Overview of Berkeley Lab's quantum computing and quantum information science capabilities

Bert de Jong

Deputy Director Quantum Systems Accelerator

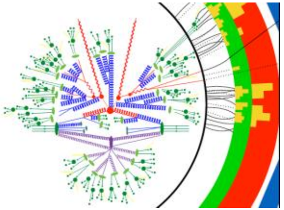
Director AIDE-QC Program

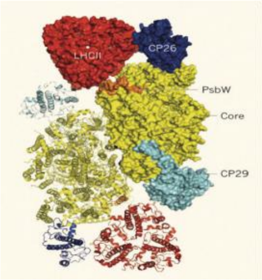
wadejong@lbl.gov

BERKELEY LAB

Promise of quantum computing is exciting

Algorithmic speedups over classical computing





Quantum simulation

Efficient optimization algorithms

“Unbreakable” encryption protocols

Moving towards quantum advantage for science

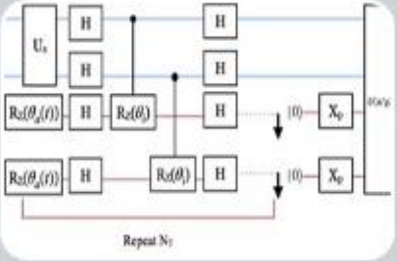
Hardware technology

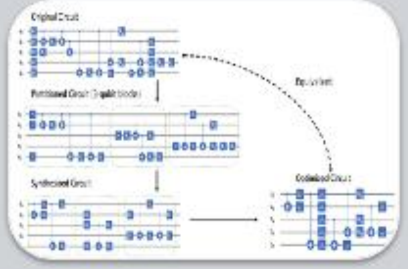
Scientific algorithms and software

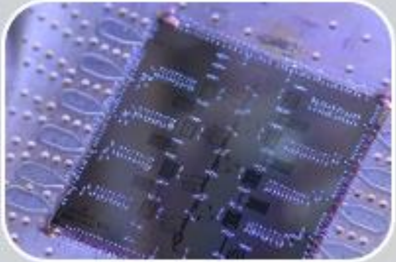
- Increasing qubit count
- Increasing lifetimes
- Increasing fidelity and reducing errors

- Reducing qubit count
- Decreasing operation counts
- Incorporating error resiliency

Full stack Quantum Information Science at Berkeley Lab







Developing Novel Algorithms and Software to Advance Science with Quantum

Programming Tools and Control Protocols to Harness the Power of Quantum Computers

Designing and Building Prototype Quantum Processors, Controls, and Sensors

Building Prototype Quantum Network and Quantum Computing Testbeds

Research programs in Quantum Information Science

Quantum Information Science Research Center

QUANTUM SYSTEMS ACCELERATOR
Catalyzing the Quantum Ecosystem

2 National Labs, 1 FFRDC, 12 Universities

Algorithms and Quantum Software

FAR-QC

⟨AIDE|QC⟩

5 National Labs, 8 Universities

Quantum at Berkeley Lab

Testbeds

AQT

QUANT-NET

Partner at Sandia

1 National Lab, 2 Universities

Quantum Science in HEP and BES

QuantISED Quest

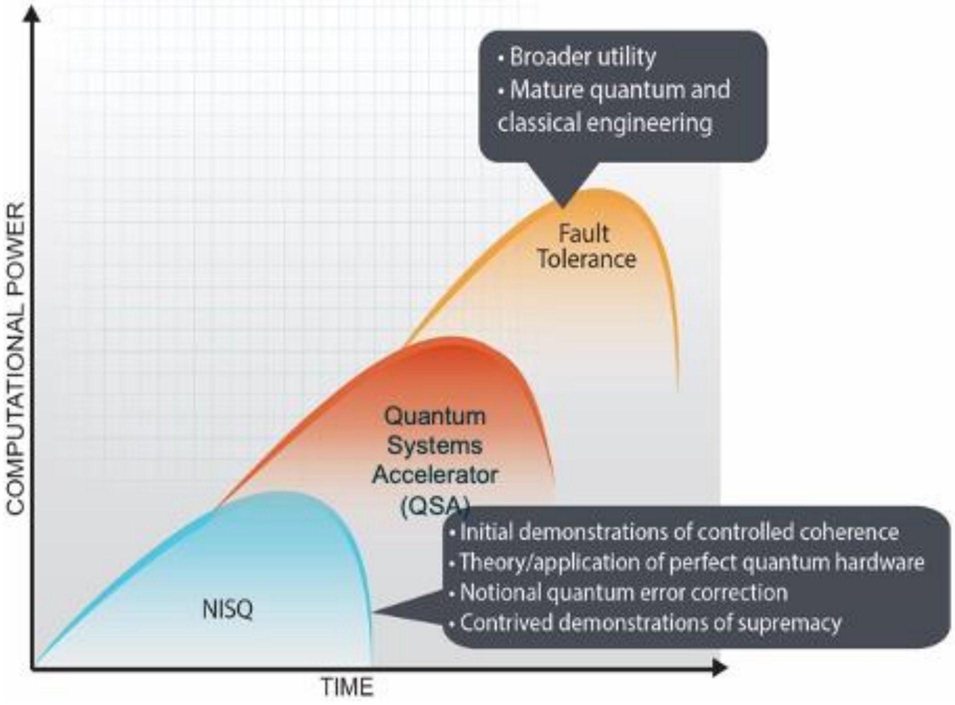
Strong correlation in chemistry and materials

New materials in QC

3 National Labs, 1 University

Quantum Systems Accelerator Vision

The QSA is catalyzing national leadership in quantum information science through <u>co-design</u> of the quantum devices, algorithms, and engineering solutions to <u>deliver certified quantum advantage</u> in Department of Energy scientific applications.



QSA addressing major challenges in quantum computing

Obstacle 1
Quantum systems are imperfect, with performance-limiting errors and coherence issues.

Obstacle 2
Current controls are not extensible and lack precision, limiting overall system size.

Obstacle 3
The domain of meaningful applications with quantified advantage on NISQ hardware is unexplored.

Obstacle 4
Lack of protocols to quantify and benchmark performance of imperfect hardware.

