# Advancing Physical Sciences on Near-Term Quantum Computers





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# What makes quantum computing so exciting?

- Speedups over classical computing
- "Unbreakable" encryption protocols
- Quantum simulation
- Efficient optimization algorithms







# Quantum computing hardware technologies



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# Many challenges with quantum hardware



ATOMS



SOLID STATE

- # of good qubits not yet enough for quantum advantage/science
- Coherence (available compute time) very short (10s-100s of ops)
- Noise and errors still pretty large
- Diverse technologies, each with its own instruction set
- Software tools and compilers are still in their infancy



# For example, gate sets in superconducting chips











Google

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IBM

Rigetti



IonQ

- Each chip has own native gate set
  - Single qubit, usually rotations, and Hadamard
  - Two-qubit, usually CNOT, CZ (Google), SWAP
- Each chip has a constrained topology
  - Ring, array, mesh, bow-tie
- Compilers needed to translate gate sets, do mapping





# Making quantum simulations feasible with NISQ

- Requires minimizing number of qubits and depth of circuit
  - Novel basis, using physical knowledge (symmetries, electron count, etc.) reduces qubit count
  - Localized Hamiltonians reduce number of interactions, reducing circuit depth and level of entanglement Interaction picture, qubitization
- Using error mitigation strategies



# Towards useful quantum computing 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



# Parton showers and interfering trees

Fermions interacting with scalar boson  $\mathcal{L} = \bar{f}_1(i\partial \!\!\!/ + m_1)f_1 + \bar{f}_2(i\partial \!\!\!/ + m_2)f_2 + (\partial_\mu \phi)^2$   $+ g_1 \bar{f}_1 f_1 \phi + g_2 \bar{f}_2 f_2 \phi + g_{12} [\bar{f}_1 f_2 + \bar{f}_2 f_1] \phi.$ 





Provasoli, Nachman, Bauer, de Jong, Quant. Sci. Tech. 5, 035004 (2020) Nachman, Provasoli, de Jong, Bauer, Phys. Rev. Lett. 126, 062001 (2021)



# Two common algorithms for quantum simulations



#### Variational Quantum Eigensolver (VQE) Algorithm 2 Algorithm 1 QPU CPU $\langle H_1 \rangle$ $\langle H_1 \rangle$ uantum module 1 $\langle H_2 \rangle$ $\langle H_2 \rangle$ uantum module 2 $\langle H_3 \rangle$ $\langle H_3 \rangle$ uantum module 3 $\langle H_N \rangle$ $\langle H_N \rangle$ uantum module n

$$H = \sum_{i\alpha} g_i^{\alpha} \left\langle \sigma_{\alpha}^i \right\rangle + \frac{1}{2} \sum_{ij\alpha\beta} g_{ij}^{\alpha\beta} \left\langle \sigma_{\alpha}^i \sigma_{\beta}^j \right\rangle + \cdots$$

Adjust the parameters for the next input state

Only prepare and measure, do the rest classically

### Quantum subspace expansion (QSE)





McClean, Schwartz, Carter, de Jong, Phys. Rev. A 95 (4), 042308 (2017)

#### **Demonstrated end-to-end simulation on Berkeley hardware**



Colless, J.I., Ramasesh, V.V., Dahlen, D., Blok, M.S., McClean, J.R., Carter, J., de Jong, W.A., Siddiqi, I. - Phys. Rev. X 8, 011021 (2018)



### Solving noisy generalized eigensolver problem a challenge



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 QSE: Real-time evolution for eigenvalue extraction

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



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.



# Variational Quantum Phase Estimation (VQPE)

Original generalized eigenvalue equation:

Unitary form:

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

$$U(\Delta t)_{j,k} = \left\langle \Psi_0 | e^{-iH(\Delta t + t_k - t_j)} | \Psi_0 \right\rangle = S_{j,k+1} = S_{j-1,k} \qquad \begin{array}{l} H_{i,j} = \left\langle \Phi_i | H | \Psi_j \right\rangle \\ S_{i,j} = \left\langle \Phi_i | \Phi_j \right\rangle \end{array}$$

**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!



# Towards engineering open quantum systems



#### 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

#### **Scientific Achievement**

A team of researchers led by Berkeley Lab developed a quantum algorithm to sample from Boltzmann distributions on quantum computers by engineering open-quantum system dynamics.

#### Significance and Impact

Our algorithm is designed to prepare robust, thermal states on quantum computers enabling finitetemperature simulations on quantum computers relevant to chemistry, materials and machine learning quantum applications.

