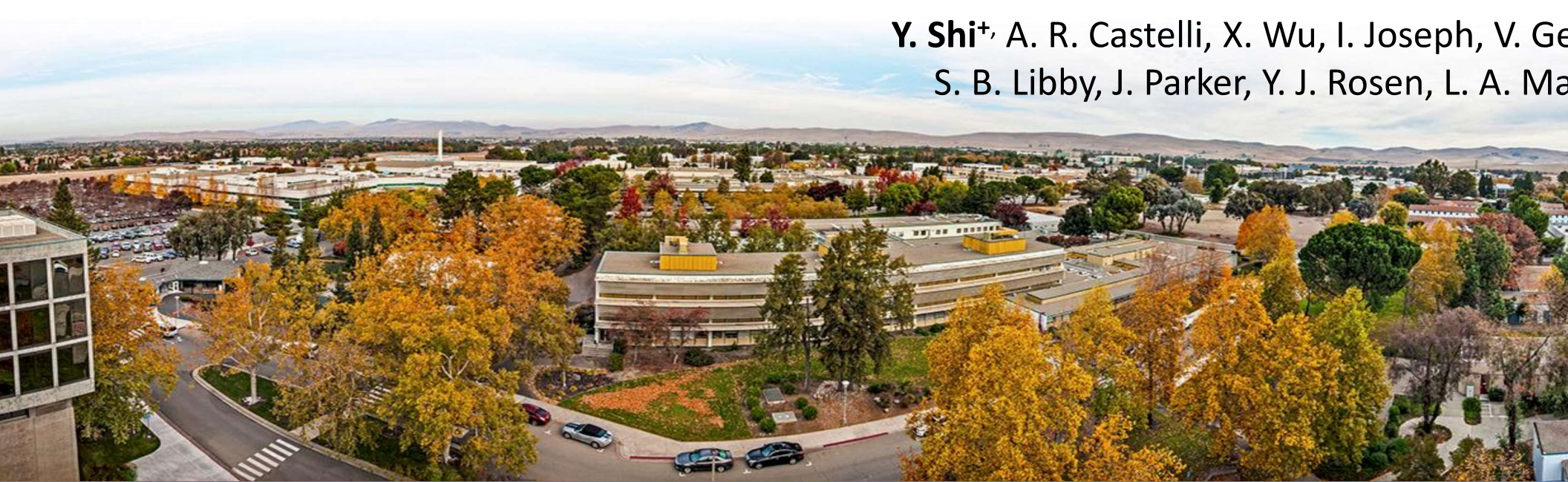


Using quantum computers to simulate a toy problem of laser-plasma interactions

HEDS Seminar
Aug 5th, 2021

Y. Shi⁺, A. R. Castelli, X. Wu, I. Joseph, V. Ge
S. B. Libby, J. Parker, Y. J. Rosen, L. A. Ma



LLNL-PRES-815947 and LLNL-PRES-823716

⁺ shi9@llnl.gov

This work was performed under the auspices of US DOE by LLNL under Contract DE-AC52-07NA27344 and was supported by DOE FES Project Quantum Leap for Fusion Energy Sciences FWP SCW1680 and LLNL-LDRD Project No. 19-FS-072. Y. S. was supported by the Lawrence Fellowship through LLNL-LDRD under Project No. 19-ERD-038.



Quantum computing: a promise yet to be fulfilled

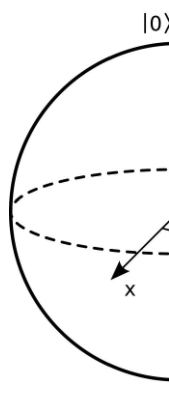
- Ideal quantum memory can hold more information
 - Classical computing uses bits: 0 or 1, binary
Specifying the state of n bits need n numbers, e.g. 101
 - Quantum computing uses qubits: 0 and 1 superpositions
Specifying the state of n qubits need 2^n numbers, e.g.

$$|\Psi\rangle = c_0|000\rangle + c_1|001\rangle + c_2|010\rangle + c_3|011\rangle + c_4|100\rangle + c_5|101\rangle + c_6|110\rangle + c_7|111\rangle$$

- Quantum algorithms may require less operations

- Ideal quantum computers offer unitary operations
Classical computers rely on irreversible operations
- Notable quantum algorithms with exponential speedup:
Quantum Fourier transform, Shor's algorithm for prime factorization, Grover's search, quantum random walk, quantum Hamiltonian simulation.