QSA Approach

Advanced quantum prototypes

- Development of atomic, ionic, superconducting platforms
- Noise resilient encodings & active error suppression
- Systems-level materials optimization

Higher fidelity control

- Integrated multichannel optical/microwave control
- Scalable FPGA/RFSoC electronic control
- Advanced metrology

Near term applications

- Platform-aware applications
- Hamiltonian emulation
- New algorithms and new science domains

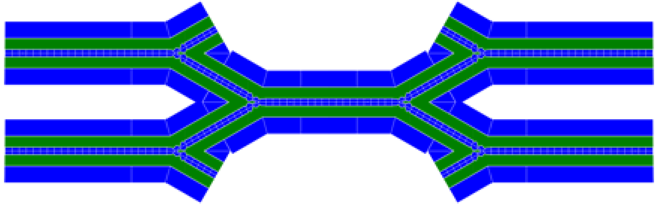
Benchmarking quantum advantage

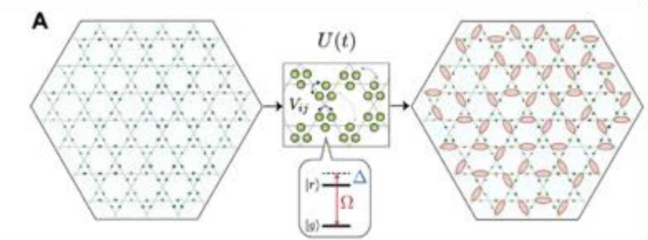
- Scalable quantum benchmarks
- Complexity analysis of quantum advantage
- Application specific benchmarking

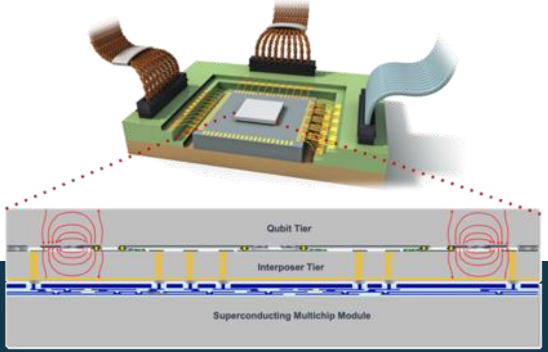
QSA is making major advances in QIS

QSA Top Achievements

- ✓ Created a **256 neutral atom** quantum simulator
- ✓ Designed and started fabricating a **200 ion trap**
- ✓ Built an **advanced 3D 4x4** qubit array with **50x reduction** in crosstalk
- ✓ Showed metrological gains **beyond the quantum projection noise limit** in a spin squeezed clock
- ✓ Developed **N-qubit entangling gates** for trapped ions
- ✓ Simulated frustrated magnetic states on a **tunable Fermi-Hubbard optical lattice**
- ✓ Demonstrated a **topological spin liquid** on a **256 neutral atom quantum simulator**
- ✓ Created and demonstrated protocols for **proof of quantumness**
- ✓ **Measured the gravitational redshift** within a millimeter atomic sample
- ✓ Taught **20 high school teachers and 32 students** at QCaMP
- ✓ Hosted quantum computer science program at **Simons Institute**







Advanced Quantum Testbed mission

To serve as an advanced superconducting platform for full-stack quantum computation, and to foster deep research collaborations with users selected through an open, competitive proposal process, synergistic with other resources available to the researcher community.

AQT delivers a unique research environment

Unique Quantum Platform

A state-of-the art open platform based on superconducting circuits for the scientific exploration of quantum computing, including quantum circuit fidelity, control/compilation, and processor architecture.

Deep User Collaborations

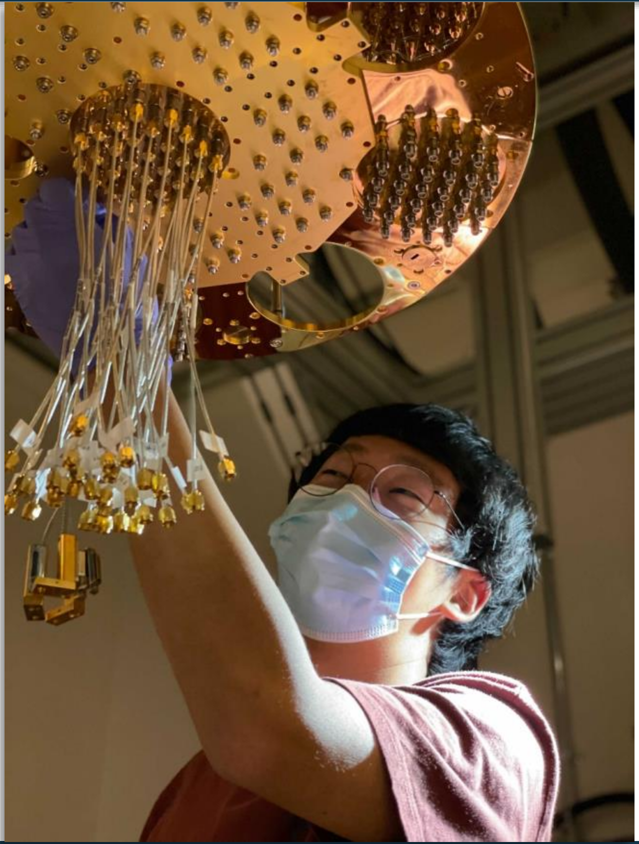
A highly-qualified team assists and partners in the development, execution, and optimization of short- and long-term scientific projects.

Broad Exploration of Technology

AQT deploys an evolving suite of circuits, controls, classical hardware, and algorithms developed at LBNL and via commercial partnerships.

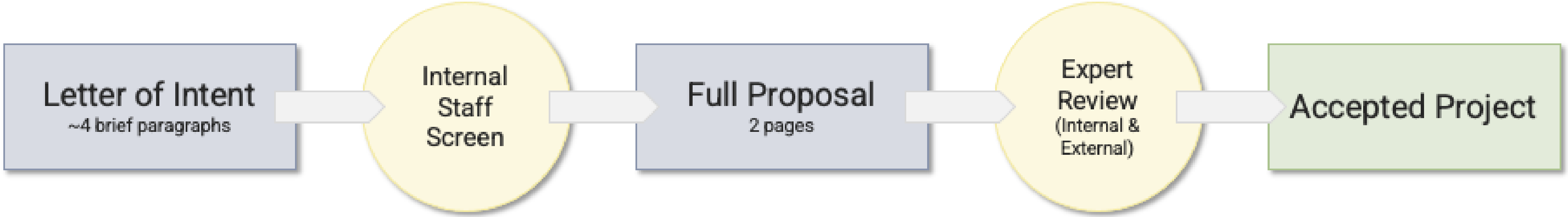
Developing Future QIS Experts

An ideal platform for training the next generation of scientists and engineers on cutting-edge hardware and real-world problems.



BERKELEY LAB

AQT runs an annual widely-announced Open Call



The proposal process is designed to have low barriers to entry with brief LOIs and proposals. Technical staff members are available throughout the proposal process to answer questions and discuss the feasibility of potential project ideas.