Metcalf, Stone, Klymko, Kemper, Sarovar, de Jong - arXiv:2103.03207



# **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.

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

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#### Non-equilibrium dynamics and thermalization in the Schwinger model

Fermion sites, uncopied or with electron/positron with electric field between fermions (green) and interaction with environment.

Demonstration below on 2 fermions sites an 1 qubit representing the environment.







Qubit use, system in green, with 4 qubits for environment for 4 cycles as mid-circuit reset was not available.

de Jong, Metcalf, Mulligan, Ploskon, Ringer, Yao, arXiv:2106.08394

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# **Computing Free Energy with Jarzynski Equality**



Challenges:

- Prepare thermal state on quantum computer
- Measure quantum work over trajectory



#### **Computing Free Energies with Fluctuation Relations on Quantum Computers**



# Programming a quantum computer

#### Scientist

#### Science problem to Algorithm



#### **High level interface**

- Domain Specific Language
- Solvers (VQE, QPA, QITE)
- Algorithm specified in any gate set

# 

**Compiled Quantum Algorithm** 

#### **Translate to processor**

- Arbitrary gates compiled into available gate set
- Processor connectivity and timing constraints enforced

#### Pulses output by AWG

Hardware



#### **Translation to hardware**

- Define pulse parameters (shape, phase, sequence)
- Reset/feedback code applied by FPGAs



#### Adapted from Irfan Siddiqi, UC Berkeley

# A far from complete list of software tools

• Frameworks from most chip providers

Provider	Framework	License	Cloud
IBM	QisKit	Minor restrictions	IBM Q-Experience
Google	Cirq	Open	
Rigetti	Forest / PyQuil	Restrictive	Rigetti QCS (beta)
Microsoft	LiQUi> / Q#	Minor restrictions	
D-Wave	qbsolv	Minor restrictions	D-Wave Leap
Xanadu	Strawberry Fields	Open	

- Academia & startups target the above
  - E.g. PyTKET (Cambridge Quantum), ProjectQ (ETH Zürich)
  - QuTiP (Academia, also RIKEN; <a href="http://qutip.org">http://qutip.org</a>)



# Quantum JIT (QJIT)

- JIT for quantum kernels in qcor
  - Flexibility to construct kernels based on runtime information
- Kernels passed as strings, output function pointer to execute
- QJIT class integration of ...
  - QCOR SyntaxHandler (map kernel to valid C++ code)
  - Clang LLVM IR CodeGen (map C++ code to LLVM Module)
  - LLVM JIT (extract function pointer from LLVM Module)
- Extended to Python...

```
#include "qcor_jit.hpp"
```

int main() {

// QJIT is the entry point to QCOR quantum kernel
// just in time compilation
QJIT qjit;

```
// Define a quantum kernel string dynamically
const auto kernel_src = R"#(__qpu__ void bell(qreg q) {
    using qcor::openqasm;
    h q[0];
    cx q[0], q[1];
    creg c[2];
    measure q -> c;
})#";
```

// Use the QJIT instance to compile this at runtime
qjit.jit\_compile(kernel\_src);

// Now, one can get the compiled kernel as a
// functor to execute, must provide the kernel
// argument types as template parameters
auto bell\_functor = qjit.get\_kernel<qreg>("bell");

// Allocate some qubits and run the kernel functor
auto q = qalloc(2);
bell\_functor(q);
q.print();

```
// Or, one can call the QJIT invoke method
// with the name of the kernel function and
// the necessary function arguments.
auto r = qalloc(2);
qjit.invoke("bell", r);
r.print();
```



#### Quantum JIT (QJIT)

nclude "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 Hamiltonia

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

}

qsim::ModelBuilder::createModel(ansatz, H, num\_qubits, num\_params); auto optimizer = createOptimizer("nlopt");

// Instantiate a VQE workflow with the nlopt optimizer

auto workflow = qsim::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;



#### from qcor import \*

# Define the deuteron hamiltonian

 $H = -2.1433 * X(0) * X(1) - 2.1433 * \langle Y(0) * Y(1) + .21829 * Z(0) - 6.125 * Z(1) + 5.907$ 

# 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 = qsim.ModelBuilder.createModel(ansatz, H,
num\_params)

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

# Create the VQE workflow

workflow = qsim.getWorkflow('vqe', {'optimizer': optimizer})

