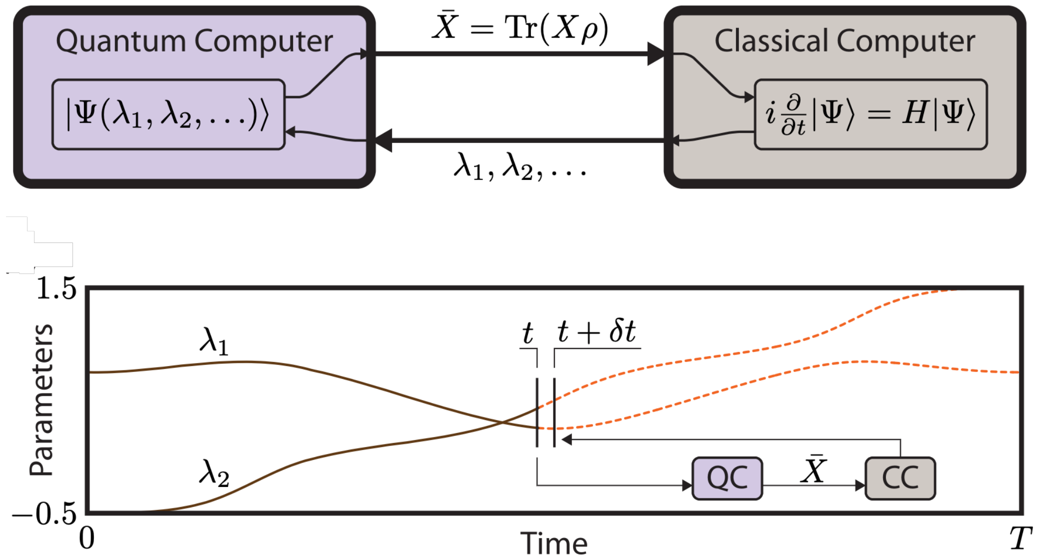
Variational Quantum Simulator

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, $|\boldsymbol{\psi}(\boldsymbol{t})\rangle = |\boldsymbol{\psi}\big(\boldsymbol{\lambda_1}(\boldsymbol{t}), \ldots, \boldsymbol{\lambda_P}(\boldsymbol{t})\big)\rangle$, which is tractable on a classical computer**



Y. Li & S. Benjamin, *Phys. Rev. X* **7**, 021050 ('17)

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