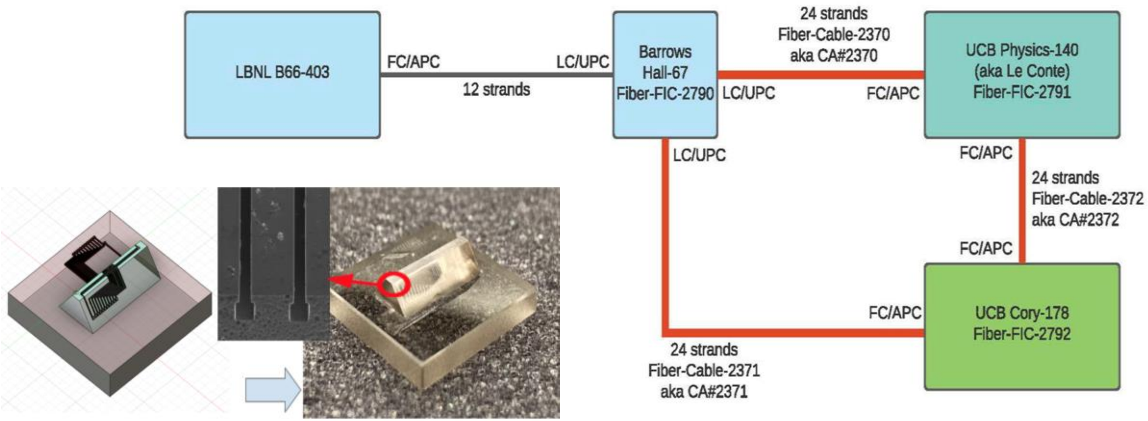
Review criteria:

- Scientific merit
- Alignment with AQT program goals and use of unique resources not available in the commercial domain
- Feasibility with testbed capabilities and resources

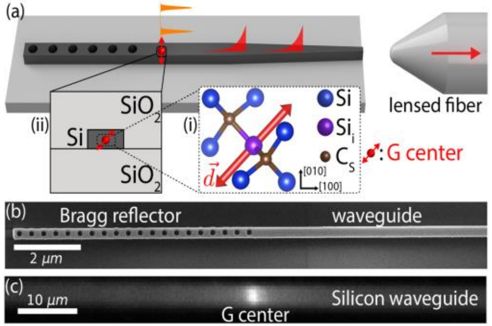
Project areas:

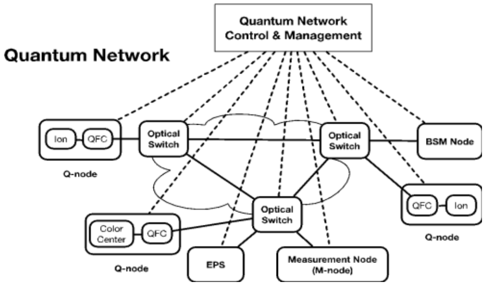
- Implementations of quantum algorithms or quantum simulations
- Quantum characterization, validation, and control routines
- Novel control hardware / firmware / software
- Novel superconducting quantum processor architectures

QUANT-NET program in a nutshell



Quantum Application Network Testbed for Novel Entanglement Technologies aims to build a proof-of-concept quantum network based on entanglement





quantnet.lbl.gov

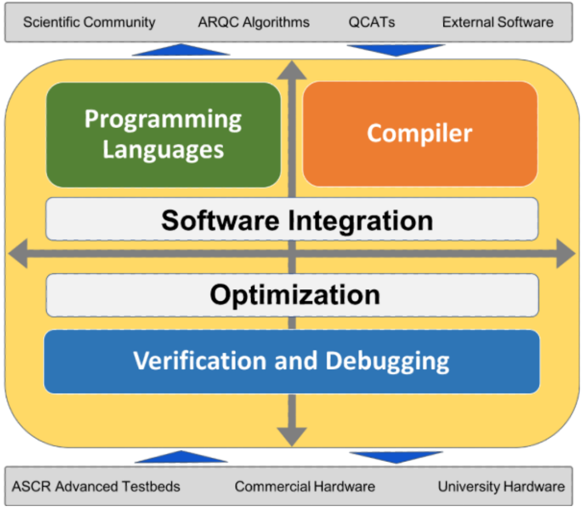
AIDE-QC program in a nutshell

We are developing and delivering an open-source computing, programming, and simulation environment that supports the large diversity of NISQ quantum computing research at DOE

Language abstractions enabling expression of algorithms across scientific domains

Cross-platform compiler with circuit synthesis, resource optimization and analysis tools

Extensible programming, compilation, and hardware-agnostic execution work flow for scientific quantum computing



Scalable techniques for verification of results from NISQ platforms

Development of debugging tools to analyze circuit execution errors

Next-gen optimization algorithms in service of quantum computing

Oak Ridge National Laboratory · Sandia National Laboratories · Argonne National Laboratory · Los Alamos National Laboratory EST. 1943 · Berkeley University of California · The University of Chicago

Flexible programming for scientists in C++ and Python

C++

```cpp
#include "qcor_qsim.hpp"

// Define a fixed ansatz as a QCOR kernel
__qpu__ void ansatz(qreg q, double theta) {
  X(q[0]);
  auto exponent_op = X(0) * Y(1) - Y(0) * X(1);
  exp_i_theta(q, theta, exponent_op);
}

int main(int argc, char **argv) {
  // Create the Deuteron Hamiltonian
  auto H = 5.907 - 2.1433 * X(0) * X(1) - 2.143 * Y(0) * Y(1) + 0.21829
* Z(0) -
           6.125 * Z(1);
  const auto num_qubits = 2;
  const auto num_params = 1;
  auto problemModel =
      QuaSiMo::ModelFactory::createModel(ansatz, H, num_qubits,
num_params);
  auto optimizer = createOptimizer("nlopt");
  // Instantiate a VQE workflow with the nlopt optimizer
  auto workflow = QuaSiMo::getWorkflow("vqe", {{"optimizer",
optimizer}});

  // Result should contain the ground-state energy along with the
optimal
  // parameters.
  auto result = workflow->execute(problemModel);

  const auto energy = result.get<double>("energy");
  std::cout << "Ground-state energy = " << energy << "\n";
  return 0;
}
```

Python

```python
from qcor import *

# Define the deuteron hamiltonian
H = -2.1433 * X(0) * X(1) - 2.1433 * \
    Y(0) * Y(1) + .21829 * Z(0) - 6.125 * Z(1) + 5.907

# Define the quantum kernel by providing a
# python function that is annotated with qjit for
# quantum just in time compilation
@qjit
def ansatz(q : qreg, theta : float):
    X(q[0])
    Ry(q[1], theta)
    CX(q[1], q[0])

# Create the problem model, provide the state
# prep circuit, Hamiltonian and note how many qubits
# and variational parameters
num_params = 1
problemModel = QuaSiMo.ModelFactory.createModel(ansatz, H,
num_params)

# Create the NLOpt derivative free optimizer
optimizer = createOptimizer('nlopt')

# Create the VQE workflow
workflow = QuaSiMo.getWorkflow('vqe', {'optimizer': optimizer})

# Execute and print the result
result = workflow.execute(problemModel)
energy = result['energy']
print(energy)
```