# Execute and print the result

result = workflow.execute(problemModel)
energy = result['energy']
print(energy)

http://aide-ac.org/Software

#### Python

# **Circuit Synthesis Language Extension in Python**

Original C++ decompose extension

\_qpu\_\_ void ccnot(qreg q) {

```
// set initial state to 111
for (int i = 0; i < q.size(); i++) {
    X(q[i]);</pre>
```

Now possible in Python

@qjit
def ccnot(q : qreg):
 # create 111
 for i in range(q.size()):
 X(q[i])
 with decompose(q) as ccnot:
 ccnot = np.eye(8)
 ccnot[6,6] = 0.0
 ccnot[7,7] = 0.0
 ccnot[6,7] = 1.0
 ccnot[7,6] = 1.0

# CCNOT should produce 110 (lsb)
for i in range(q.size()):
 Measure(q[i])

#### Can leverage Numpy

```
@qjit
def all_x(q : qreg):
    with decompose(q) as x_kron:
        sx = np.array([[0, 1],[1, 0]])
        x_kron = np.kron(np.kron(sx,sx),sx)
    for i in range(q.size()):
        Measure(q[i])
```

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Measure(q[i]);

# Composable Programming of Hybrid Workflows for Quantum Simulation



Defining the antiferromagnetic (AF) Heisenberg problem model and simulating its dynamics with Quantum Simulation Modeling (QuaSiMo) library.

#### **Scientific Achievement**

We developed a composable design scheme for quantum simulation applications using the QCOR hardware-agnostic programming language into the QuaSiMo library.

#### Significance and Impact

The QuaSiMo library enables rapid synthesis of hybrid algorithms and workflows using a common, reusable methods and data structures for quantum simulation applications.



Results for the staggered magnetization of the AF Heisenberg model using quantum dynamics simulations with the QuaSiMo library

T. Nguyen, L. Bassman, D. Lyakh, A. McCaskey, V. Leyton-Ortega, R. Pooser, W. Elwasif, T. S. Humble and W. A. de Jong, "Composable Programming of Hybrid Workflows for Quantum Simulation,"in press arXiv:2101.08151 (2021)



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# **Compiling...General Synthesis Problem**

#### Unitary



Quantum Compilation: Given unitary U, find decomposition in terms of gates G from a (universal) fixed gate set





#### **Enables:**

- Algorithm discovery
- Gate set and hardware exploration
- Global circuit optimization



# **Berkeley Quantum Synthesis Toolkit**



#### QSearch – Developed by Advanced Quantum Testbed

### QFAST – Developed by QAT4Chem and AIDE-QC

Qfactor – Collaboration LANL (Cincio) and LBNL (Younis)



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# https://github.com/BQSKit

#### QFAST: Conflating Search with Numerical Optimization in Quantum Synthesis

#### **Scientific Achievement**

We show how to increase scalability of "optimal" quantum synthesis by replacing search based algorithms with one step of numerical optimization

#### Significance and Impact

NISQ hardware requires short depth circuits, compilers have limits. QFAST can produce short circuits, hierarchical approach enables both scalability and retargetability/portability. QFAST is topology aware.

- 1. QFAST reduces depth 6.3X average, up to 30X
- 2. 10x shorter circuits than state-of-the-art

Ed Younis (LBL), Koushik Sen (UCB), Kathy Yelick (LBL), Costin Iancu (LBL) - QCE21 Best Paper Award



Simulation Time Step



#### **Constant-Depth Circuits for Dynamic Simulations on QC**

#### **Scientific Achievement**

A method for generating circuits which are constant in depth with increasing time-step, thus enabling dynamic simulations on nearterm quantum computers out to arbitrarily long simulation times.

#### Significance and Impact

High-fidelity simulation results for long-time dynamic simulations of quantum materials can be obtained on currently available quantum computers.

5-spin TFIM 5 spins 300 ---- 4 spins Constant Depth Gate Count 007 ······ 3 spins N 100 Constant Depth 10 15 20 25 15 20 25 30 35 30 35 5 10 40 0 5 Simulation Timestep Simulation Timestep 5-spin XY 600 5 spins ---- 4 spins Gate Count 3 spins ¥ 200 15 20 25 15 20 25 30 10 30 10 35 0 5 35 5 40 Simulation Timestep Simulation Timestep

Bassman, Van Beeumen, Younis, Smith, Iancu, de Jong Mat. Theory, accepted (2021) - arXiv:2103.07429 Comparison of simulation results and CX gate count for the TFIM and the XY model using the constant-depth circuits versus the IBM-compiled circuits.