Idealized quantum algorithms require error correction, not yet operational

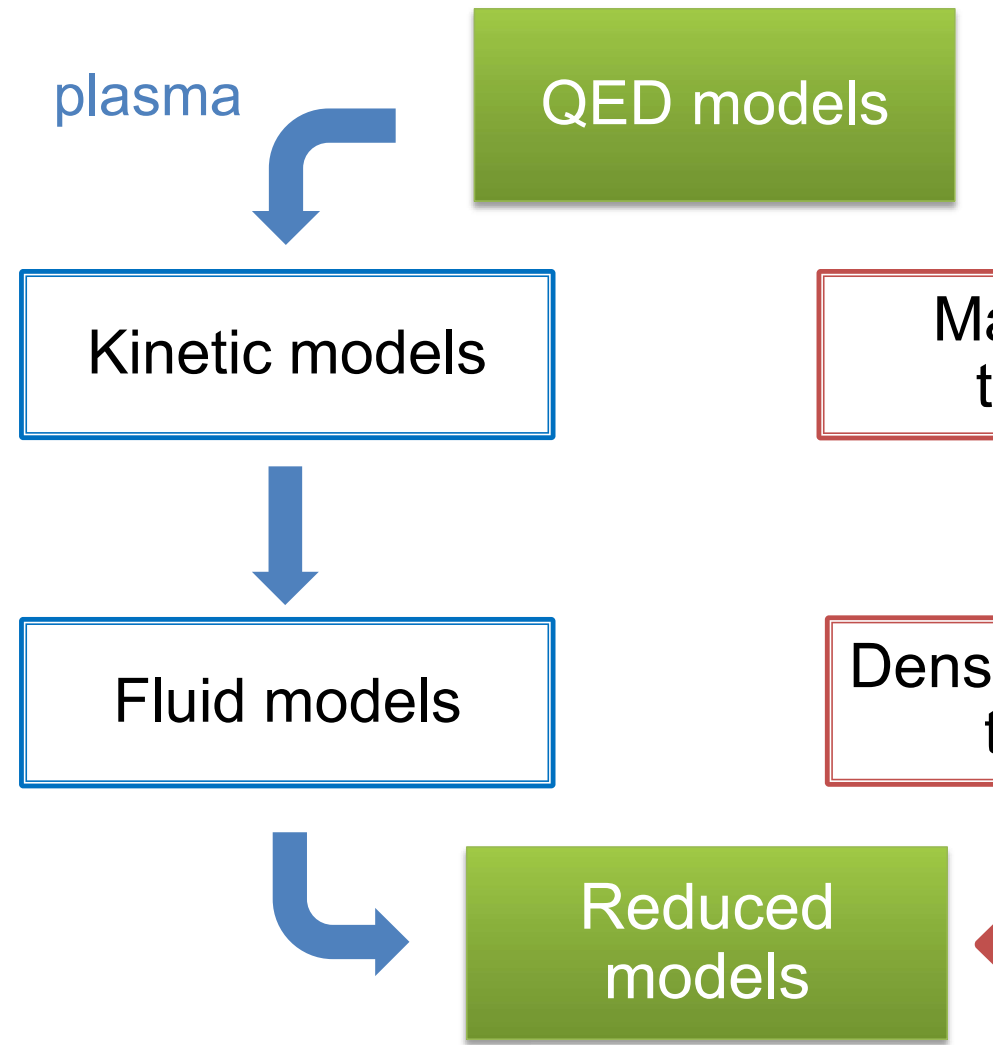


Bloch sphere superposition

$$|\psi\rangle = \cos \frac{\theta}{2} |0\rangle$$

QC may help condensed matter. How about plasmas

- Quantum computing (QC) is believed to offer advantages for condensed matter problems via quantum Hamiltonian simulations
- Plasma problems usually classical and nonlinear. But hierarchy of plasma models analogous to condensed matter models
- Plasma and condensed matter are directly connected at the level of QED and reduced models



