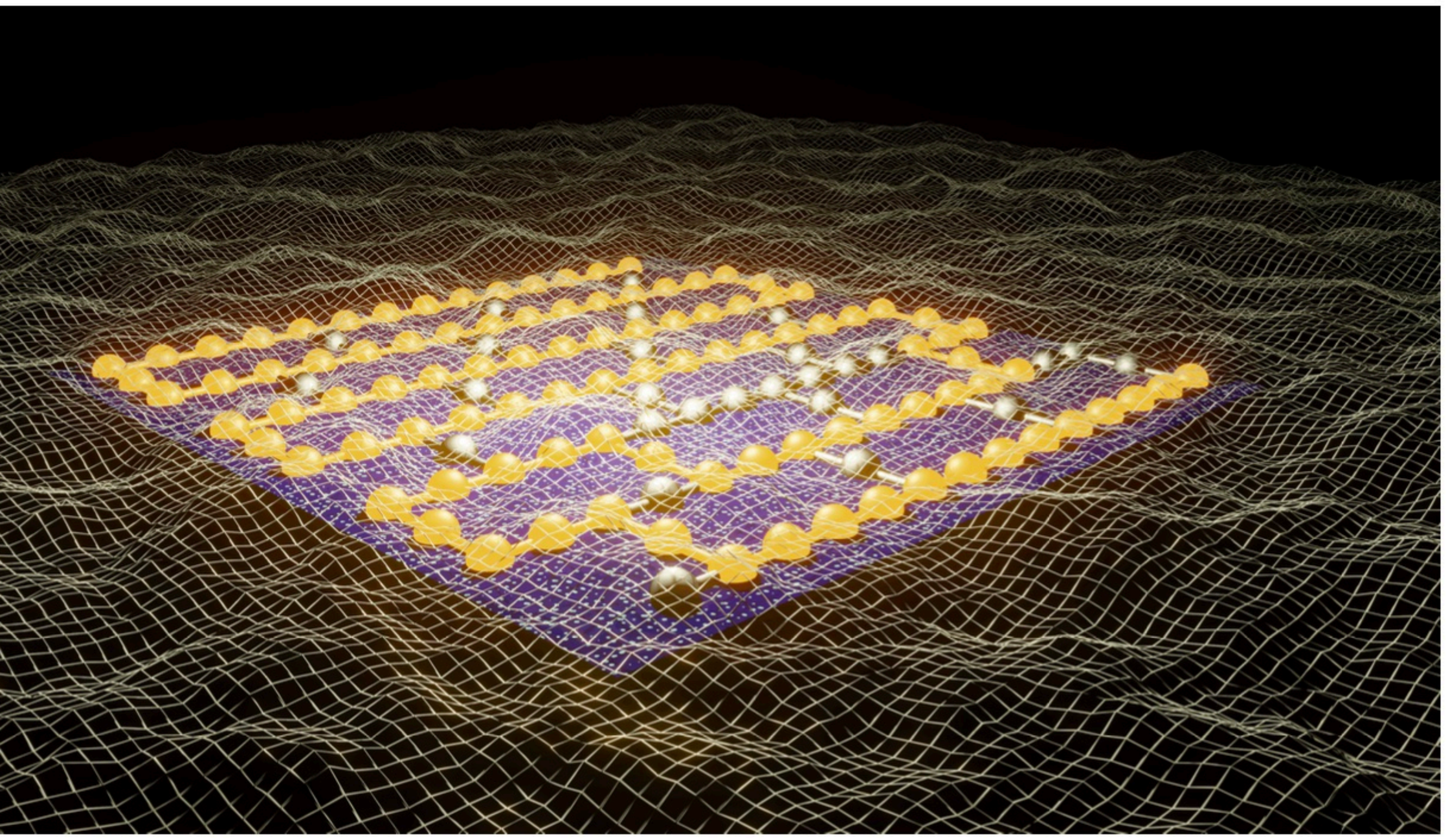
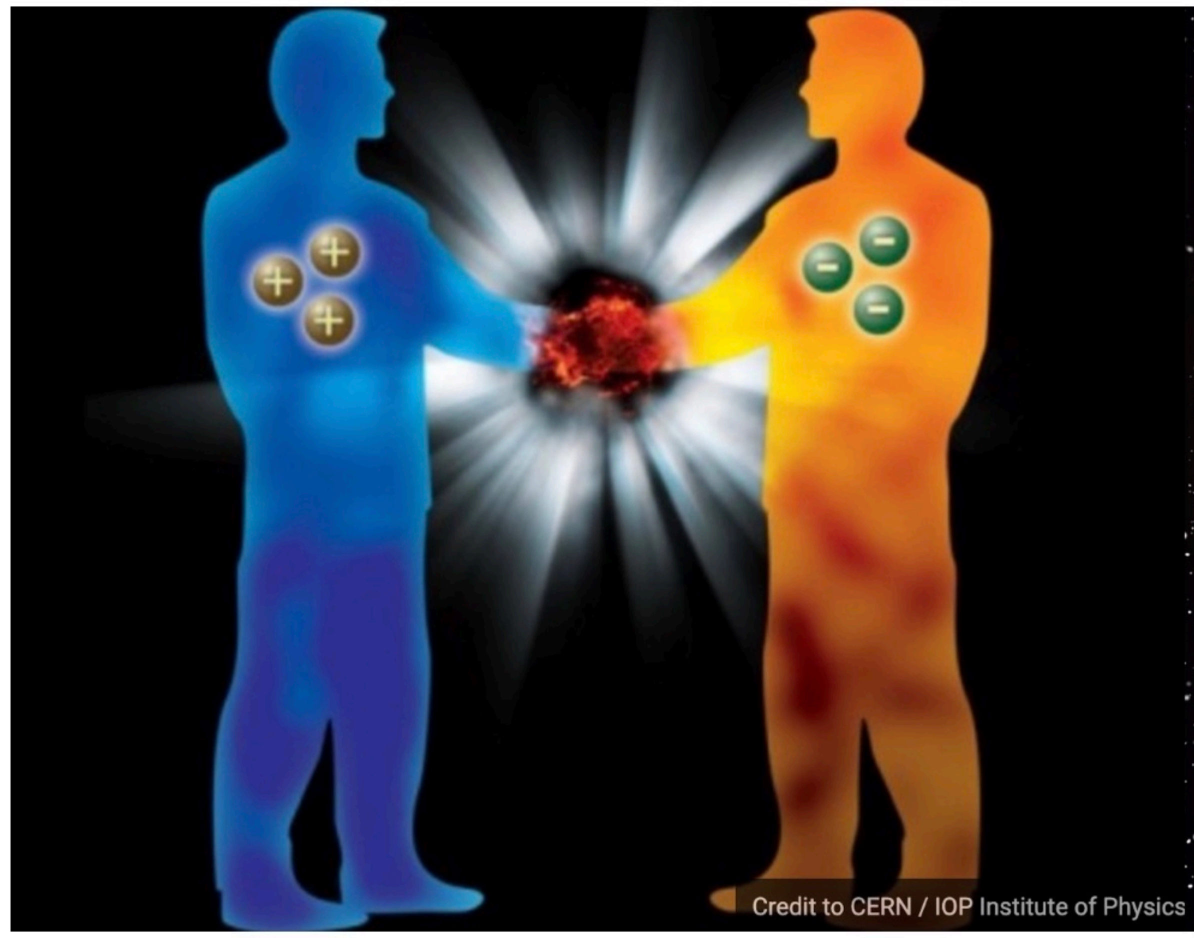
WORKSHOP ON
SOFTWARE INFRASTRUCTURE
FOR ADVANCED
NUCLEAR PHYSICS
COMPUTING JUNE 20-22, 2024