# QUEst: Robust Generation of Quantum Circuit Approximation Using Synthesis

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#### **Scientific Achievement**

We provide a sound and scalable method for generating circuit approximations. Approximations significantly reduce circuit depth, while providing same output quality. On NISQ, approximations improve output quality.

#### Significance and Impact

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Resource efficiency is an important measure of circuit performance. Our technique can be directly used for circuit optimization in NISQ and fault-tolerant quantum computing. In NISQ, we provide additional capability for very good error mitigation.

- We show 30%-80% depth reduction on many important algorithms
- We show fidelity improvements of 30% on noisy systems, independent of noise level
- The program output is accurate enough for science purposes
- Although computationally intensive, the technique scales up to high qubit counts (up 128 qubits demonstrated)

Patel, Younis, Bassman, Tiwari, de Jong, Iancu ASPLOS 2022 - https://arxiv.org/abs/2108.12714



# **AIDE-QC** software stack available

- Binary installs for various platforms
- Extensive user and developer guide with examples *http://aide-ac.org/Software https://aide-qc.github.io/deploy*



# **Qubit errors due to relaxation and decoherence**

#### T<sub>1</sub>: relaxation, dampening

- Environment exchanges energy with the qubit, mixing the two states by stimulated emission or absorption
- Important during read-out
- Intuitively time to decay from |1> to |0>

#### T<sub>2</sub>: dephasing

- Environment creates loss of phase memory by smearing energy levels, changing phase velocity
- Important during "computation", bounds circuit depth (number of consecutive gates)

#### • Intuitively time for $\phi$ to get imprecise





# Noisy intermediate-scale quantum devices



#### • Right now quantum computing is still a *physics experiment*

- Noise is everywhere
- Measurement errors



#### **Correcting read-out error bias:** Learning from noisy high-energy physics



# **Regularized matrix inversion approaches**



-35- HEP QuantiSED

Nachman et al., npj Quant. Inform. 6, 84 (2020)

parameter

# **Building error detection/correction into algorithms**



[[4,2,2]] error correction code, with 2 logical qubits





# **Error corrected circuits drastically improve results**



#### H<sub>2</sub> molecule on 2/6 qubits with minimal basis



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

#### Tackling noise in quantum operations without error correction



#### Ying Li and Simon C. Benjamin - Phys. Rev. X 7, 021050 (2017)



# Limits of error mitigation with linear extrapolation

- Primary challenge in circuits are CNOTs
- What if your circuit has 16 CNOTs...or more?
  - Would require 16+32 and 16+32+32 CNOTs to add 1 and 2 layers of identities to extrapolate
- Alternative is adding fewer identities (RIIM)
  - Including fewer identities and using polynomial fits

 $\max\left[\delta, \epsilon^{n_{\max}}, \Delta_{\text{shot}}\right]$ 

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HEP QuantiSED

He et al., Phys. Rev. A 102, 012426 (2020)

#### Practical error-mitigation strategy for superconducting qubits



**Effect of mitigation:** Time evolution of a sixqubit magnetic model calculated without and with error mitigation.

#### Longest time = 220 CNOTs

#### **Scientific Achievement**

Design of a practical mitigation strategy for reducing errors and noise present in quantum computers based on superconducting qubits.

#### **Significance and Impact**

Combination of both existing and own mitigation approaches that address various error sources improves accuracy for quantum circuits with hundreds of gates.

#### **Research Details**

- *Readout error correction* mitigates readout errors occurring during a measurement.
- Randomized compiling mitigates coherent gate errors and converts them to incoherent noise.
- Noise correction with *noise estimation circuits* mitigates global depolarizing noise.
- Error extrapolation mitigates local depolarizing noise.



Urbanek, Nachman, Pascuzzi, He, Bauer, de Jong, Phys. Rev. Lett. 127, 270502 (2021)

# Interdisciplinary team at LBNL

#### **Physics**

- Mekena Metcalf
- Miro Urbanek
- Lindsay Bassman
- Katie Klymko
- Ben Nachman
- Christian Bauer
- James Mulligan
- Matheusz Ploskon
- Felix Ringer
- Xiaojun Yao



#### **Error mitigation**

- Wim Lavrijsen
- Ben Nachman
- Christian Bauer
- Miro Urbanek

#### Mathematics

- Daan Camps
- Roel van Beeumen
- Julie Mueller

#### Compilers

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- Costin lancu
- Ed Younis









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# **HEP QuantiSED**

# qat4chem.lbl.gov aide-qc.org berkeleyquantum.org thequantuminformationedge.org







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