Example reduced model: three-wave interactions

- Interesting problems are usually **nonlinear**
 - Lowest order: cubic couplings, common in nonlinear media
 - Examples: laser-plasma interactions, turbulence, nonlinear optics, lattice QED ...
 - Classical resonant interactions described by three-wave envelope equations

$$d_t A_1 = g A_2 A_3, \quad d_t A_2 = -g^* A_1 A_3^\dagger, \quad d_t A_3 = -g^* A_1 A_2^\dagger$$

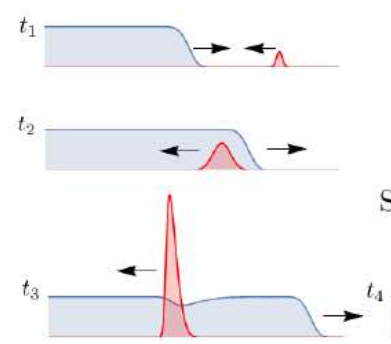
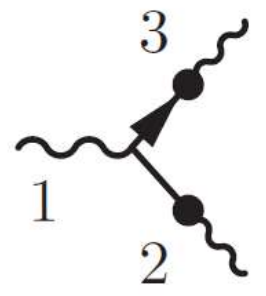
$$d_t = \partial_t + \mathbf{v}_j \cdot \nabla, \quad \mathbf{v}_j = \partial \omega_j / \partial \mathbf{k}_j$$

Coupling coefficient

- Quantized version $[A_j, A_l^\dagger] = \delta_{jl}$

$$\text{Interaction Hamiltonian } H_I = ig A_1^\dagger A_2 A_3 - ig^* A_1 A_2^\dagger A_3^\dagger$$

- Quantum hardware usually lacks native cubic couplings: **nonnative**
Can we program cubic interactions on general-purpose quantum computers



Simulating **nonnative** interaction is challenging

- Standard approach to quantum Hamiltonian simulation
 - Hardware Hamiltonian: determined by device architecture

$$H_0 = \sum_{k=1}^m H_k$$

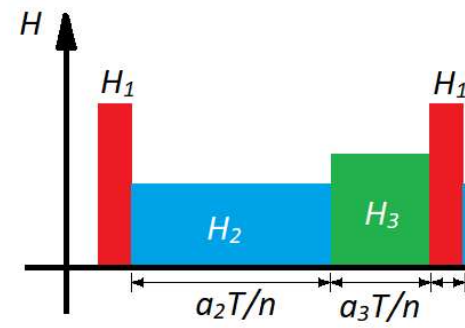
- Hamiltonian of the physical system: likely different from H_0

$$H = \sum_{k=1}^m a_k H_k$$

- Lie-Trotter-Suzuki approximation when terms in H are natively available

$$\exp(-iHT) = \lim_{n \rightarrow \infty} [\prod_{k=1}^m U_k(a_k T/n)]^n$$

$$U_k(t) = \exp(-iH_k t) \quad \leftarrow \text{require native } H_k$$



- What if H contains terms that are nonnative?
Implement general unitary is exponentially expensive!

It's difficult! OK, let's say we can do it. Does it help?

- Example application: laser-plasma interactions
 - Plasma parameters evolve under laser drives
 - Laser propagation/scattering affected by plasma conditions

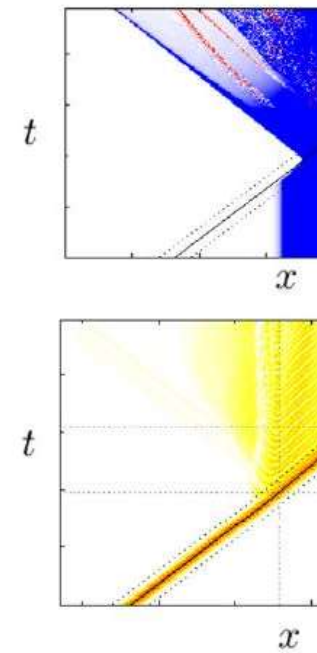
- Simulating real-time dynamics: expensive!