Software Infrastructure for Advanced Nuclear Physics Computing

IQuS - The InQubator for Quantum Simulation

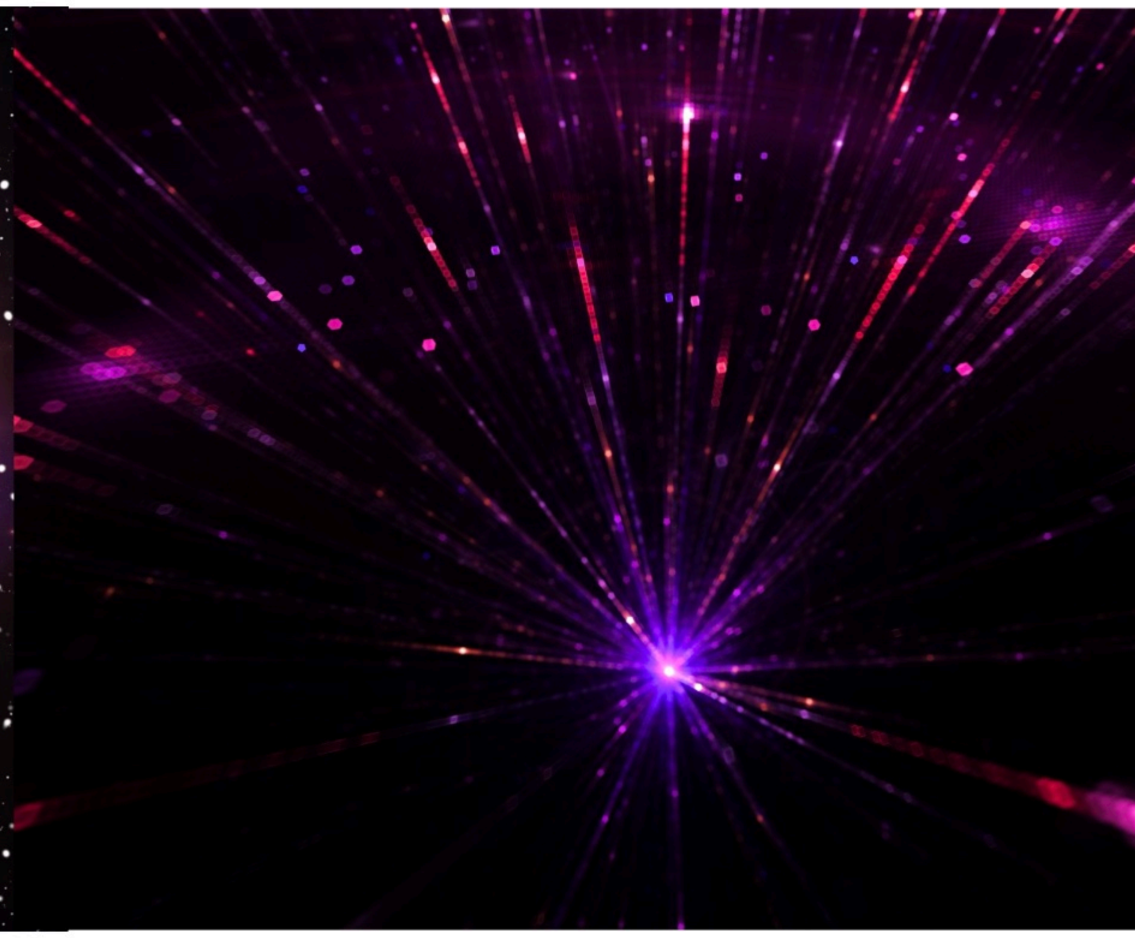




Credit to CERN / IOP Institute of Physics

The Matter-Antimatter Asymmetry

Astrophysical Environments



Collisions and Reactions

Martin Savage
University of Washington

Thomas Jefferson National Accelerator Facility, June 20-22, 2024

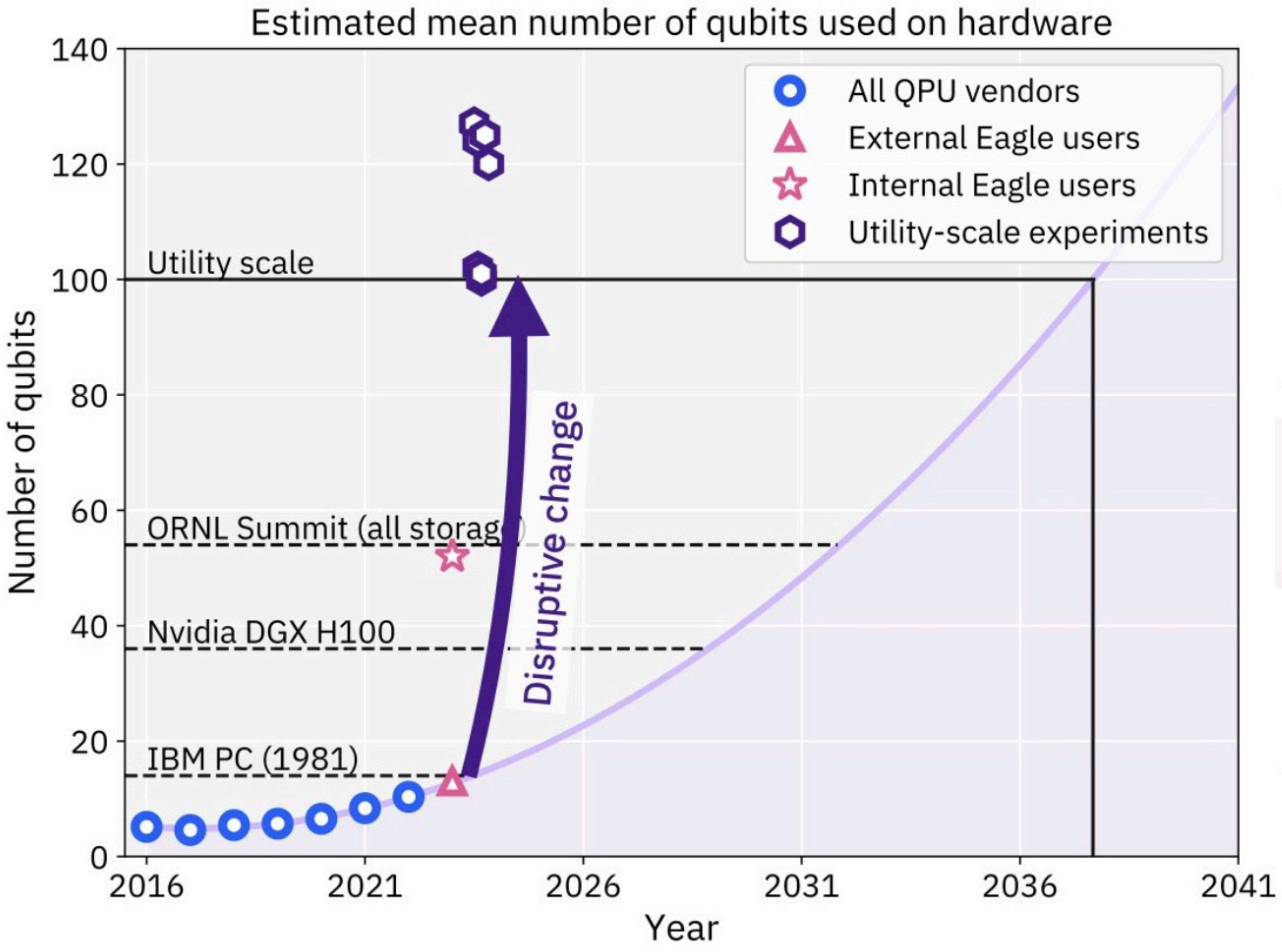
IQuS

DEPARTMENT OF ENERGY • UNITED STATES OF AMERICA

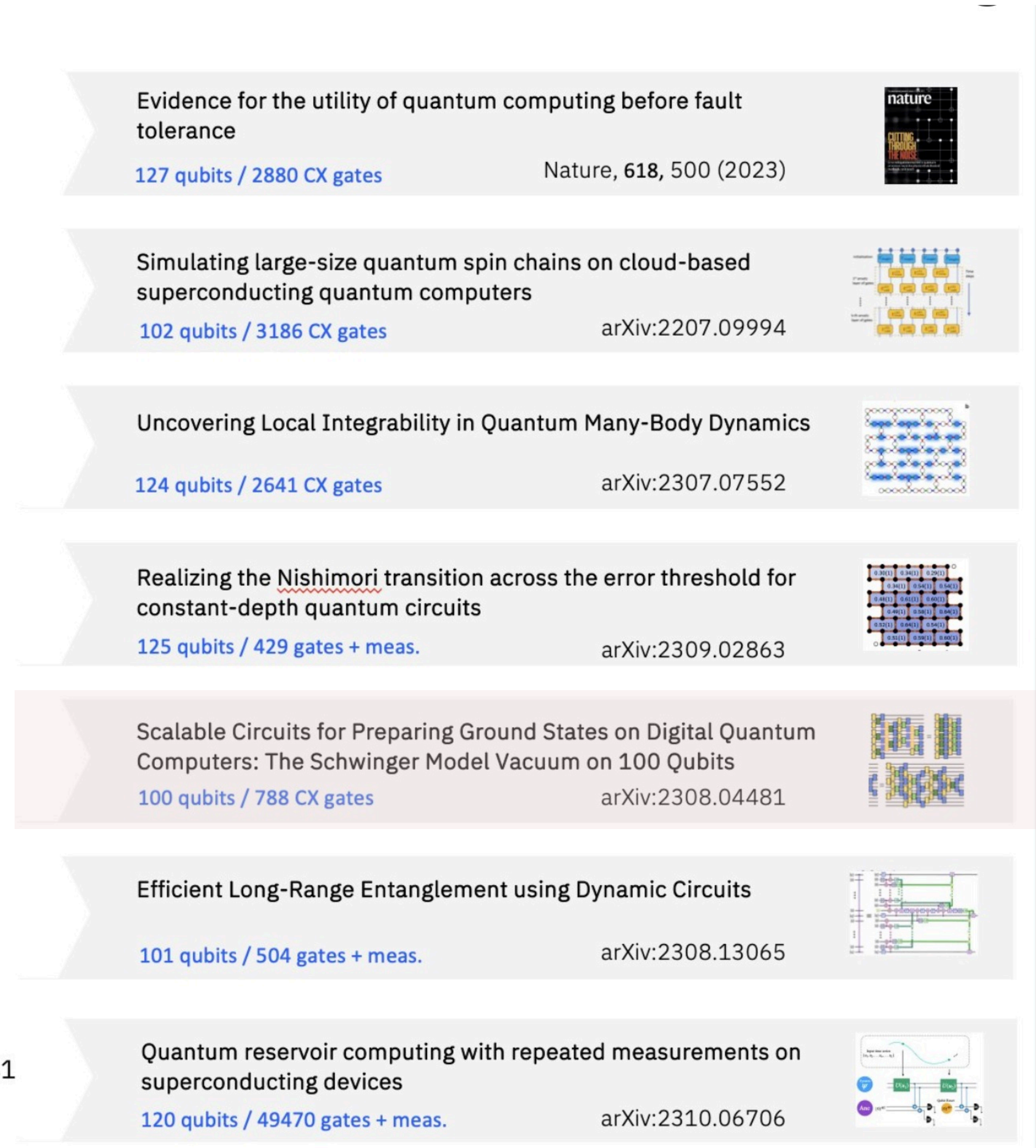
IBM Defines the *The Utility Scale*

December 2023, IBM Summit

With quantum systems composed of 100+ qubits, researchers are beginning to explore algorithms and applications at scales beyond brute-force classical computation using IBM Quantum systems.



IBM Quantum



Evidence for the utility of quantum computing before fault tolerance
127 qubits / 2880 CX gates
Nature, **618**, 500 (2023)

Simulating large-size quantum spin chains on cloud-based superconducting quantum computers
102 qubits / 3186 CX gates
arXiv:2207.09994

Uncovering Local Integrability in Quantum Many-Body Dynamics
124 qubits / 2641 CX gates
arXiv:2307.07552

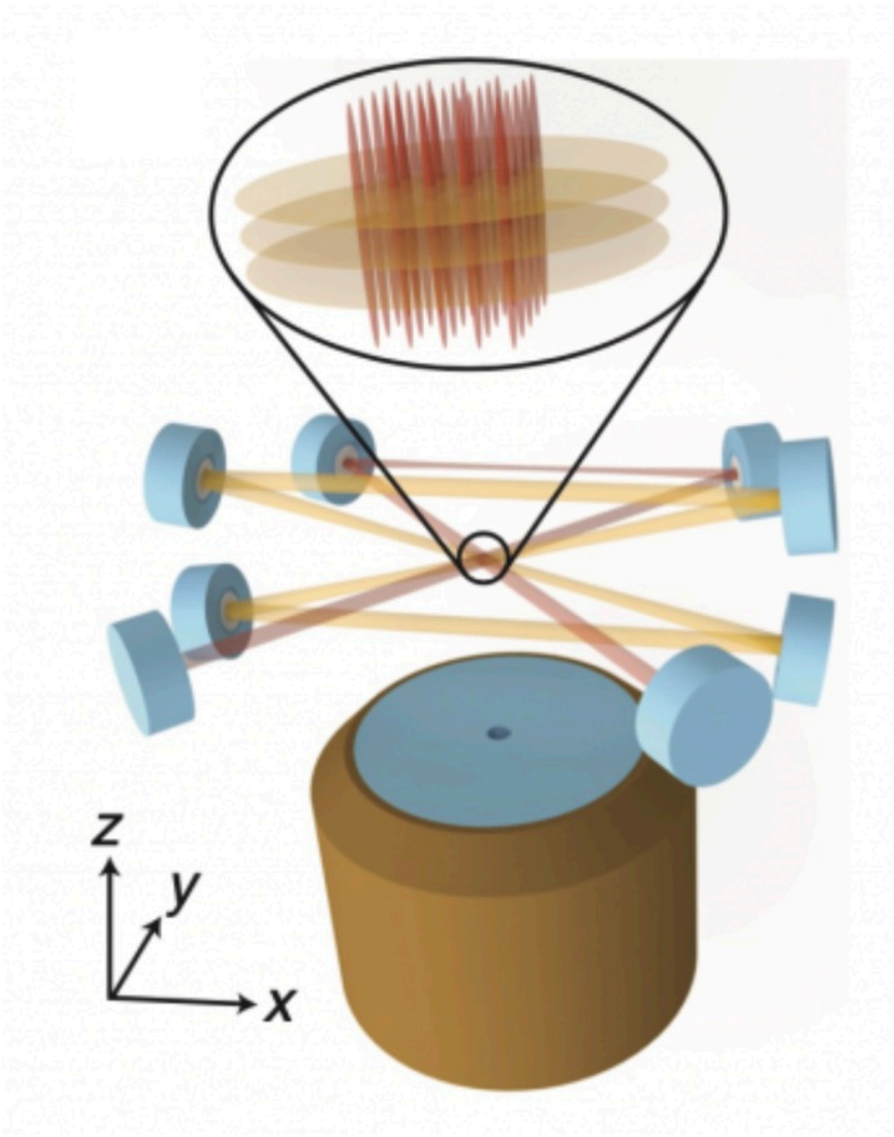
Realizing the Nishimori transition across the error threshold for constant-depth quantum circuits
125 qubits / 429 gates + meas.
arXiv:2309.02863

Scalable Circuits for Preparing Ground States on Digital Quantum Computers: The Schwinger Model Vacuum on 100 Qubits
100 qubits / 788 CX gates
arXiv:2308.04481

Efficient Long-Range Entanglement using Dynamic Circuits
101 qubits / 504 gates + meas.
arXiv:2308.13065

Quantum reservoir computing with repeated measurements on superconducting devices
120 qubits / 49470 gates + meas.
arXiv:2310.06706