Compilers are a critical piece in the tool chain

Quantum
the open journal for quantum science

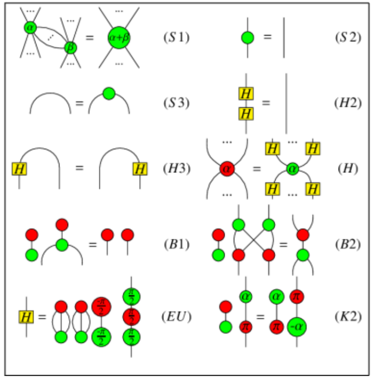
PAPERS PERSPECTIVES

Graph-theoretic Simplification of Quantum Circuits with the ZX-calculus

Ross Duncan[1,2], Aleks Kissinger[3], Simon Perdrix[4], and John van de Wetering[5]

[1]University of Strathclyde, 26 Richmond Street, Glasgow G1 1XH, UK
[2]Cambridge Quantum Computing Ltd, 9a Bridge Street, Cambridge CB2 1UB, UK
[3]Department of Computer Science, University of Oxford
[4]CNRS LORIA, Inria-MOCQUA, Université de Lorraine, F 54000 Nancy, France
[5]Institute for Computing and Information Sciences, Radboud University Nijmegen

Published: 2020-06-04, volume 4, page 279
Eprint: arXiv:1902.03178v6
Doi: https://doi.org/10.22331/q-2020-06-04-279
Citation: Quantum 4, 279 (2020).

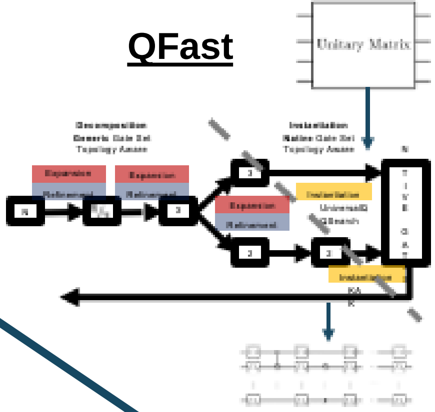


t|ket⟩ ™

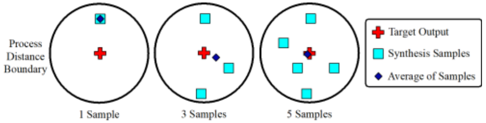
Compilation is an NP-hard problem

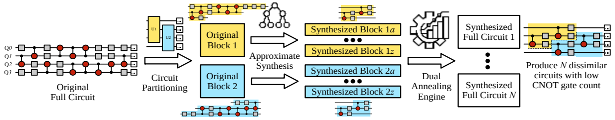
BQSKit
https://bqskit.lbl.gov

QFast



QUEST

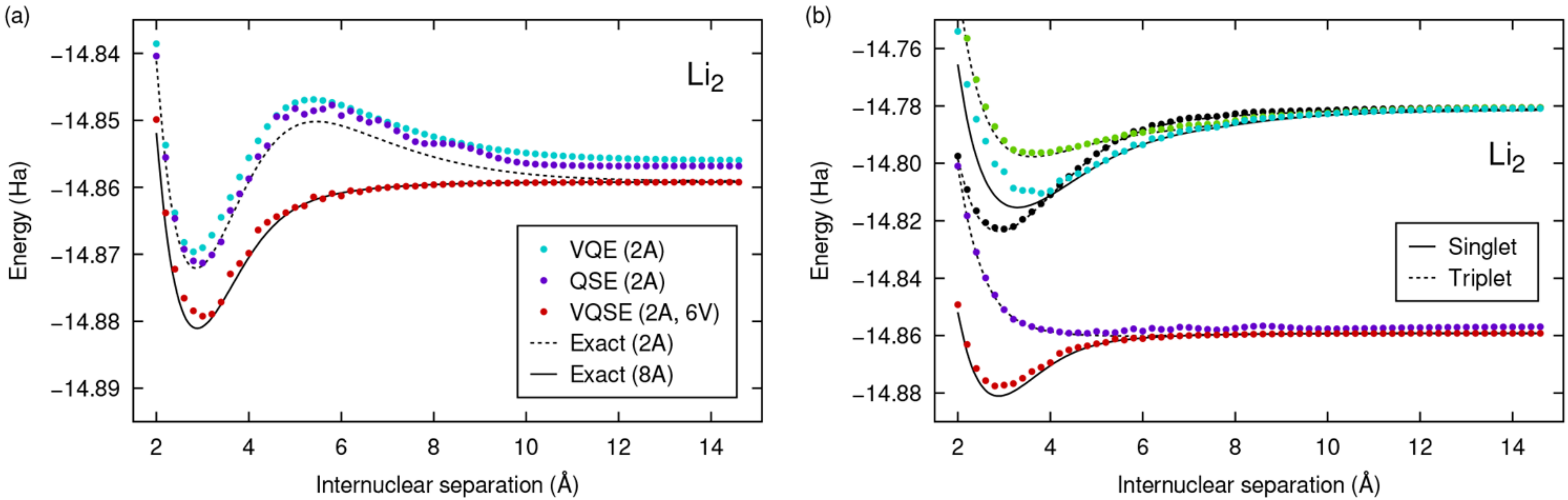




and for large qubit counts needs HPC

BERKELEY LAB

Towards chemical accuracy for battery relevant systems



Special care needs to be taken in general eigensolver due to noise in data!

$$HC = SCE$$

Urbanek, Van Beeumen, et al., J. Chem. Theory Comput. 16, 5425 (2020)

Building on Quantum Subspace Expansion: Real-time evolution for eigenvalue extraction

Real time evolution to generate a basis of expansion states: $|\Phi_{j,0}\rangle = e^{-iHt_j}|\Psi_0\rangle$

$|\Psi_0\rangle$ $\quad |\Phi_{1,0}\rangle$ $\quad |\Phi_{2,0}\rangle$ $\quad |\Phi_{3,0}\rangle$ $\quad \ldots$ $\quad |\Phi_{N,0}\rangle$

Initial vector

Use as a basis to solve: $H\Psi = ES\Psi$

$$H_{i,j} = \langle \Phi_i | H | \Phi_j \rangle$$
$$S_{i,j} = \langle \Phi_i | \Phi_j \rangle$$

Possible to extract eigenstates by the cancellation of phases of components of the initial vector.

Promising because unlike imaginary, real time evolution is native to quantum computing.