- Plasma states $|g(t + \Delta t/2)\rangle = \mathcal{A}(t)|g(t - \Delta t/2)\rangle$
- Laser states $|a(t + \Delta t)\rangle = \mathcal{G}(t + \Delta t/2)|a(t)\rangle$

- Sub problem: D -level photon occupation

- Classical: computing next state by matrix multiplication, $O(D^2)$ operations
- Quantum: computing next state by applying cubic gates, $O(1)$ operations
 - Need 1-parameter family of cubic gates
 - Initial states simple, readout only needed at final step

Cubic gates have overhead, but once precompiled, operations cheap for each



Solving cubic problem: mapping in action space

■ Naive mapping in **energy space**

- Direct mapping from resonant levels in energy space to hardware space restricted by
 - (1) Tunability of level spacings and coupling
 - (2) Unwanted terms in native Hamiltonian
 - (3) Inefficient representation: 0 or 1 per qubit

$$H = igA_1^\dagger A_2 A_3 - ig$$

$$\omega_1 \left(\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} \right) \begin{array}{l} \omega_2 \\ \omega_3 \end{array} \quad |n_j\rangle = \frac{(A_j^\dagger)^{n_j}}{\sqrt{n_j!}}$$

■ More versatile mapping in **action space**

- Action operators commute with Hamiltonian

$$S_2 = n_1 + n_3, \quad S_3 = n_1 + n_2$$

$$[H, S_2] = [H, S_3] = 0$$

- Simultaneous eigen states of H , S_2 and S_3

$$|\psi\rangle = \sum_{j=0}^{\min(s_2, s_3)} c_j |s_2 - j, s_3 - s_2 + j, j\rangle$$

$$\text{---} \quad j = D = \min(s_2, s_3)$$

⋮

⋮

⋮

⋮

⋮

⋮

⋮

⋮

⋮

⋮

⋮

⋮

⋮

⋮

⋮

⋮

⋮

⋮

⋮

⋮

⋮

⋮

⋮

⋮

⋮

⋮

⋮

$$|\psi_j\rangle = |s_2 - j, s_3 - s_2 + j, j\rangle$$

$$|n_1, n_2, n_3\rangle = |n_1\rangle \otimes |n_2\rangle \otimes |n_3\rangle$$

Temporal three-wave problem = Hamiltonian simulation

- Occupation amplitudes satisfy Schrödinger equations

$$i\partial_t c_j = ig h_{j+\frac{1}{2}} c_{j+1} - ig^* h_{j-\frac{1}{2}} c_{j-1}$$

$$h_{j-\frac{1}{2}} = \sqrt{j(s_2 + 1 - j)(s_3 - s_2 + j)}$$

$$h_{-\frac{1}{2}} = h_{D+\frac{1}{2}} = 0$$

- Observables can be post processed from occupation probabilities

$$\langle n_1 \rangle = \sum_{j=0}^{s_2} (s_2 - j) |c_j|^2$$

$$\langle n_2 \rangle = \sum_{j=0}^{s_2} (s_3 - s_2 + j) |c_j|^2$$

$$\langle n_3 \rangle = \sum_{j=0}^{s_2} j |c_j|^2$$

- Quantum number operators satisfy Heisenberg equations

$$\begin{aligned} \partial_t^2 n_1 &= -\partial_t^2 n_2 = -\partial_t^2 n_3 \\ &= 2|g|^2 [s_2 s_3 - (2s_2 + 2s_3 + \dots)] \end{aligned}$$

- Classical expectation values satisfy slightly different equations

$$\begin{aligned} \partial_t^2 \langle n_1 \rangle &= -\partial_t^2 \langle n_2 \rangle = -\partial_t^2 \langle n_3 \rangle \\ &= 2|g|^2 [s_2 s_3 - (2s_2 + 2s_3 + \dots)] \end{aligned}$$

- Quantum system behaves like classical system when wave packet is localized and spontaneous emission is subdominant

Simplest nontrivial case requires $D = 3 = (1+1/2)$ qu

- Readily realizable on hardware for $s_2=2$ and $s_3=s$. Hamiltonian matrix tridiagonal

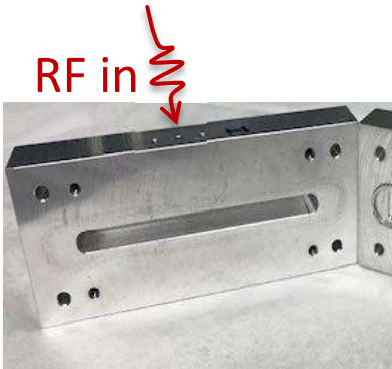
$$h(\theta, s) = \begin{pmatrix} 0 & e^{i\theta} \sqrt{2(s-1)} & 0 \\ e^{-i\theta} \sqrt{2(s-1)} & 0 & e^{i\theta} \sqrt{2s} \\ 0 & e^{-i\theta} \sqrt{2s} & 0 \end{pmatrix} \quad \begin{array}{l} h = H/|g| \\ \exp(i\theta) = ig/|g| \end{array} \quad \begin{array}{l} |2, s-2\rangle \\ |1, s-1\rangle \\ |0, s\rangle \end{array}$$