Select Recent Advances in Quantum Computing



Cold-Atom arrays with Optical Tweezers

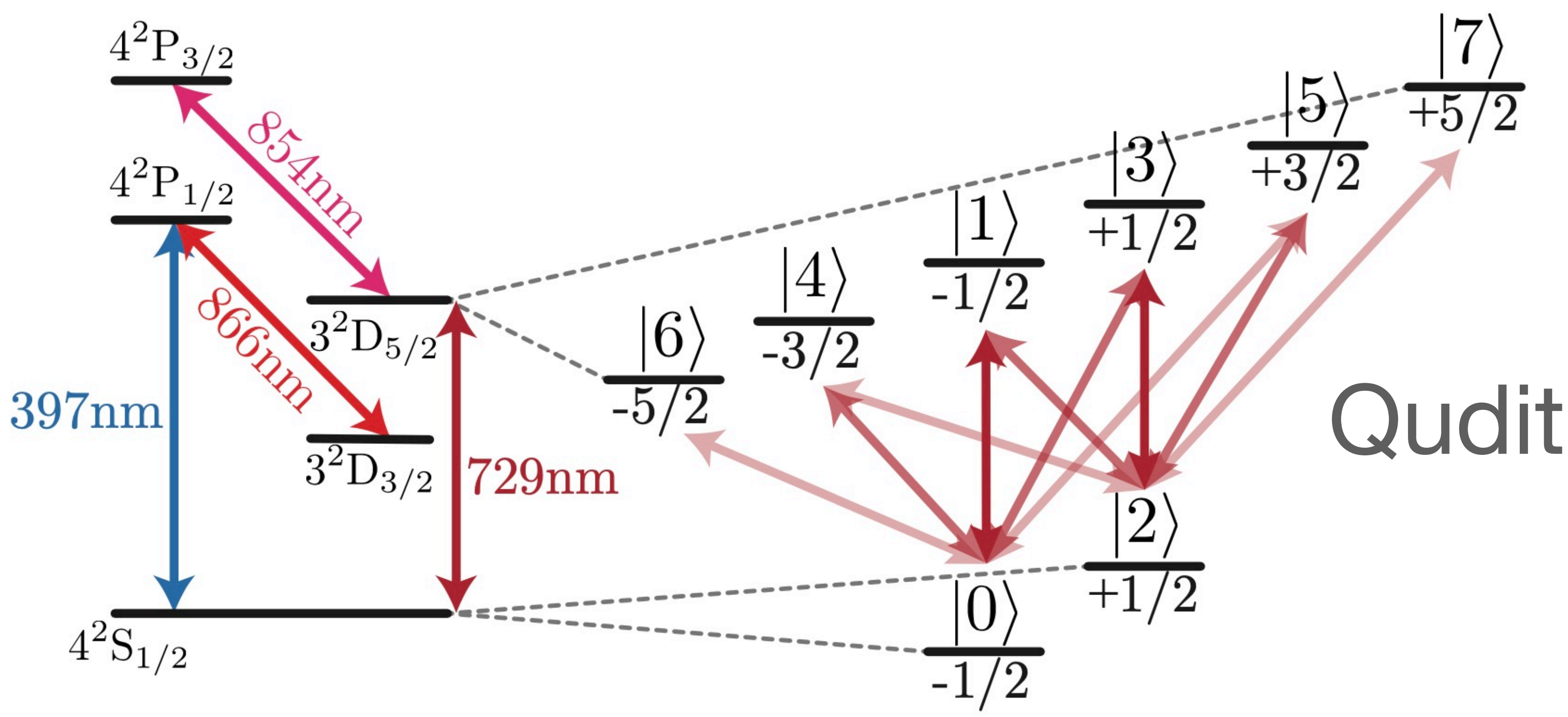
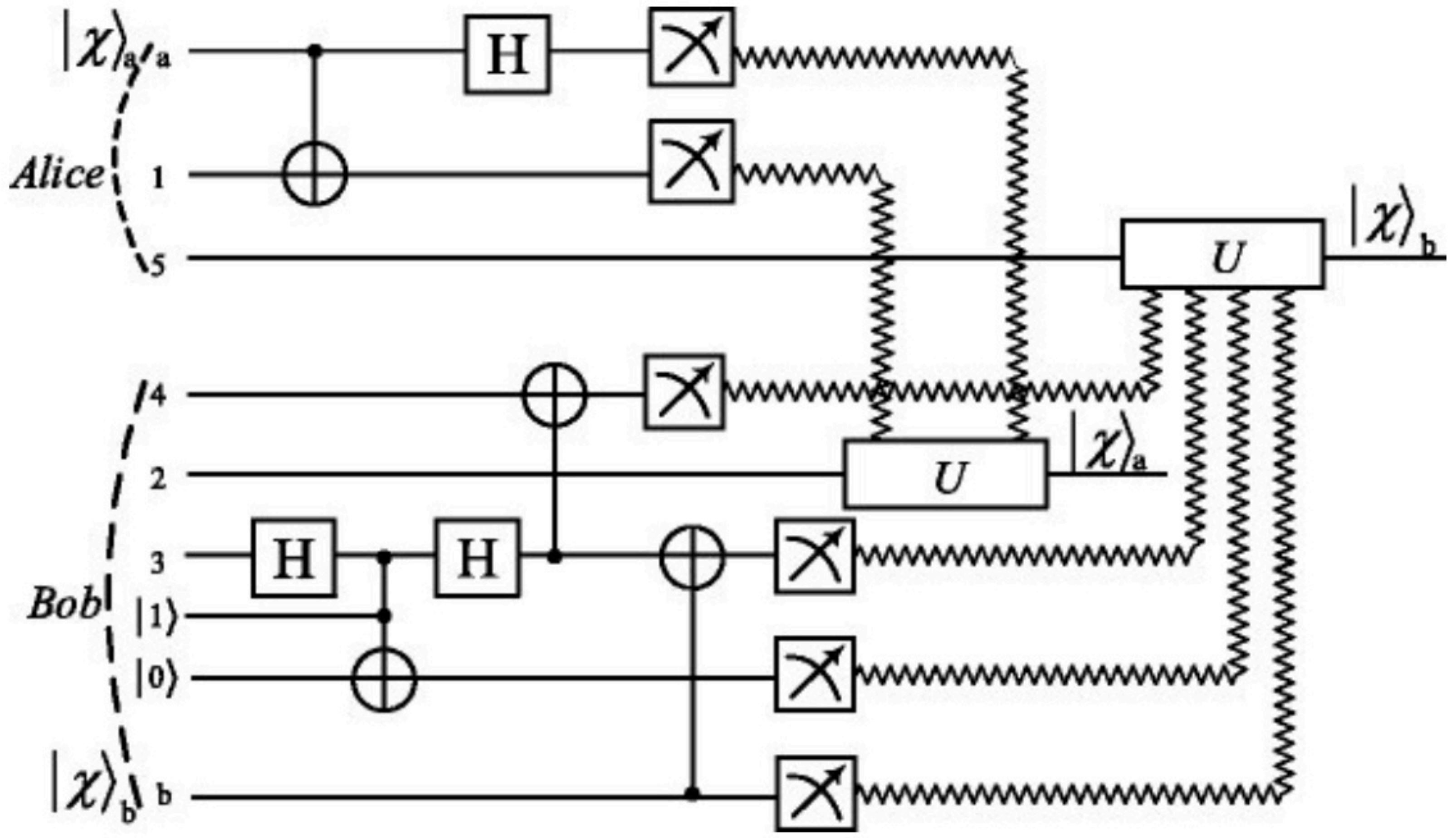


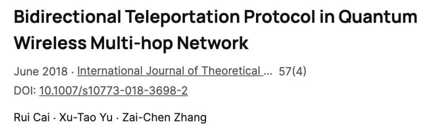
FIG. 1. **Level scheme of the ^{40}Ca$^+$ ion.**

Qudits with trapped ions

4 Logical Qubits
32-qubit H2-1 trapped ions
(Quantinuum-Microsoft)



Mid-circuit measurements



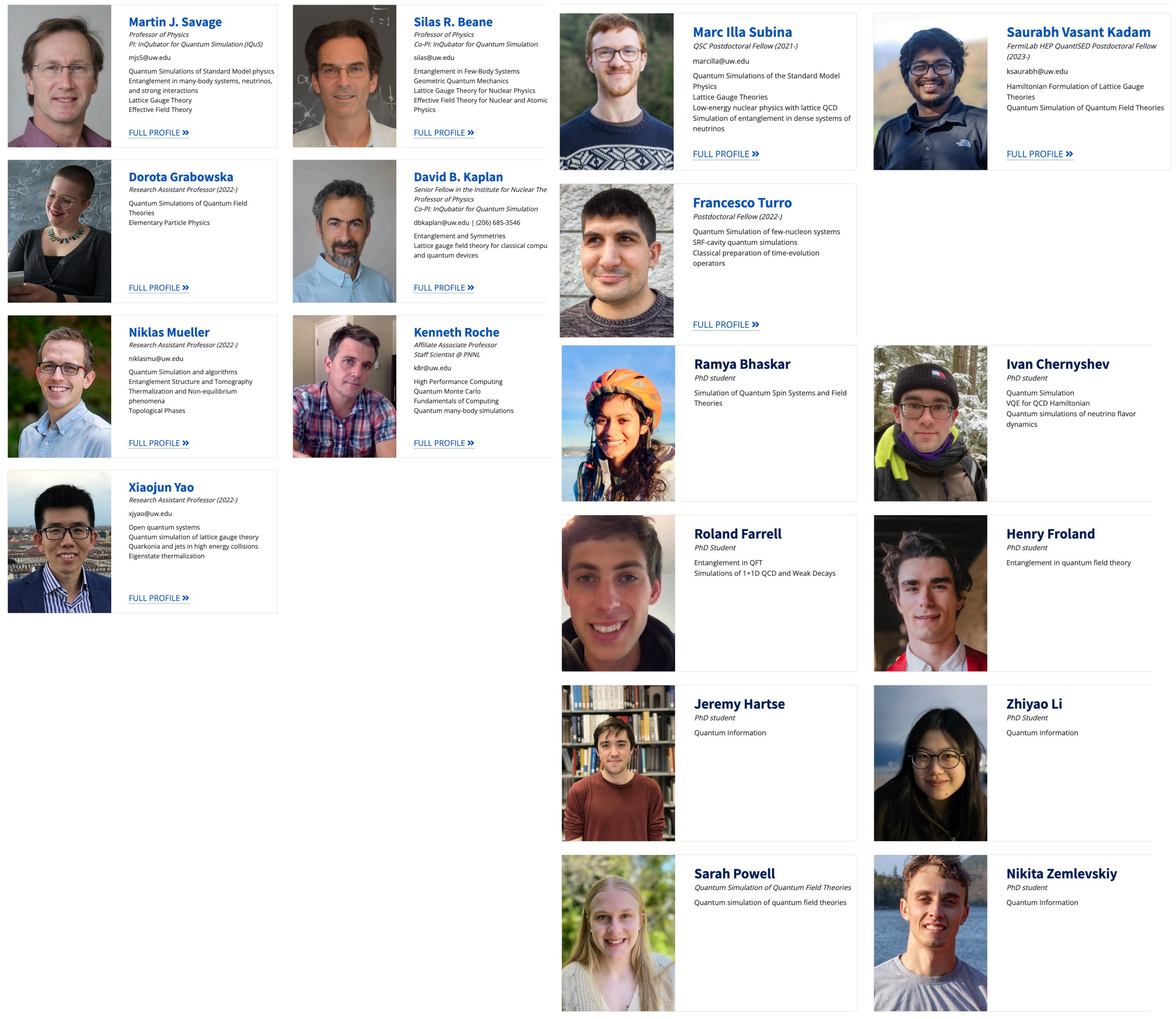
Bidirectional Teleportation Protocol in Quantum Wireless Multi-hop Network

June 2018 · International Journal of Theoretical ... 57(4)
DOI: 10.1007/s10773-018-3698-2

Rui Cai · Xu-Tao Yu · Zai-Chen Zhang

IQuS InQubator for Quantum Simulation

Workshops
Research
Visitors



Martin J. Savage
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PI: InQubator for Quantum Simulation (IQuS)
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Quantum Simulations of Standard Model physics
Entanglement in many-body systems, neutrinos, and strong interactions
Lattice Gauge Theory
Effective Field Theory
FULL PROFILE »

Dorota Grabowska
Research Assistant Professor (2022-)
Quantum Simulations of Quantum Field Theories
Elementary Particle Physics
FULL PROFILE »

Niklas Mueller
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Quantum Simulation and algorithms
Entanglement Structure and Tomography
Thermalization and Non-equilibrium phenomena
Topological Phases
FULL PROFILE »

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Open quantum systems
Quantum simulation of lattice gauge theory
Quarkonia and jets in high energy collisions
Eigenstate thermalization
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Entanglement in Few-Body Systems
Geometric Quantum Mechanics
Lattice Gauge Theory for Nuclear Physics
Effective Field Theory for Nuclear and Atomic Physics
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Lattice gauge field theory for classical compu
and quantum devices
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Quantum Monte Carlo
Fundamentals of Computing
Quantum many-body simulations
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Quantum Simulations of the Standard Model Physics
Lattice Gauge Theories
Low-energy nuclear physics with lattice QCD
Simulation of entanglement in dense systems of neutrinos
FULL PROFILE »

Francesco Turro
Postdoctoral Fellow (2022-)
Quantum Simulation of few-nucleon systems
SRF-cavity quantum simulations
Classical preparation of time-evolution operators
FULL PROFILE »

Ramya Bhaskar
PhD student
Simulation of Quantum Spin Systems and Field Theories

Roland Farrell
PhD Student
Entanglement in QFT
Simulations of 1+1D QCD and Weak Decays

Jeremy Hartse
PhD student
Quantum Information

Sarah Powell
Quantum Simulation of Quantum Field Theories
Quantum simulation of quantum field theories

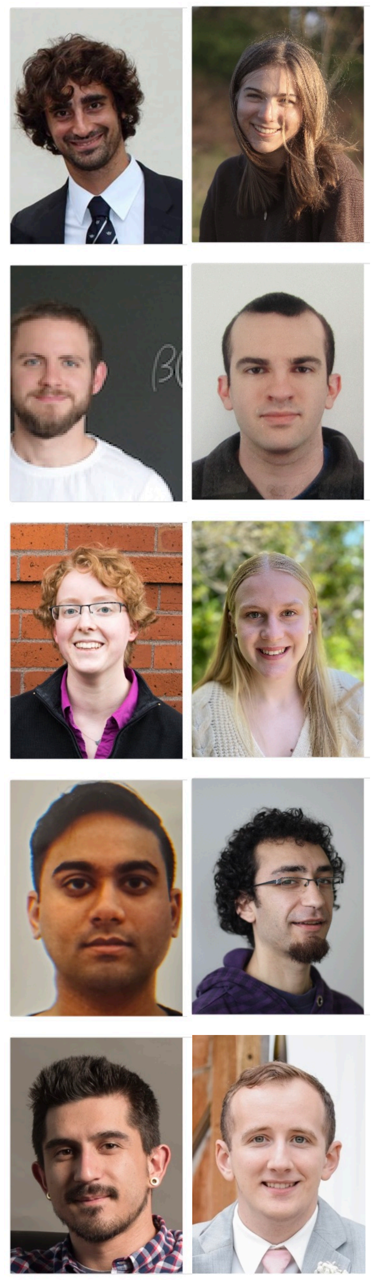
Saurabh Vasant Kadam
FermiLab HEP QuantISED Postdoctoral Fellow (2023-)
ksaurabh@uw.edu
Hamiltonian Formulation of Lattice Gauge Theories
Quantum Simulation of Quantum Field Theories
FULL PROFILE »