Klymko, de Jong, Tubman et al., PRX Quantum 3 (2022)

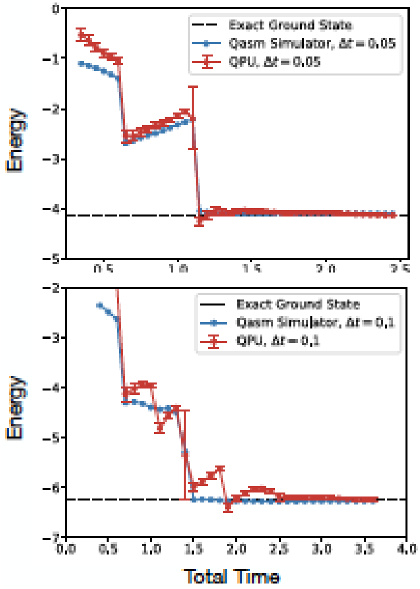
Building on quantum subspace expansion to extract excited states: Variational Quantum Phase Estimation (VQPE)

Original generalized eigenvalue equation: Unitary form:

$$H\mathbf{c} = ES\mathbf{c} \quad \longrightarrow \quad U(\Delta t)\mathbf{c} = e^{-iE\Delta t} S\mathbf{c}$$

$$U(\Delta t)_{j,k} = \langle \Psi_0 | e^{-iH(\Delta t + t_k - t_j)} | \Psi_0 \rangle = S_{j,k+1} = S_{j-1,k}$$

Autocorrelation Function Toeplitz structure!

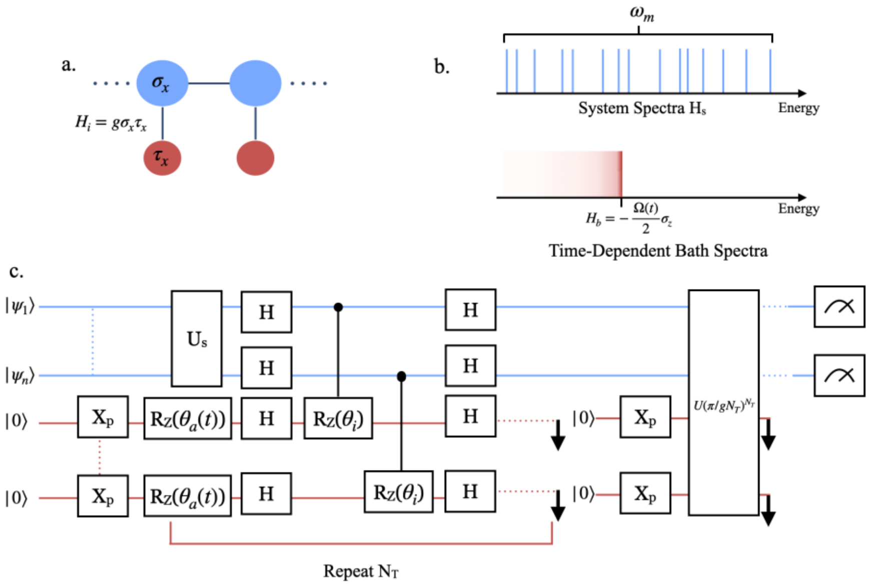


Toeplitz structure means that we only need a ***linear*** number of measurements instead of quadratic

Approach allows extraction of the maximal number of excited states!

Klymko, de Jong, Tubman et al., PRX Quantum 3 (2022)

Quantum Markov Chain Monte Carlo with Driven Dissipative Dynamics on Quantum Computers



a) Principal qubits (blue) locally connected to ancilla qubits (red). b) Time-dependent ancilla frequency combs the system energy spectra and resonantly exchanges energy with different energy transitions in the system at different times c) Quantum circuit to implement the interaction cycle dynamical map

Development of a quantum algorithm to sample from Boltzmann distributions on quantum computers by engineering open-quantum system dynamics

Algorithm can prepare robust, thermal states on quantum computers enabling finite-temperature simulations on quantum computers relevant to chemistry, materials and machine learning quantum applications

Metcalf, Stone, Klymko, Kemper, Sarovar, de Jong Quant. Sci. Tech. ***7****, 025017 (2022)*

Open quantum systems in heavy-ion collisions

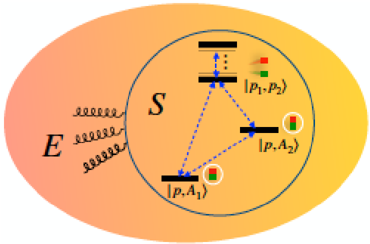
Two-level system of heavy quark-antiquark pair (H_s) interacting with quark-gluon plasma (H_e) via interaction Hi with strength g.

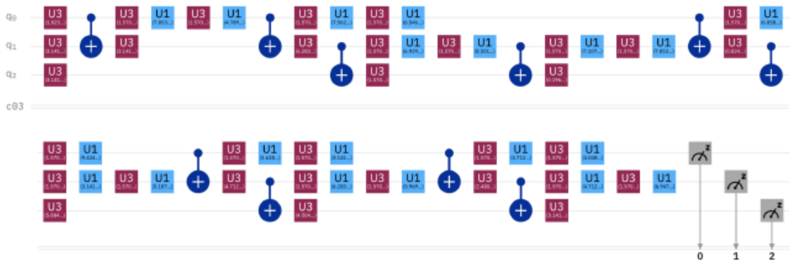
$$H_S = H_{S0} = -\frac{\Delta E}{2} Z$$

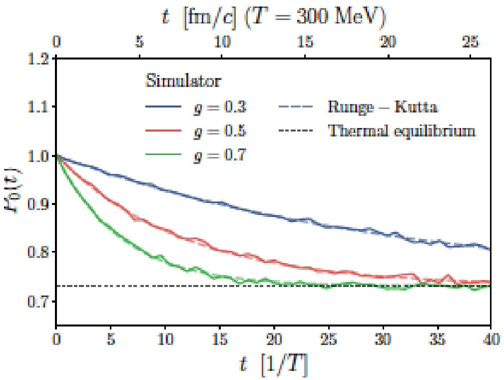
$$H_E = \int \mathrm{d}^3x \left[\frac{1}{2}\Pi^2 + \frac{1}{2}(\nabla\phi)^2 + \frac{1}{2}m^2\phi^2 + \frac{1}{4!}\lambda\phi^4\right]$$