- Solution to 3-level problem known analytically. Unitary to be implemented on

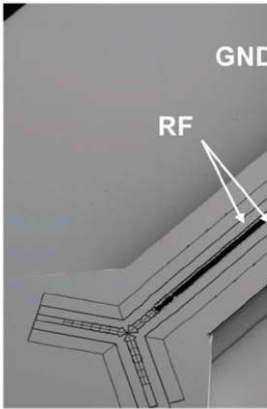
$$U = \begin{pmatrix} \frac{(s-1) \cos \lambda\tau + s}{2s-1} & -ie^{i\theta} \sqrt{\frac{s-1}{2s-1}} \sin \lambda\tau & e^{2i\theta} \frac{\sqrt{s(s-1)}}{2s-1} (\cos \lambda\tau - 1) \\ -ie^{-i\theta} \sqrt{\frac{s-1}{2s-1}} \sin \lambda\tau & \cos \lambda\tau & -ie^{i\theta} \sqrt{\frac{s}{2s-1}} \sin \lambda\tau \\ e^{-2i\theta} \frac{\sqrt{s(s-1)}}{2s-1} (\cos \lambda\tau - 1) & -ie^{-i\theta} \sqrt{\frac{s}{2s-1}} \sin \lambda\tau & \frac{s \cos \lambda\tau + s - 1}{2s-1} \end{pmatrix} \quad \begin{array}{l} U = \exp(-iH\tau) \\ \lambda = \sqrt{2s-1} \\ U_2 = \begin{pmatrix} \cos \lambda\tau & -i \sin \lambda\tau \\ i \sin \lambda\tau & \cos \lambda\tau \end{pmatrix} \end{array}$$

Solving test problems: What quantum devices are a

- Leading architectures under development
 - **Superconducting qubits:** Nonlinear oscillators as registers. Control/readout by microwave pulses. Fabrication techniques already in use in semiconductor industry
 - **Trapped-ion qubits:** Hyperfine levels as registers. Control by electrodes, lasers, or microwaves. Readout by lasers. Potentially more versatile connection topology
 - **Photonic qubits:** Photon states as registers. Control by network of beam splitters and interferometers. Readout by single-photon detectors. Potentially miniaturizable and programable at room temperature
 - **Nuclear spins:** Angular momentum states of selected isotopes in B field as registers. Control/readout by electromagnetic pulses. Potentially operable at room temperature
- Noisy intermediate-scale quantum (NISQ) era: many qubits available, but not fault tolerant ...