Ivan Chernyshev
PhD student
Quantum Simulation
VQE for QCD Hamiltonian
Quantum simulations of neutrino flavor dynamics

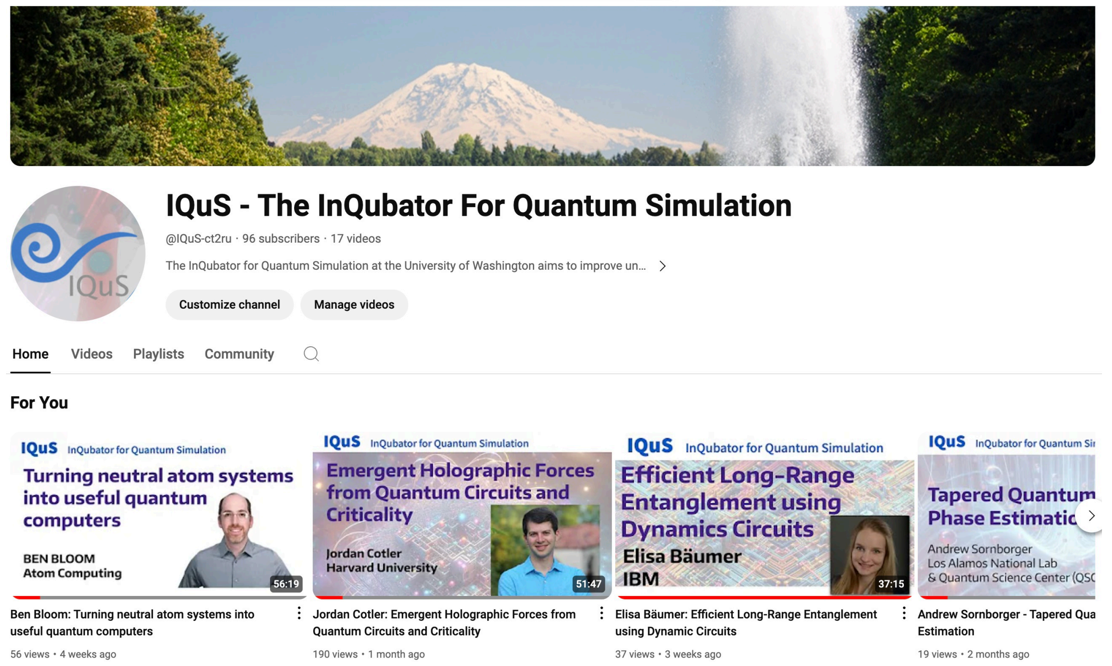
Henry Froland
PhD student
Entanglement in quantum field theory

Zhiyao Li
PhD Student
Quantum Information

Nikita Zemlevskiy
PhD student
Quantum Information



TO ACCELERATE PROGRESS AT THE INTERFACE OF QUANTUM INFORMATION AND NUCLEAR PHYSICS



IQuS - The InQubator For Quantum Simulation
@IQuS-ct2ru · 96 subscribers · 17 videos
The InQubator for Quantum Simulation at the University of Washington aims to improve un...

For You

IQuS InQubator for Quantum Simulation
Turning neutral atom systems into useful quantum computers
BEN BLOOM
Atom Computing
56:19
Ben Bloom: Turning neutral atom systems into useful quantum computers
56 views • 4 weeks ago

IQuS InQubator for Quantum Simulation
Emergent Holographic Forces from Quantum Circuits and Criticality
Jordan Cotler
Harvard University
51:47
Jordan Cotler: Emergent Holographic Forces from Quantum Circuits and Criticality
190 views • 1 month ago

IQuS InQubator for Quantum Simulation
Efficient Long-Range Entanglement using Dynamics Circuits
Elisa Bäumer
IBM
37:15
Elisa Bäumer: Efficient Long-Range Entanglement using Dynamic Circuits
37 views • 3 weeks ago

IQuS InQubator for Quantum Si
Tapered Quantum
Phase Estimatio
Andrew Sornborger
Los Alamos National Lab
& Quantum Science Center (QSC
Andrew Sornborger - Tapered Qua
Estimation
19 views • 2 months ago

DOE OFFICE OF NUCLEAR PHYSICS

UW DEPARTMENT OF PHYSICS

W
DEPARTMENT OF PHYSICS

UW COLLEGE OF ARTS & SCIENCES

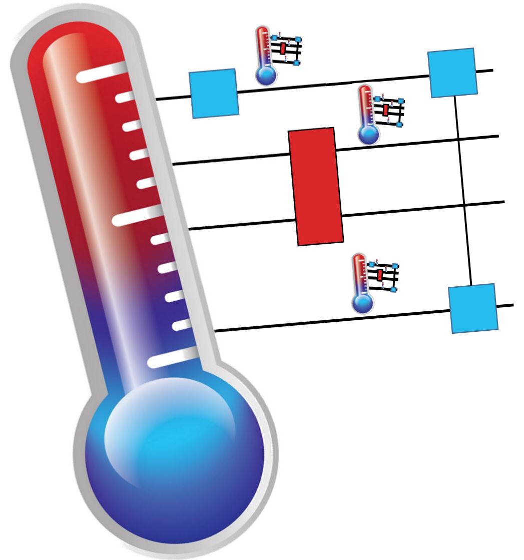
W
ARTS & SCIENCES

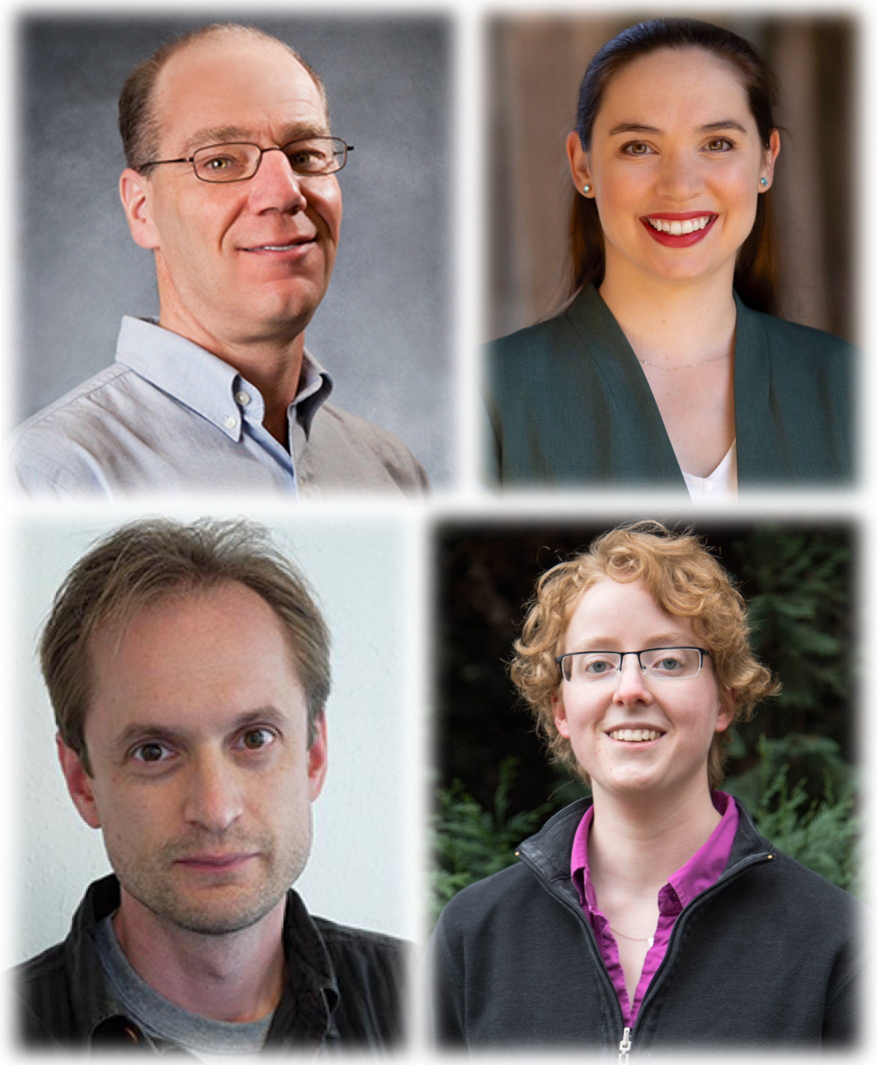
INSTITUTE for NUCLEAR THEORY

Workshops

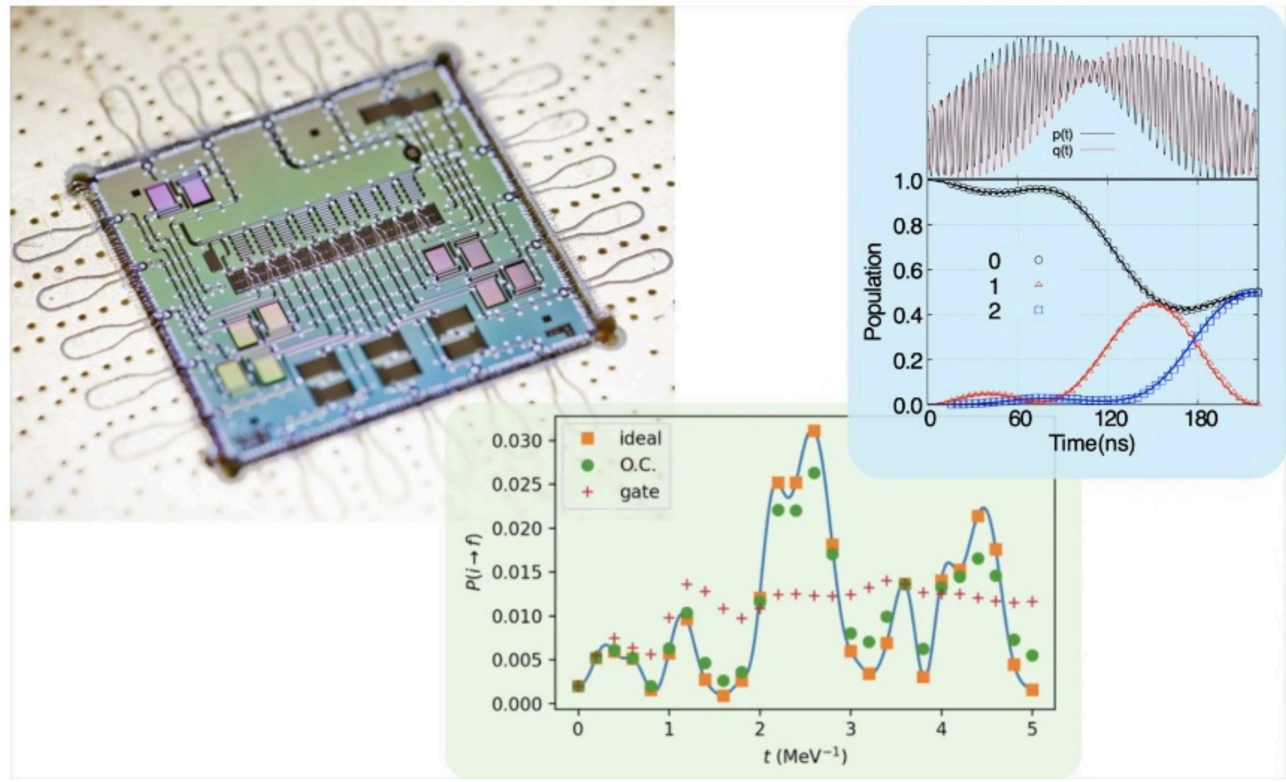
At the Interface of Quantum Sensors and Quantum Simulations (22-3b)

Organizers: Doug Beck (UIUC), Natalie Klco (Caltech), Crystal Noel (UMD) and Joel Ullom (NIST)