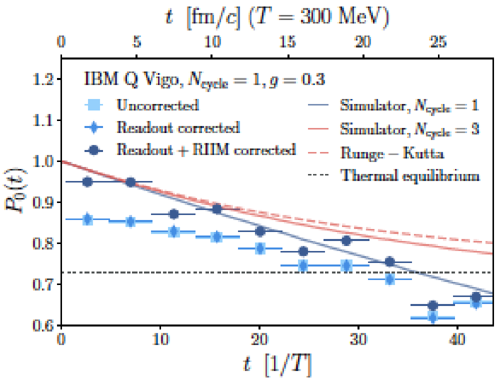
$$H_I = gX \otimes \phi(x=0)\,,$$

$$L_j = \frac{\sqrt{\Gamma_j}}{2}(X - (-1)^j iY)\,,$$









*de Jong, Metcalf, Mulligan, Ploskon, Ringer, Yao, Phys. Rev. D **104**, 051501 (2021)*

Adaptive Variational Quantum Dynamics Simulations

Variational form

$$|\Psi[\boldsymbol{\theta}]\rangle = \prod_{\mu=0}^{N_\theta - 1} e^{-i\theta_\mu A_\mu} |\Psi_0\rangle$$

Time dependent variational parameters

Von Neuman equation

$$\frac{d\rho}{dt} = \mathcal{L}[\hat{\rho}]$$

Real time: $\mathcal{L}[\hat{\rho}] = -i[\mathbf{H}, \hat{\rho}]$

Imaginary time: $\mathcal{L}[\hat{\rho}] = -\{\mathbf{H}, \hat{\rho}\} + 2\langle \mathbf{H} \rangle \hat{\rho}$

McLachlan distance

$$L^2 \equiv \left\| \sum \frac{\partial \hat{\rho}[\boldsymbol{\theta}]}{\partial \theta_\mu} \dot{\theta}_\mu - \mathcal{L}[\hat{\rho}[\boldsymbol{\theta}]] \right\|^2$$

$$= \sum_{\mu\nu} M_{\mu\nu} \dot{\theta}_\mu \dot{\theta}_\nu - 2 \sum_\mu V_\mu \dot{\theta}_\mu + \mathrm{Tr}[\mathcal{L}[\hat{\rho}[\boldsymbol{\theta}]]^2]$$

Distance between exact and variational time evolution

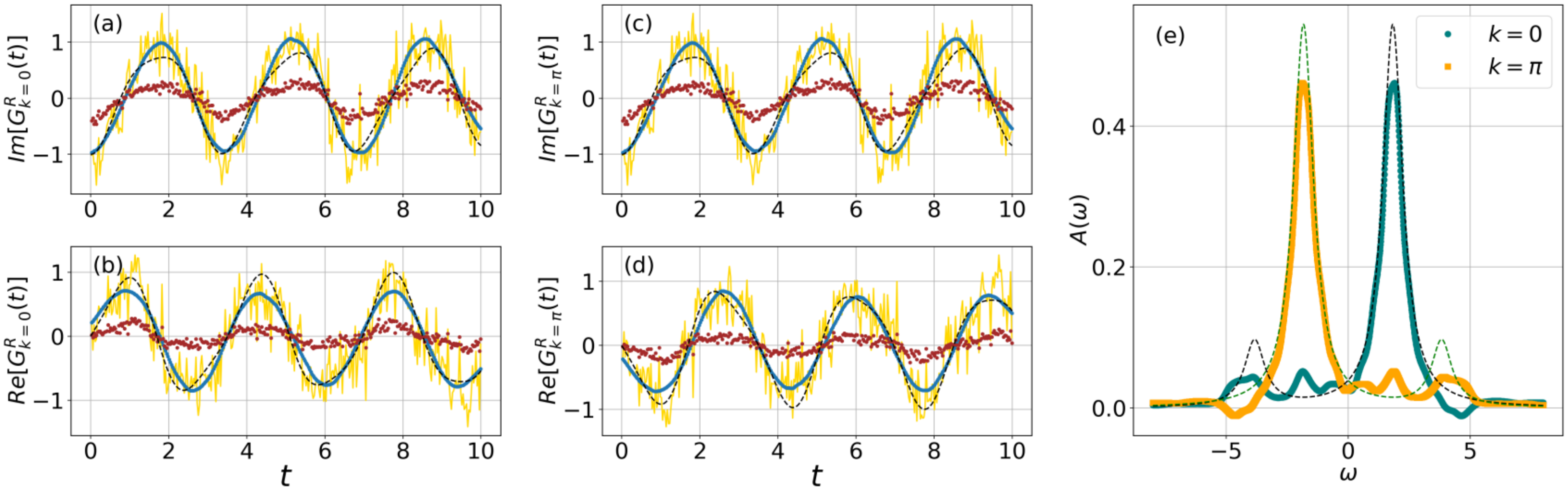
$$\sum_{\mu\nu} M_{\mu\nu} \dot{\theta}_\mu = V_\mu$$

$M_{\mu\nu}$ and V_μ are measured on QPU

Variable / Time Evolution	Ansatz type	$M_{\mu\nu}$	V_μ
Imaginary	$\mathcal{U}(\theta)\,\lvert 0\rangle$	$2\,\mathrm{Re}\left[\frac{\partial\langle\Psi[\theta]\rvert}{\partial\theta_\mu}\frac{\partial\lvert\Psi[\theta]\rangle}{\partial\theta_\nu} + \frac{\partial\langle\Psi[\theta]\rvert}{\partial\theta_\mu}\lvert\Psi[\theta]\rangle\frac{\partial\langle\Psi[\theta]\rvert}{\partial\theta_\nu}\lvert\Psi[\theta]\rangle\right]$	$\mathrm{Re}\left\{\frac{\partial\langle\Psi\rvert}{\partial\theta_\mu}\lvert\Psi\rangle\langle\Psi\rvert H\lvert\Psi\rangle - \frac{\partial\langle\Psi\rvert}{\partial\theta_\mu}H\lvert\Psi\rangle\right\}$
Real	$\mathcal{U}(\theta)\,\lvert 0\rangle$	$2\,\mathrm{Re}\left[\frac{\partial\langle\Psi[\theta]\rvert}{\partial\theta_\mu}\frac{\partial\lvert\Psi[\theta]\rangle}{\partial\theta_\nu} + \frac{\partial\langle\Psi[\theta]\rvert}{\partial\theta_\mu}\lvert\Psi[\theta]\rangle\frac{\partial\langle\Psi[\theta]\rvert}{\partial\theta_\nu}\lvert\Psi[\theta]\rangle\right]$	$-\,\mathrm{Im}\left\{\frac{\partial\langle\Psi\rvert}{\partial\theta_\mu}\lvert\Psi\rangle\langle\Psi\rvert H\lvert\Psi\rangle - \frac{\partial\langle\Psi\rvert}{\partial\theta_\mu}H\lvert\Psi\rangle\right\}$