Superconducting



Ion trap at Sandia Nat

Realize cubic gates using standard gates

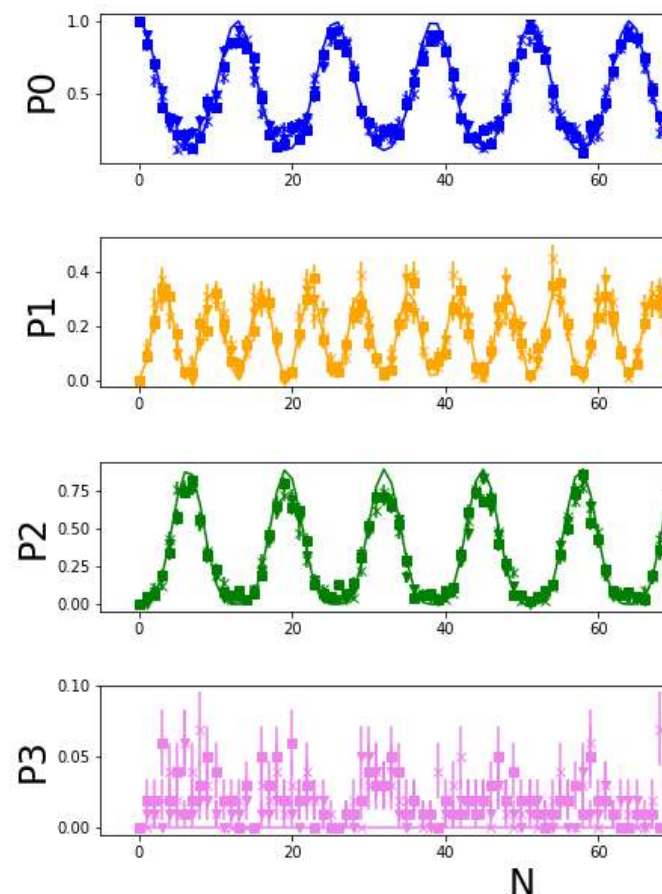
Quantum Cloud Services

Hardware: superconducting transmon qubits on 2D lattice, utilized Aspen-4-2Q-A

- Imbed 3 levels in 2 qubits:
Utilize 00, 01, and 10 states
- Compile into standard gates¹, approximate single-step unitary matrix by

1	RZ(pi) 0	10	RX(pi/2) 1
2	RX(1.570796326794897) 0	11	RZ(0.39864643091397856) 1
3	RZ(-0.9553166181245063) 0	12	RX(-pi/2) 1
4	RX(1.5707963267948948) 1	13	CZ 0 1
5	CZ 0 1	14	RZ(-2.186276035465287) 0
6	RX(pi/2) 0	15	RX(pi/2) 0
7	RZ(0.48989794855663593) 0	16	RZ(-1.7141260552949023) 1
8	RX(-pi/2) 0	17	RX(-1.5707963267948928) 1
9	RZ(1.42746659829489) 1		

1. arXiv:1608.03355, (2017)

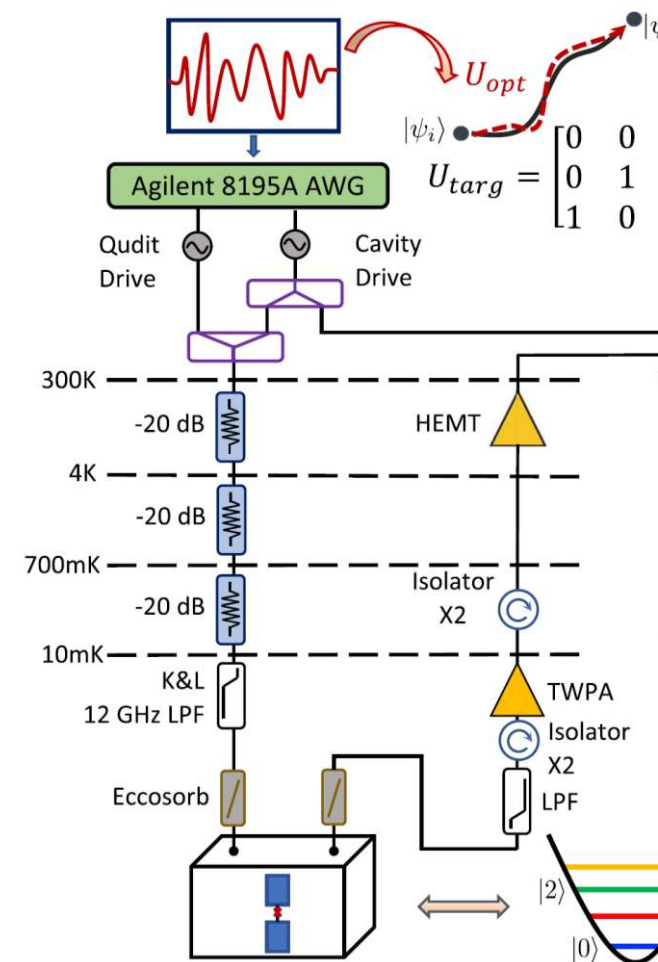
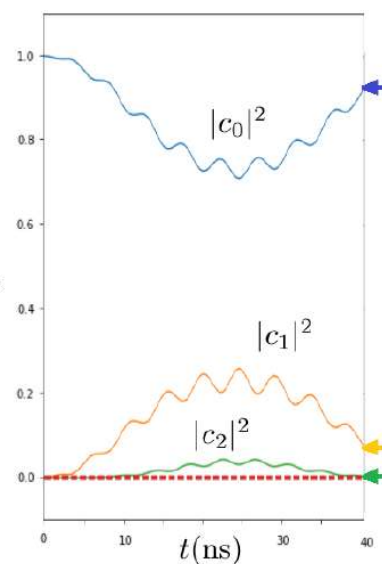
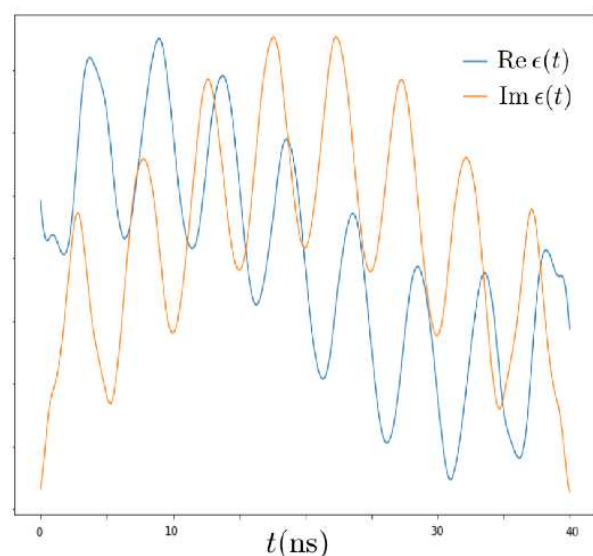