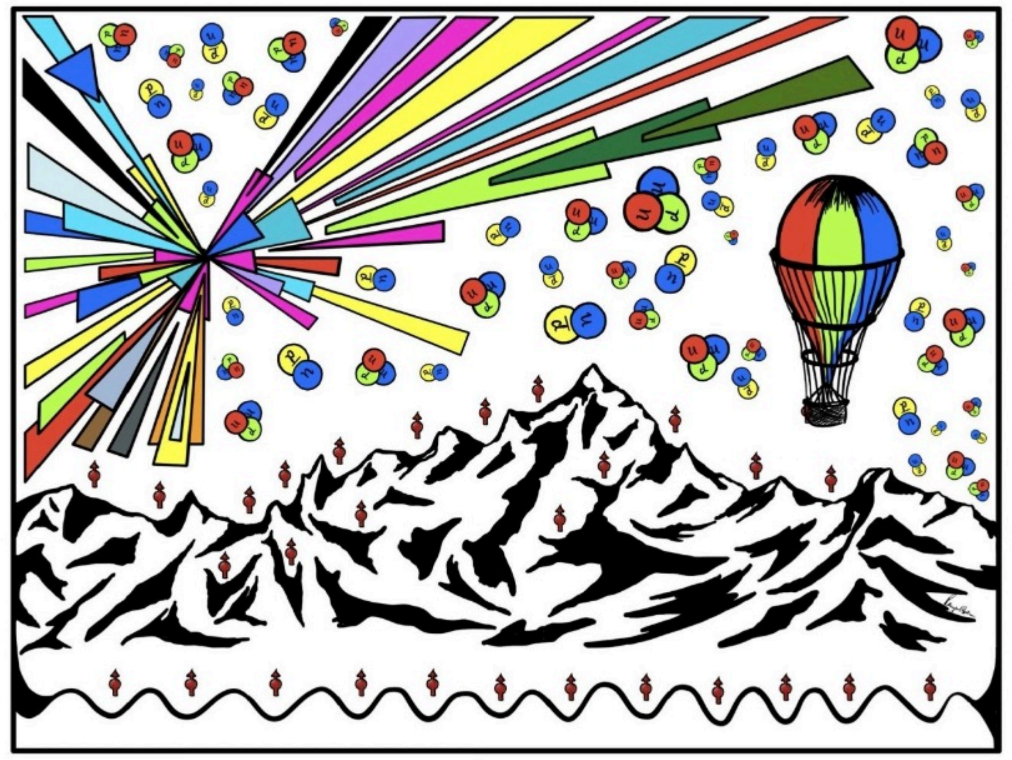




Pulses, Qudits and Quantum Simulations



Thermalization, from Cold Atoms to Hot Quantum Chromodynamics

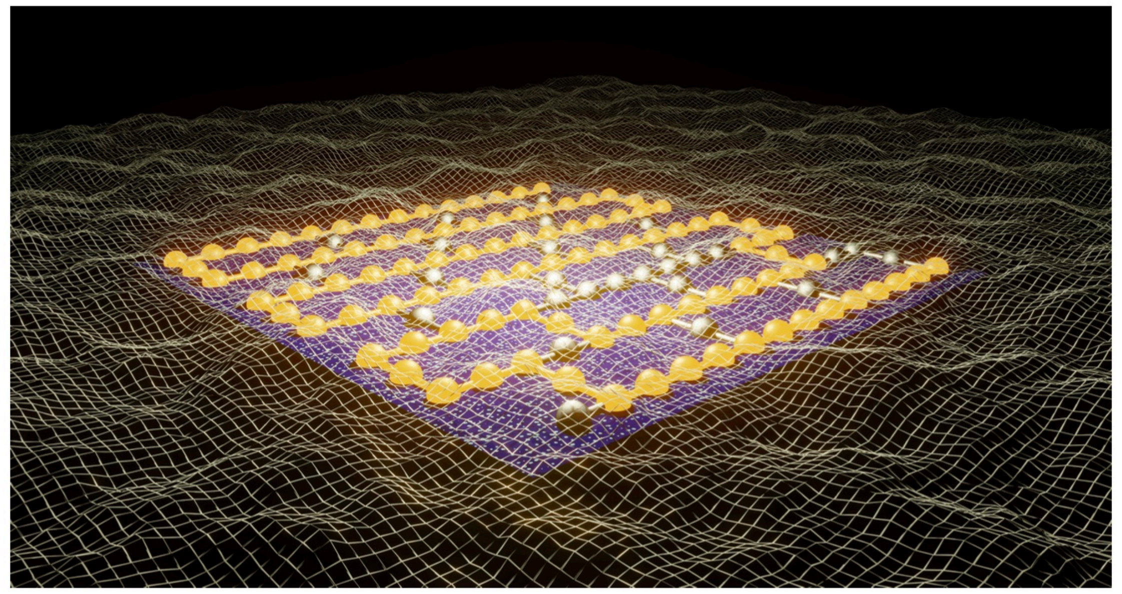


IQuS - Research Directions

Access to Quantum Computers through OLCF+QSC essential

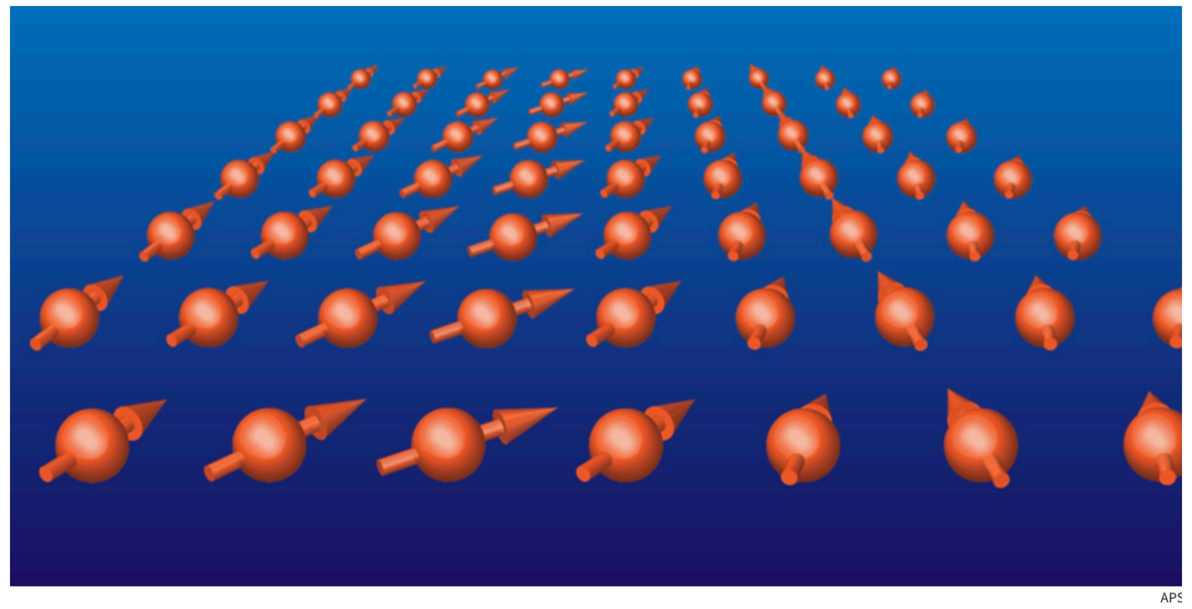
Access to HPC through NERSC+DOE+OSG+AWS+UW essential

Generally, software relies on Technology company stacks, plus NP ``on top''



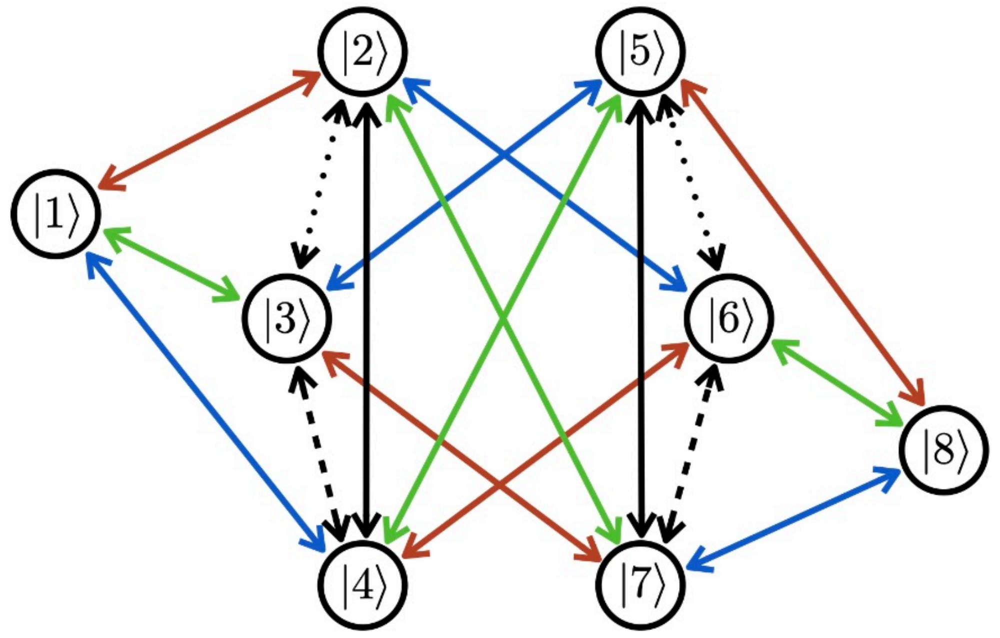
Lattice Gauge Theories

IBM+Quantinuum (OLCF)



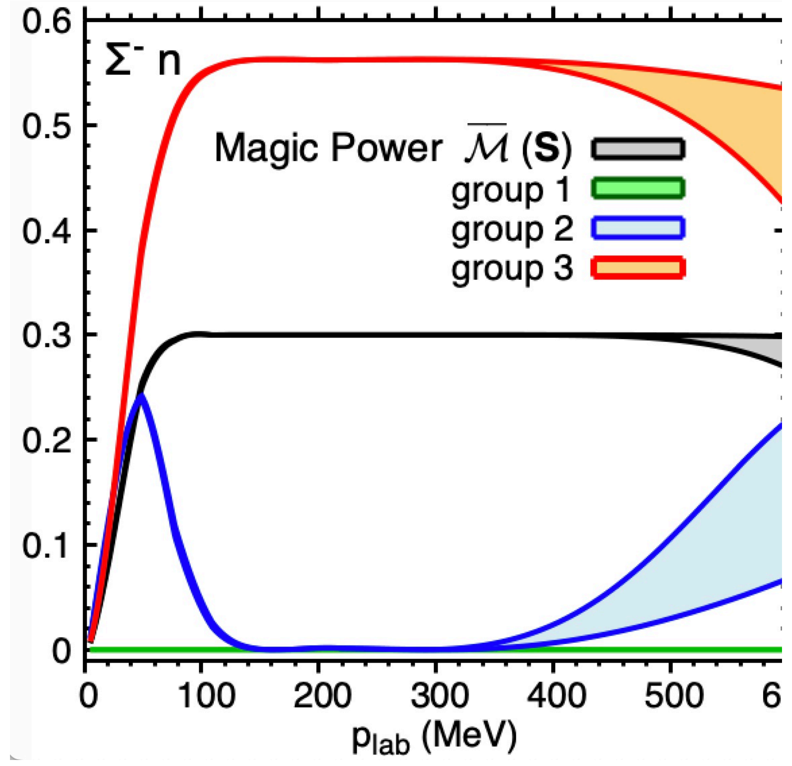
Spin Systems, Cold Atoms

[AWS - Quera]