Accuracy is limited by the form of the ansatz

Using AVQDS to calculate Green’s functions



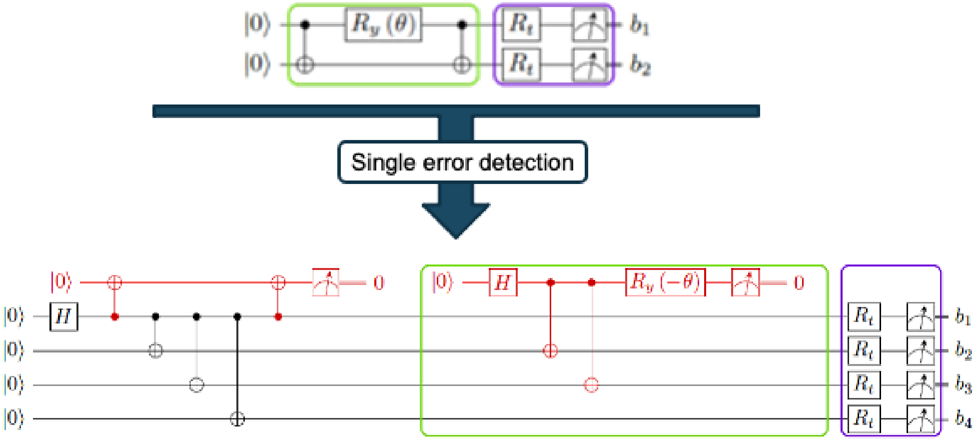
Retarded Green’s function versus time

Spectral function

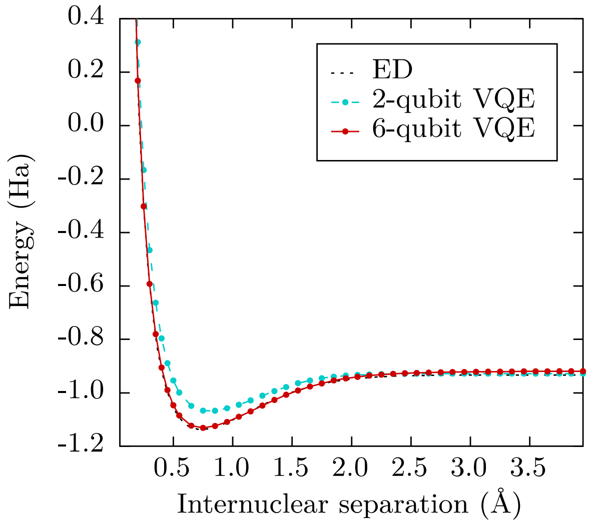
Two site Hubbard model on 4 qubits of IBM Kolkata quantum computer

Imaginary part of $G^R(\omega)$ using Pade approximation

Simple error detection and mitigation works



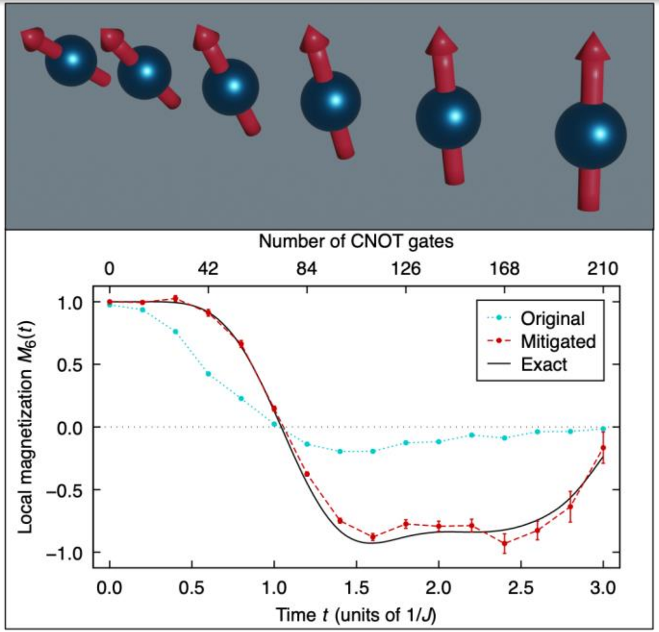
[[4,2,2]] error correction code



2 logical qubit H_2 molecule on 6 qubits with minimal basis

Urbanek et al, Phys. Rev. A 102, 022427 (2020)

Accurate magnetic materials simulation with quantum computers



Effect of mitigation: Time evolution of a six-qubit magnetic model calculated without and with error mitigation.

Longest time = 210 CNOTs

Scientific Achievement

Design of a practical mitigation strategy for drastically reducing errors and noise present in quantum computers based on superconducting qubits opens new opportunities for scientific discovery.

Significance and Impact

Combination of both existing and LBNL's new mitigation approaches enables larger scale simulations leading to quantum circuits with hundreds of operations to be run on quantum computers.

Additional Details

- Only Google has done better, but with simplified problems
- Team science, requiring physicists, chemists, computer scientists and applied mathematicians needed to achieve this result
- Science "Cutting Through the Noise" highlighted on CSA website, DOE ASCR Web Highlight in development, picked up by science outlets
- Would require a Quantum Volume of > 48,000; Current hardware as QV of 2048!

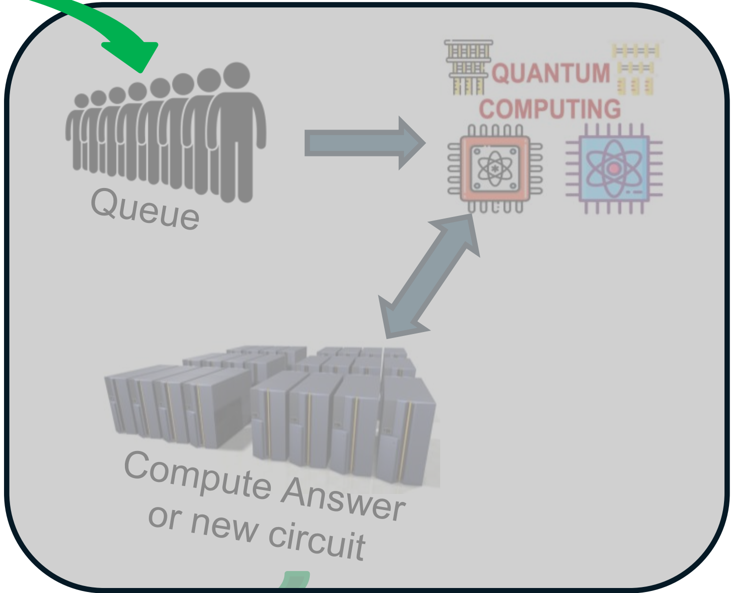
Using cloud-based quantum computer as black box