Tracks exact dynamics if all
simplification $[U(\Delta\tau)]^N =$

Realize cubic gates using optimal control

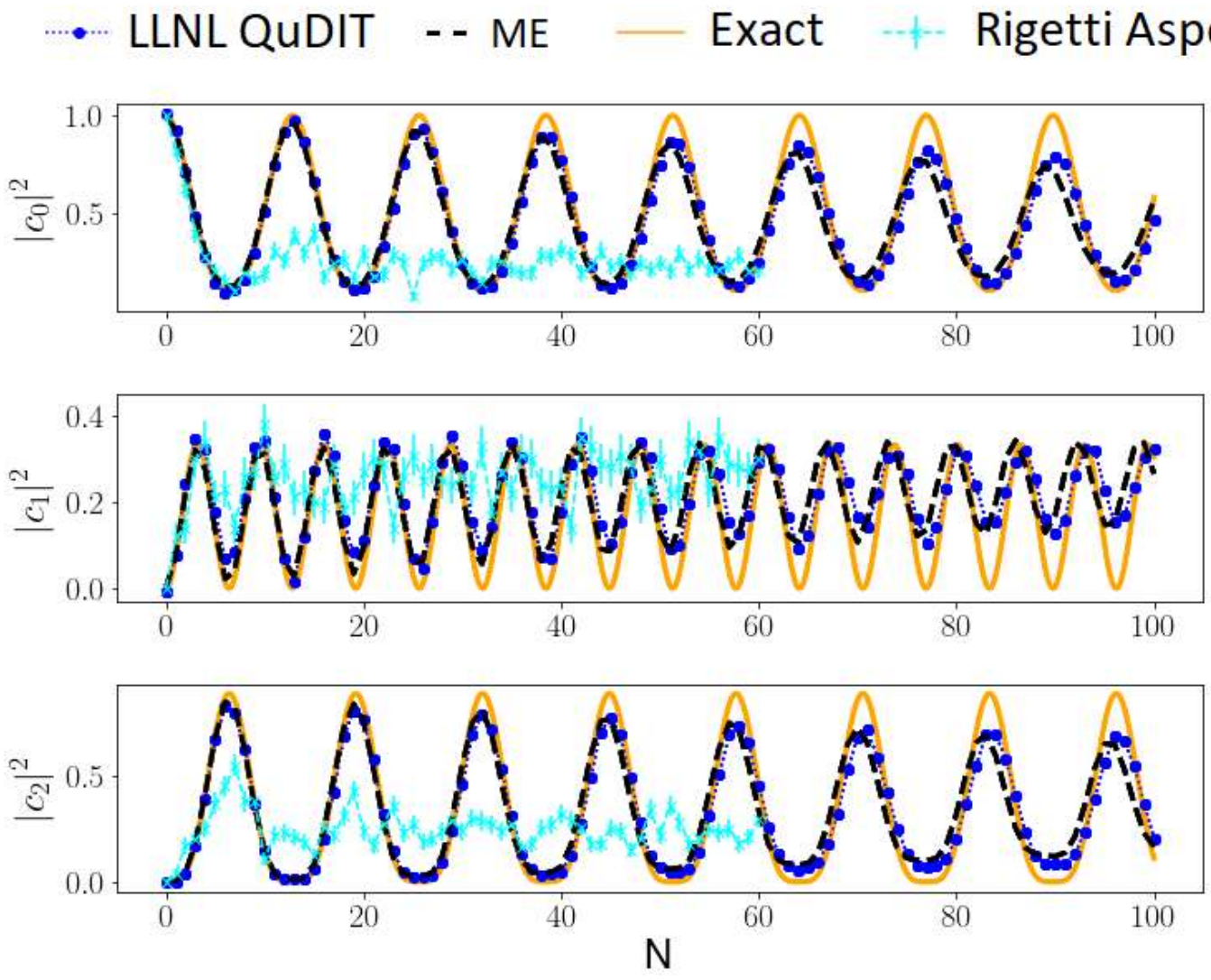
LLNL QuDIT¹

- Hardware: transmon inside a 3D microwave cavity, utilize three levels of a single qudit
- Control by customized waveform, single-step pulse optimized using GRAPE algorithm²



1. Phys. Rev. Lett. 125, 170502 (2010)
2. Comput. Phys. Commun. 184, 1 (2013)

Use precompiled gates to simulate real-time dynam



- Long-time evolution requires a customized gate. Results from the Master Equation (ME) and are close to Exact
- Short-time dynamics with shallow gates, sequences of standard gates perform
- Decay and dephasing of fidelity after ~100 gates for both standard/cu

1. Phys. Rev. A 103, 062608 (2021)

Interpolated control pulses may also achieve high fi

- Numerical optimizations expensive, shortcut by interpolation. Works well for 3-level parametric gates

Target Hamiltonian

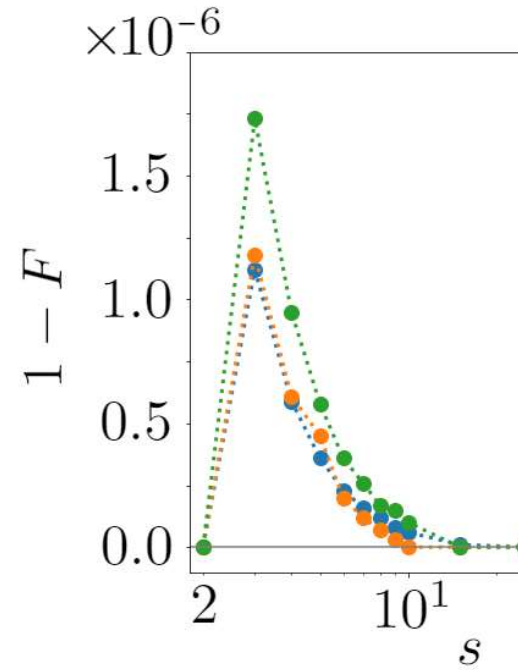
$$h(s) = \frac{\sqrt{2s}}{(1 - 2^{-1/2})} \left[(1 - \xi)K(2) + (\xi - 1/\sqrt{2})K(\infty) \right]$$

$$\xi(s) = \sqrt{1 - 1/s}$$

$$K(2) = \begin{pmatrix} 0 & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad K(\infty) = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

Control pulse

$$\epsilon_I(s) = [(1 - \xi)\epsilon_O(2) + (\xi - 1/\sqrt{2})\epsilon_O(\infty)] / (1 - 1/\sqrt{2})$$



Fidelity:

$F(\rho, \sigma) = \text{tr} \sqrt{\rho \sigma}$
 density matrices ρ, σ
 σ : optimized pulse
 ρ : interpolated pulse

Cubic gates as building blocks for future application

- Cubic gates can be programmed, no need for native cubic couplings
Action space mapping reduces nonlinear problem to Hamiltonian simulation
- **Quantum computers useful for simulating nonlinear/nonnative interactions**
- Simulations realized on Rigetti Aspen-4 using standard gates, on LLN using customized gates, and both limited by decoherence up to ~ 100 gates
- **Customized gates enable larger simulation depth on NISQ hardware**
- Future directions:
 - Generalize mapping to other nonlinear interactions
 - Implement gates on hardware with more qubits/higher fidelity
 - Utilize N-wave gates as building blocks for realistic applications



**Lawrence Livermore
National Laboratory**