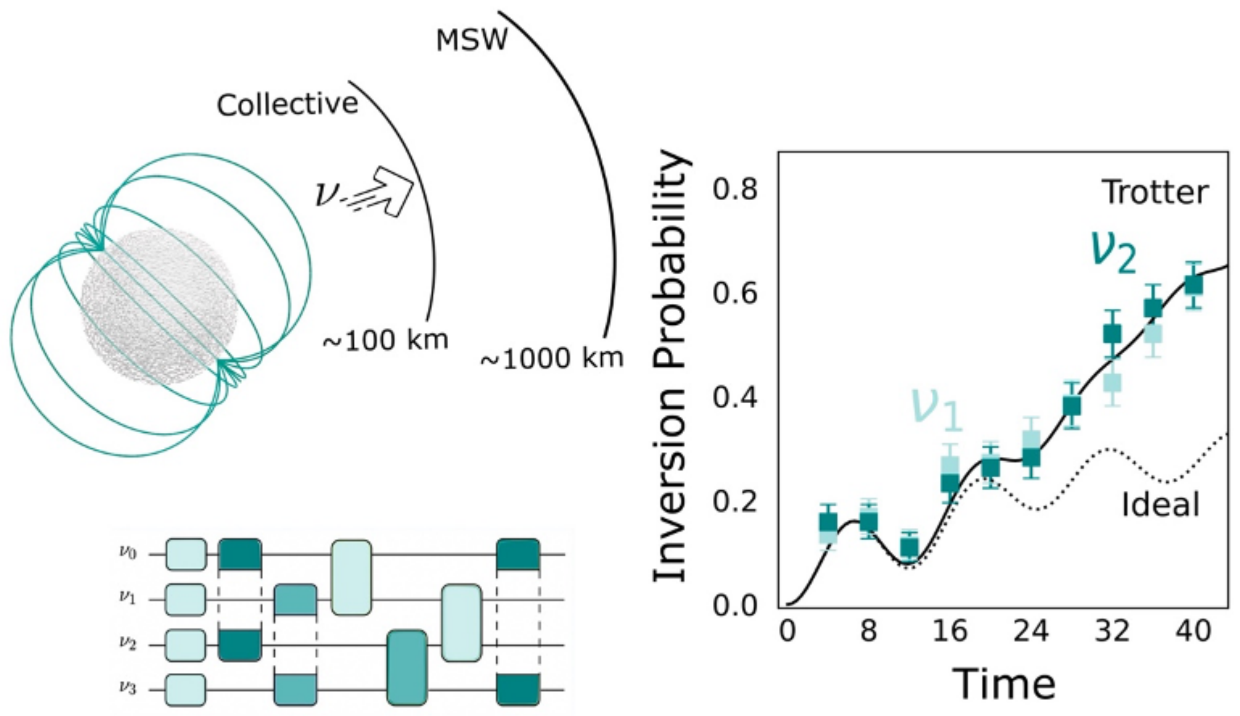


Qudits for NP

Hardware development

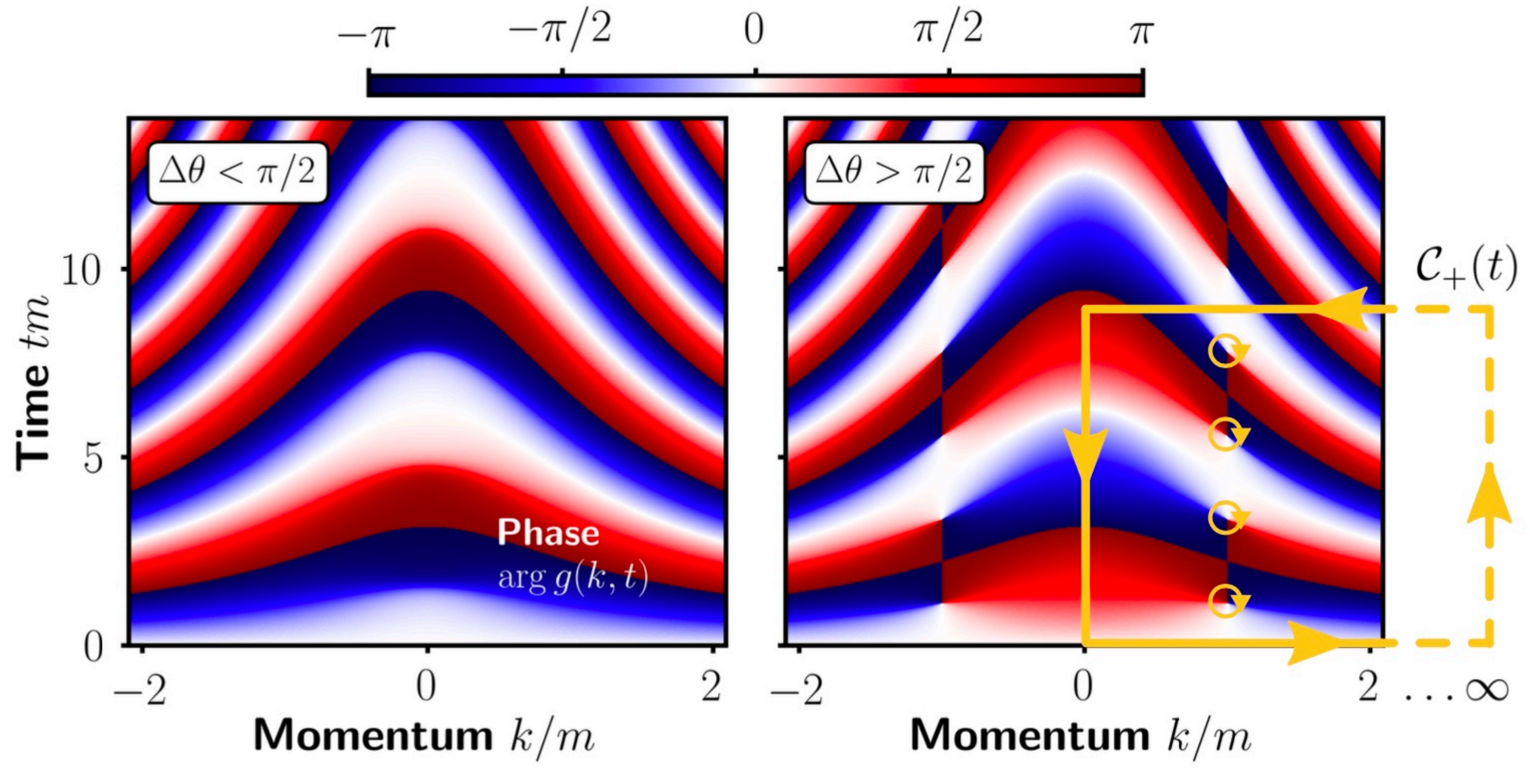


Complexity

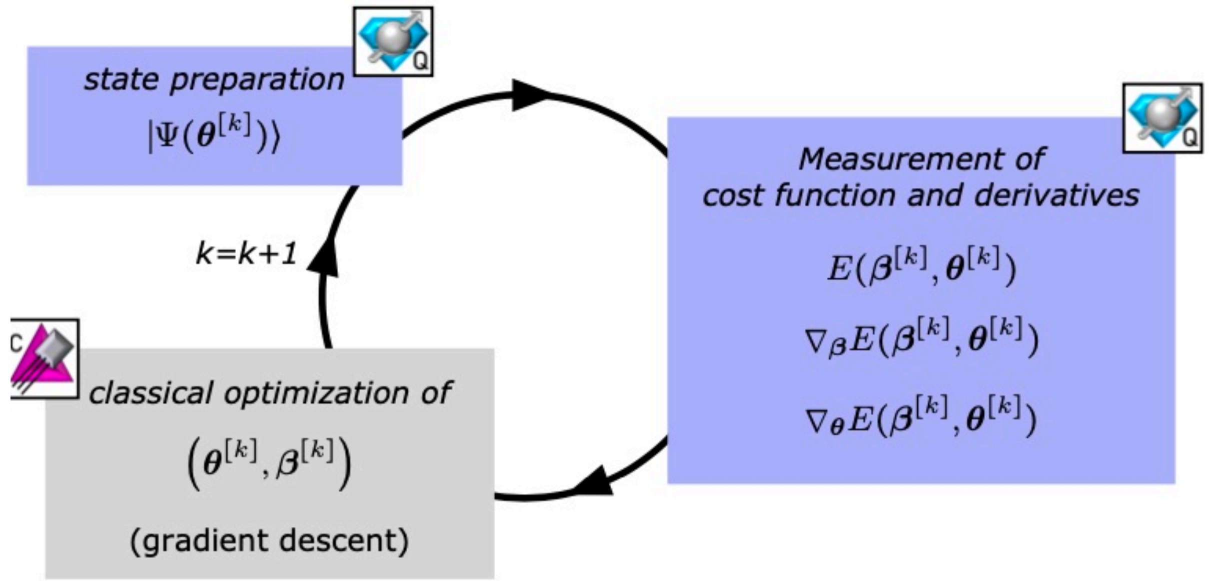


Neutrinos

(QSC+OLCF)



Topological Phases and dynamics (IonQ+MS)



state preparation $|\Psi(\boldsymbol{\theta}^{[k]})\rangle$

Measurement of cost function and derivatives

$E(\boldsymbol{\beta}^{[k]}, \boldsymbol{\theta}^{[k]})$

$\nabla_{\boldsymbol{\beta}} E(\boldsymbol{\beta}^{[k]}, \boldsymbol{\theta}^{[k]})$

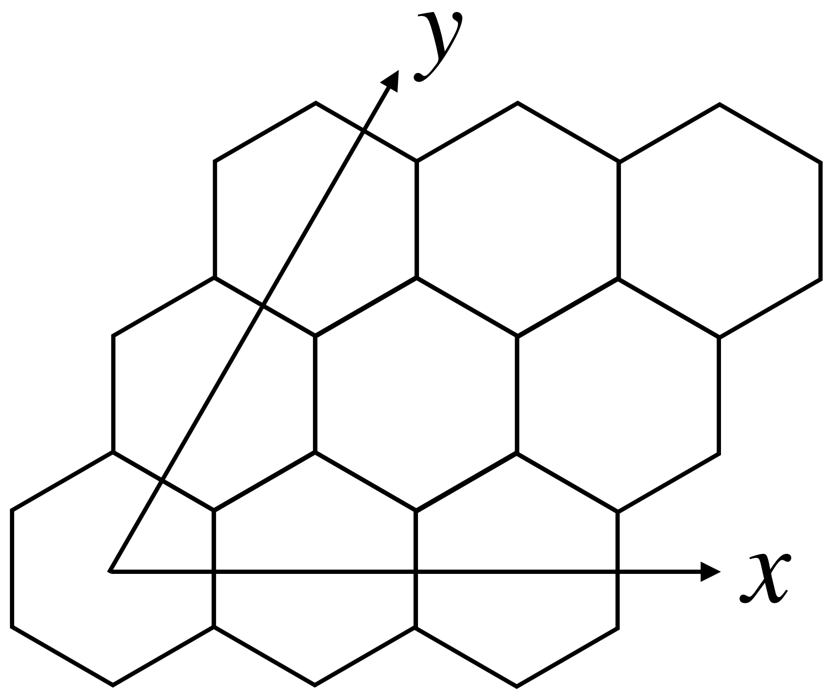
$\nabla_{\boldsymbol{\theta}} E(\boldsymbol{\beta}^{[k]}, \boldsymbol{\theta}^{[k]})$

k=k+1

classical optimization of $(\boldsymbol{\theta}^{[k]}, \boldsymbol{\beta}^{[k]})$

(gradient descent)

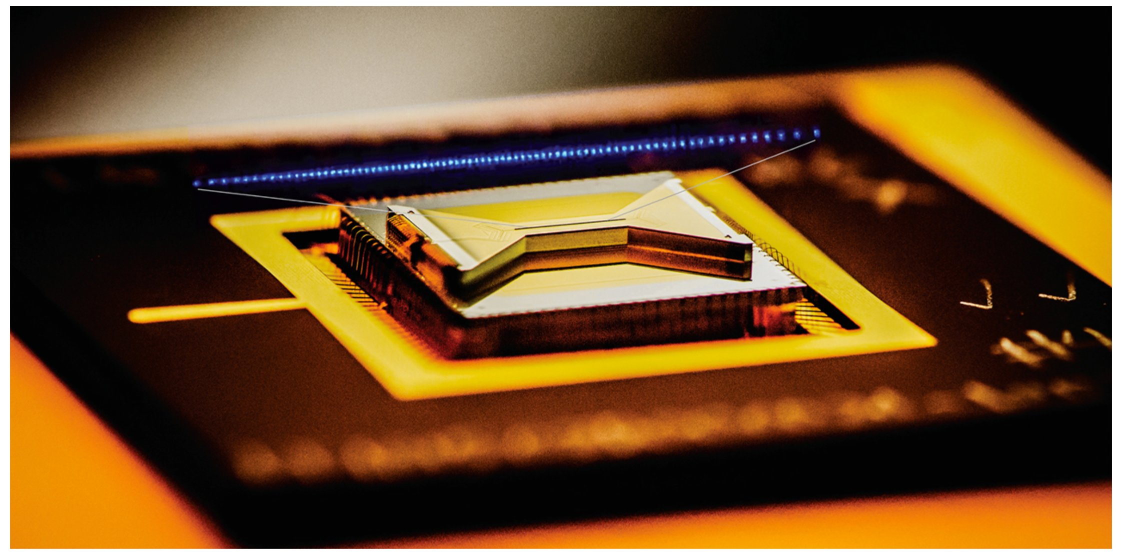
Hamiltonian Learning of EFT (IBM)