User

```
from SomeSimulationPackage import Molecule, SCFDriver
from SomeSimulationPackage import GroundStateEigensolver

molecule = Molecule(geometry=[['H', [0., 0., 0.]], ['H', [0., 0., 0.735]]],
                    charge=0, multiplicity=1)
driver = SCFDriver(molecule = molecule, basis='sto3g')

calc = GroundStateEigensolver(algorithm=VQE, qubits=4)
res = calc.solve(driver)
```

Final answer

Cloud Provider



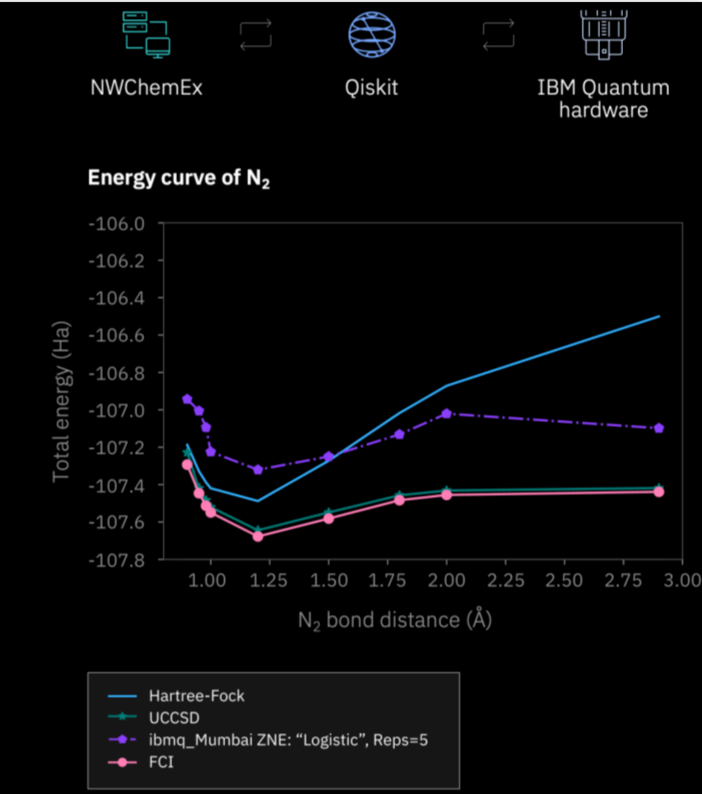
Target is the end-users in academia and industry without quantum knowledge

MCSCF with Qiskit requires iterations between quantum and HPC

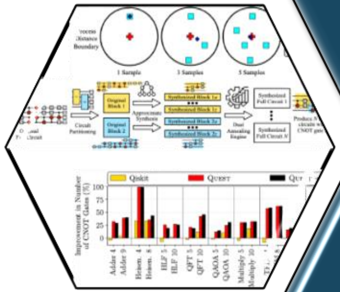
HPC codes with quantum acceleration:

Quantum chemistry's MCSCF requires a tight loop and integration into large HPC codes

```
nux.initialize()

# load modules
mm = pluginplay.ModuleManager()
nwx_quantum.load_modules(mm)

# iterate over bond dissociation
for distance in np.arange(0.7, 3.1, 0.25):
    # setup molecule
    mol = nux.get_molecule_from_xyz(
        xyz=f"2\n\nN 0 0 0\nN 0 0 {distance}", coord="ang"
    )
    # get hamiltonian
    H = nux.get_hamiltonian(mol)
    H_e = simde.type.els_hamiltonian(H)
    # construct basis set
    aos = nwchemex.apply_basis("sto-3g", mol)
    # find HF solution as initial guess
    [phi0] = mm.at("SCF Wavefunction").run_as[simde.CanonicalReference](
        H_e, aos
    )
    # setup active space
    as0 = casscf.select_active_space(phi0, 4, 4)

    # run Quantum-based CASSCF
    [E] = mm.at("FileBasedMCSCF").run_as[simde.ConfigurationInteractionEnergy](
        H_e, phi0, as0
    )
```

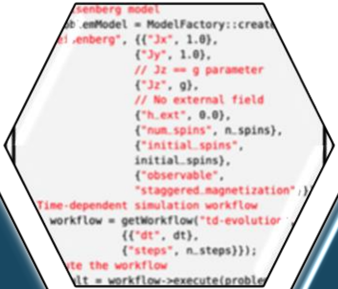


AIDE-QC is advancing the software ecosystem



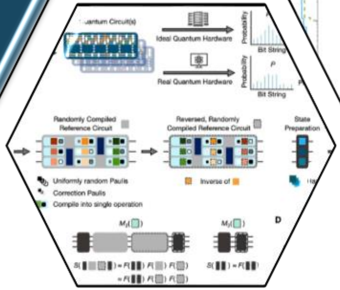
New programming language abstractions

Scalable, hardware-agnostic compilers

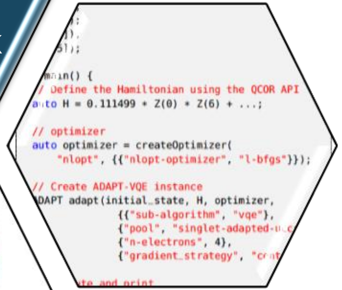


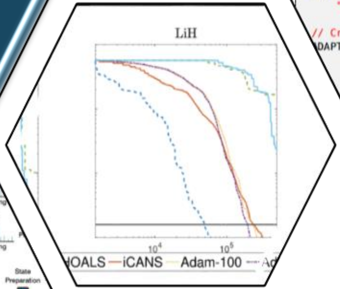
Scalable approaches for debugging and verification

Novel optimization methods for quantum computing



Extensible hardware-agnostic software stack





Exponential speedup not only factor for quantum advantage

Power: 20 MW + 10 MW for cooling
Cost: US$600M (estimated cost)
Space: 2225 m^2 (7,300 sq ft)
24,000 house holds

Quantum computers could solve **larger problems faster** compared to classical computing hardware

Quantum computers are **cheaper and use less energy** than classical computers, increasing accessibility to large scale computing

Race to the moon delivered many ancillary technologies

Quantum-inspired algorithms speedup classical computing

Novel quantum hardware technologies find way into classical computing hardware

Better understanding of quantum physics to lead to advances in classical computing

CMOS sensor, using integrated circuits….

Race for a universal quantum computer is already showing impacts beyond quantum computing

Acknowledgements

This work was supported by DOE
Office of Advanced Scientific Computing Research (ASCR)
through the QAT and ARQC
Office of Basic Energy Sciences (BES)
Quantum Systems Accelerator

Member of the ORNL IBM Q Network

This research used computing resources of the National Energy Research Scientific Computing Center

quantum.lbl.gov
quantumsystemsaccelerator.org
aide-qc.org
aqt.lbl.gov

Bert de Jong
wadejong@lbl.gov