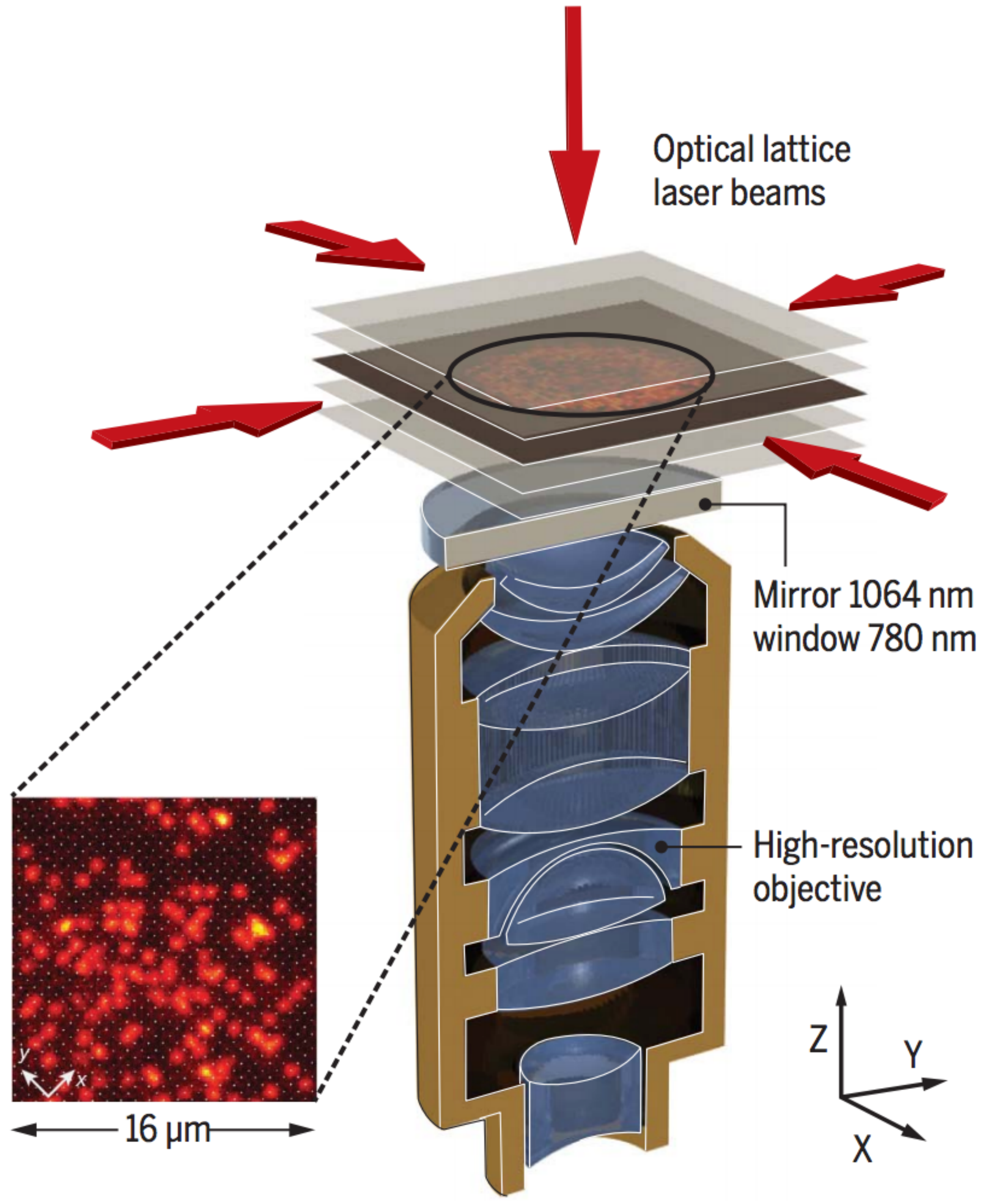


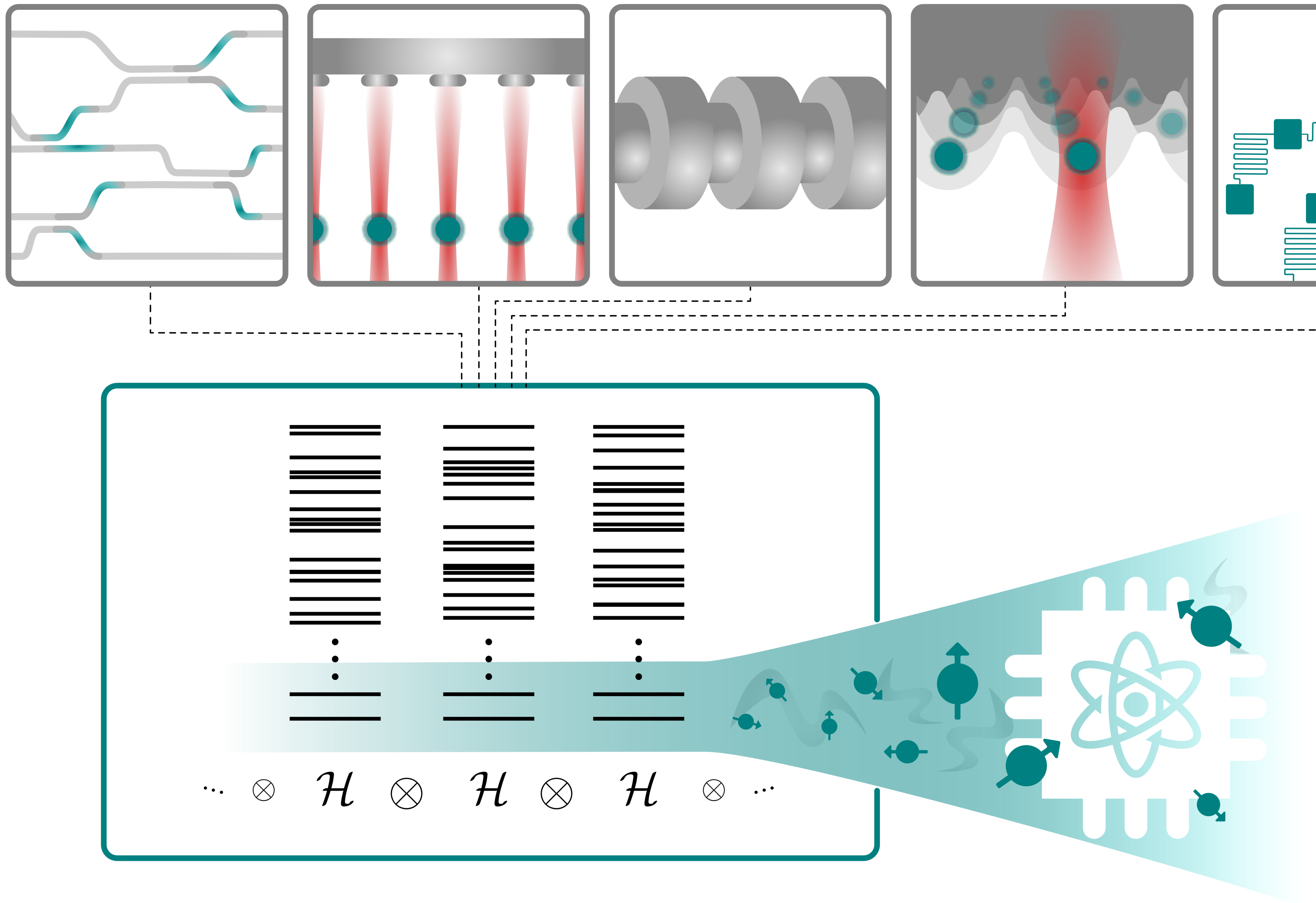
Transport SU(2) LGT

IBM+Quantinuum (OLCF)

Encoding Systems in Multi-Hilbert Space, Hybrid Devices, Embedded in Large-Scale HPC

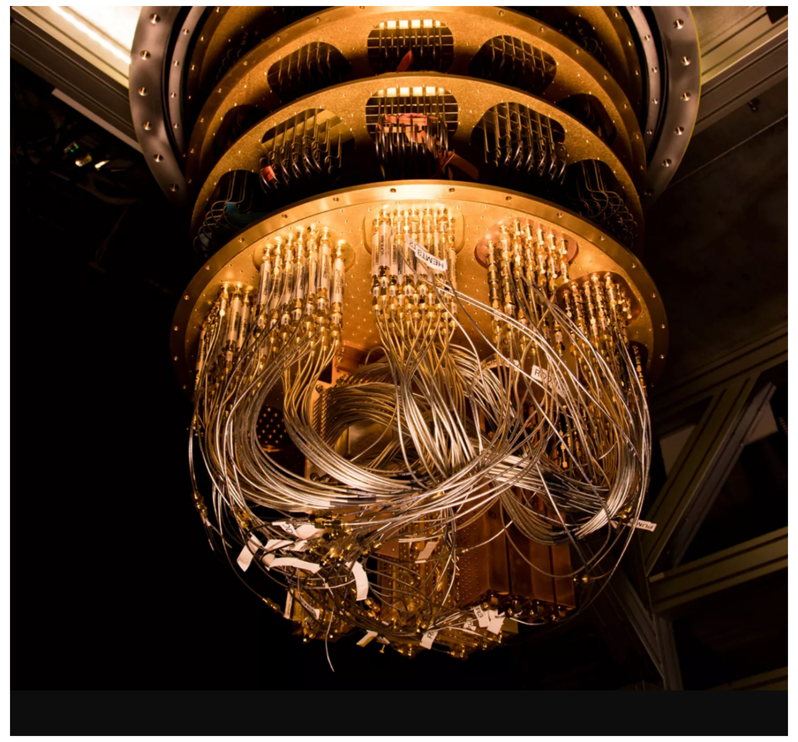


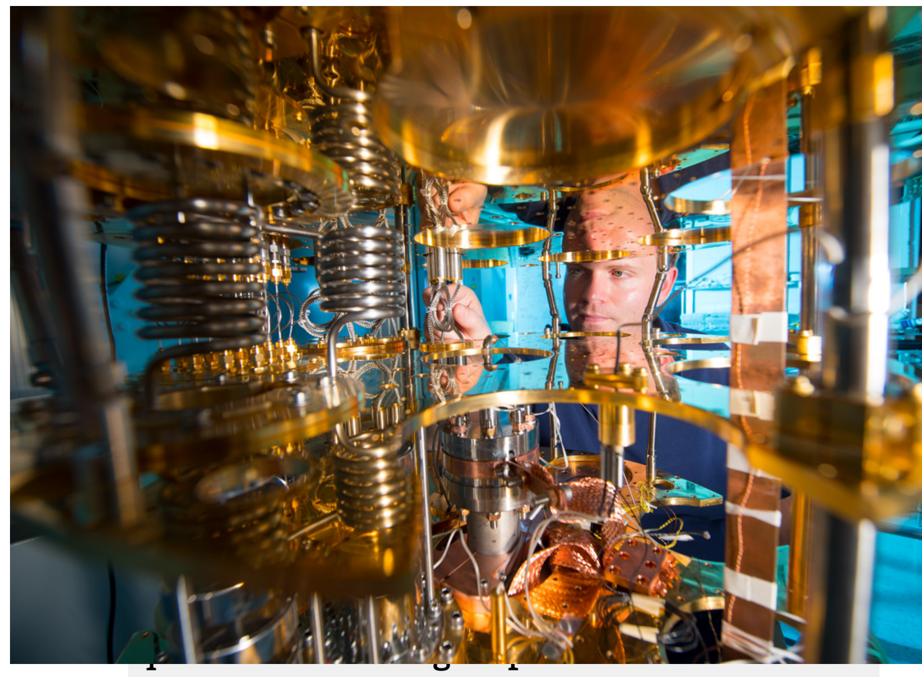


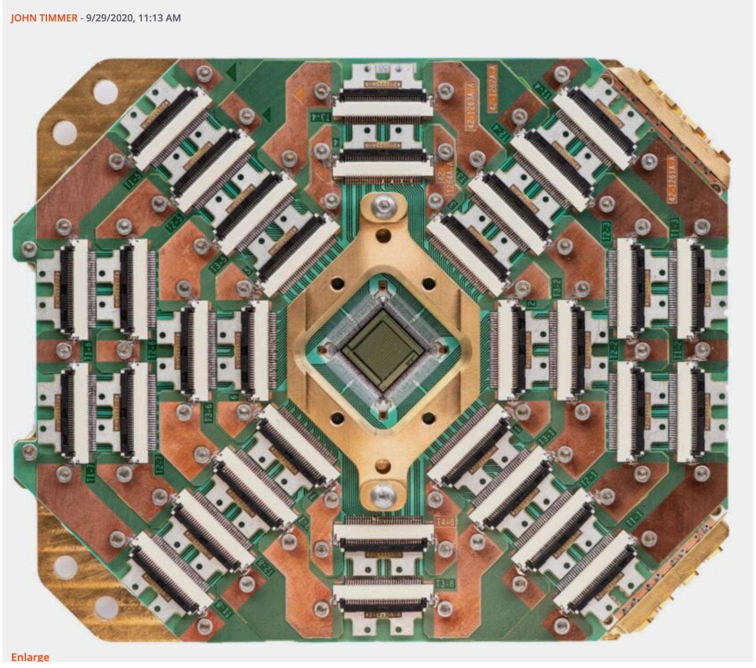


Map scalar, fermion and vector systems

Optimize for target observables - Physics Aware







What's it take to make a chip with over a million Josephson junctions?

JOHN TIMMER - 9/29/2020, 11:13 AM

Enlarge

Human-intensive and HPC-intensive

A Case Study

Scalable Circuits for Preparing Ground States on Digital Quantum Computers: The Schwinger Model Vacuum on 1
Roland C. Farrell, Marc Illa, Anthony N. Ciavarella, Martin J. Savage. e-Print: 2308.04481 [quant-ph]

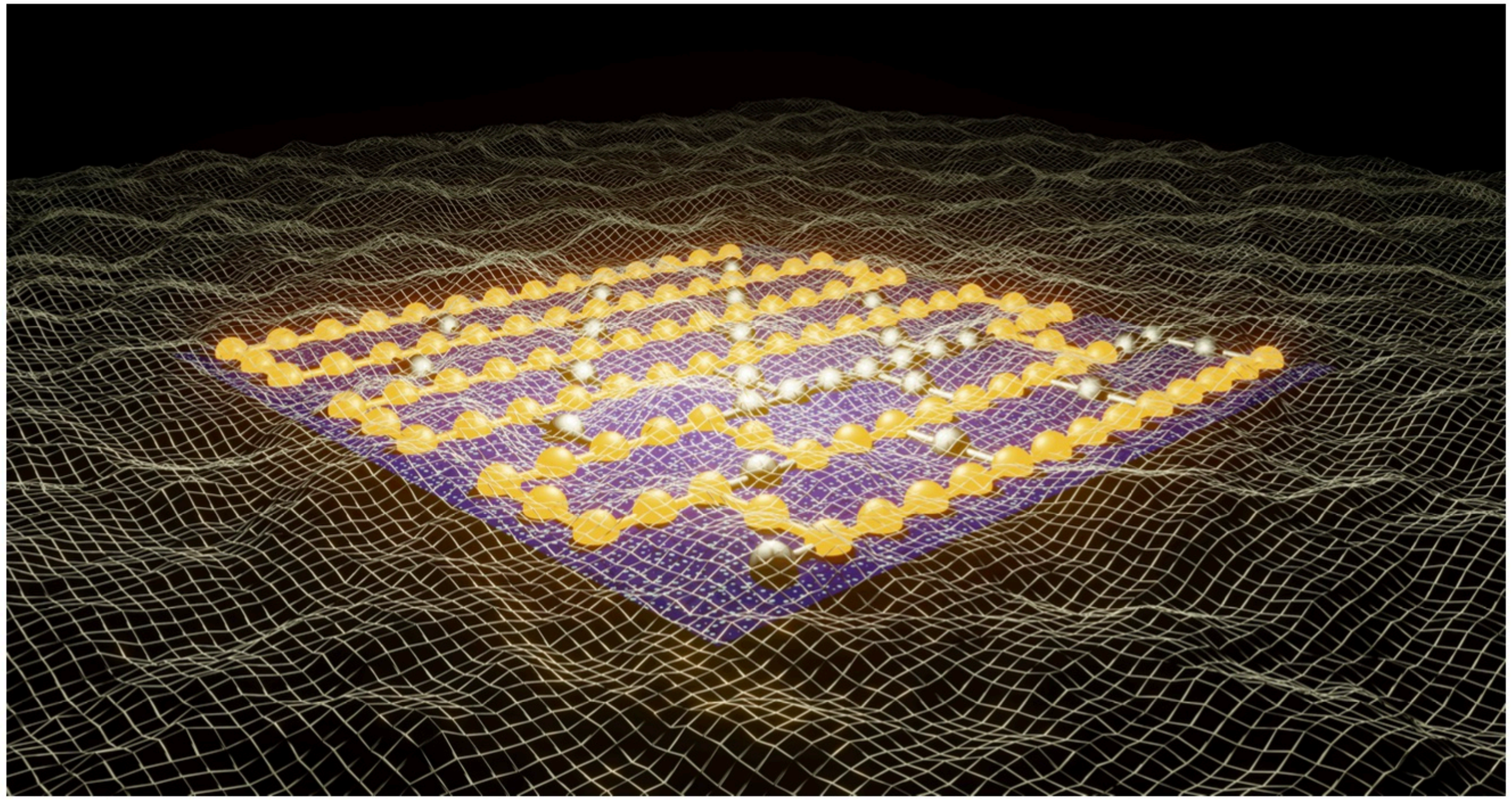
Quantum Simulations of Hadron Dynamics in the Schwinger Model using 112 Qubits
Roland C. Farrell, Marc Illa, Anthony N. Ciavarella, Martin J. Savage. e-Print: 2401.08044 [quant-ph]

IBM, OLCF, QSC, NERSC, OSG, Local

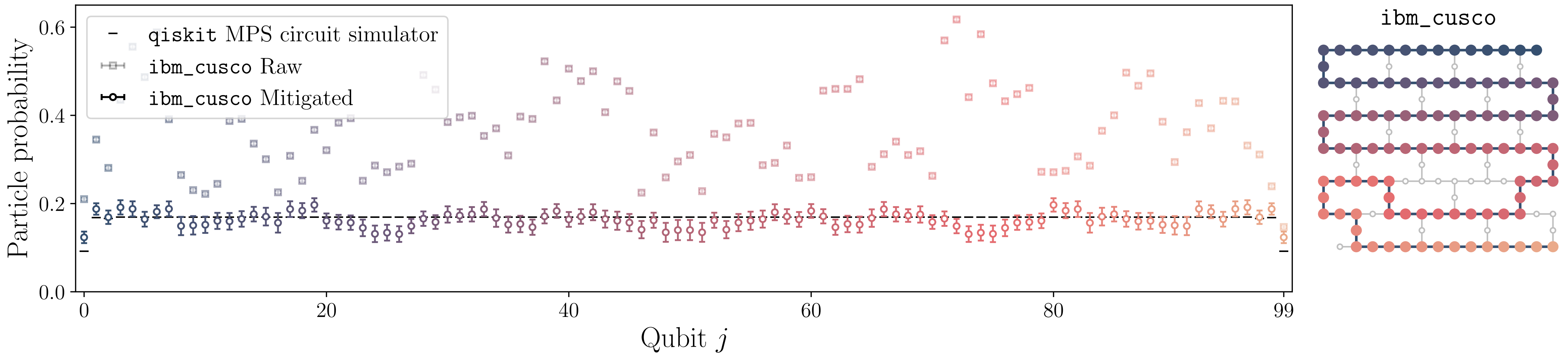
Trotter, Twirling, DD, ODR, SPAM, Transpilation…
qiskit, Mathematica, python, cirq, Julia, …
ADAPT-VQE, strong-coupling, HPC-optimizations

Scalable Quantum Circuits for Confining Theories -

Simulating the Schwinger Model using more than 100 qubits and One Trillion CNOT Gates



Roland Farrell, Marc Illa, Anthony Ciavarella, MJS

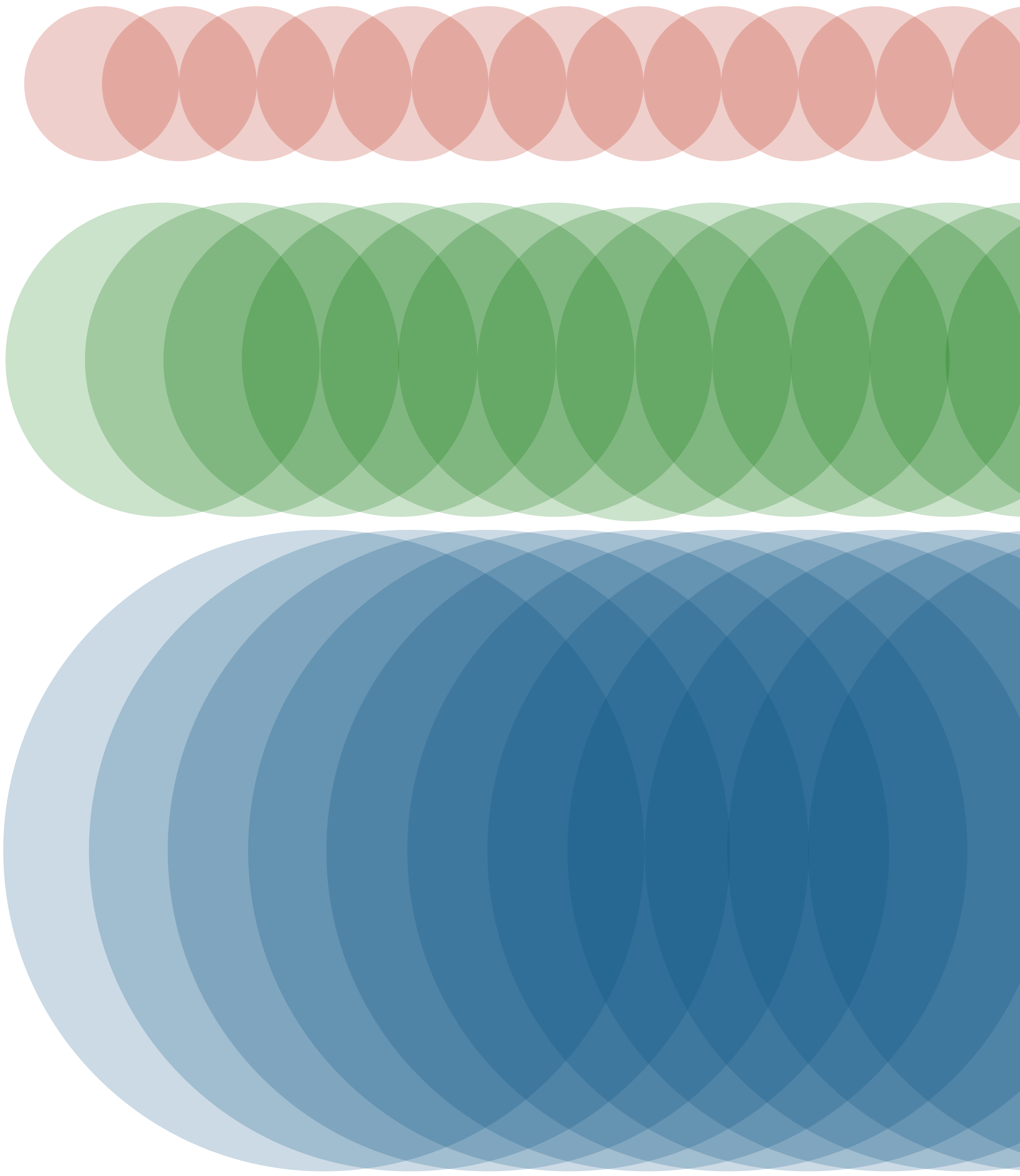


Confinement and Scalable Circuits

Physics Awareness

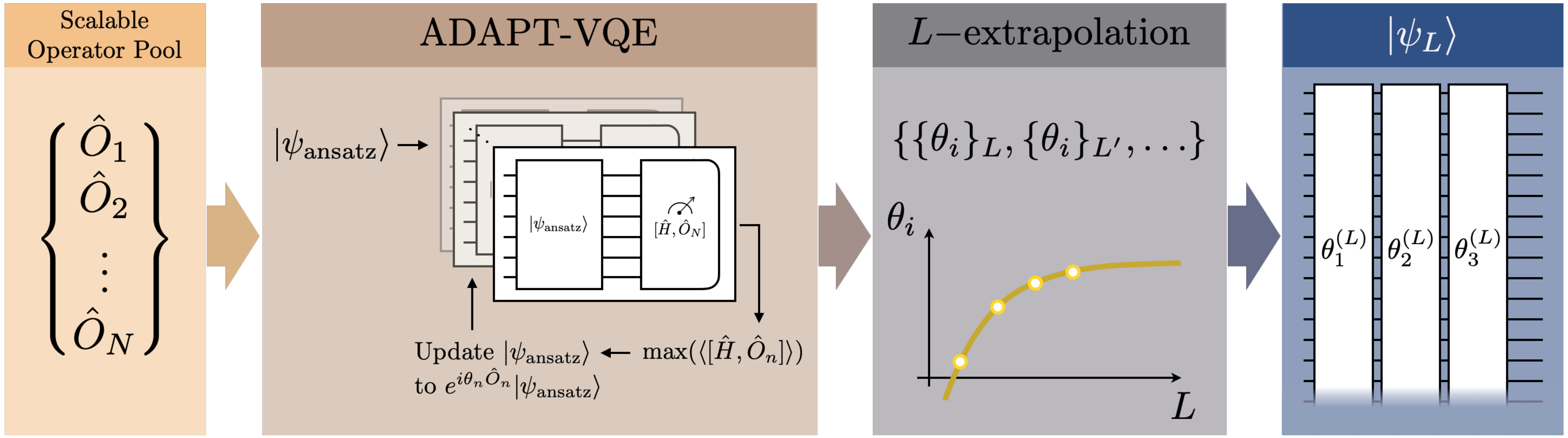
$$\hat{H} = \hat{H}_m + \hat{H}_{kin} + \hat{H}_{el} = \frac{m}{2}\sum_{j=0}^{2L-1}\left[(-1)^j \hat{Z}_j + \hat{I}\right] + \frac{1}{2}\sum_{j=0}^{2L-2}\left(\hat{\sigma}_j^+\hat{\sigma}_{j+1}^- + \text{h.c.}\right) + \frac{g^2}{2}\sum_{j=0}^{2L-2}\left(\sum_{k\leq j}\hat{Q}_k\right)^2$$

Local Nearest Neighbor Non-local



Symmetries and Confinement

Classical Extrapolations



Classical Optimization

Quantum Implementation

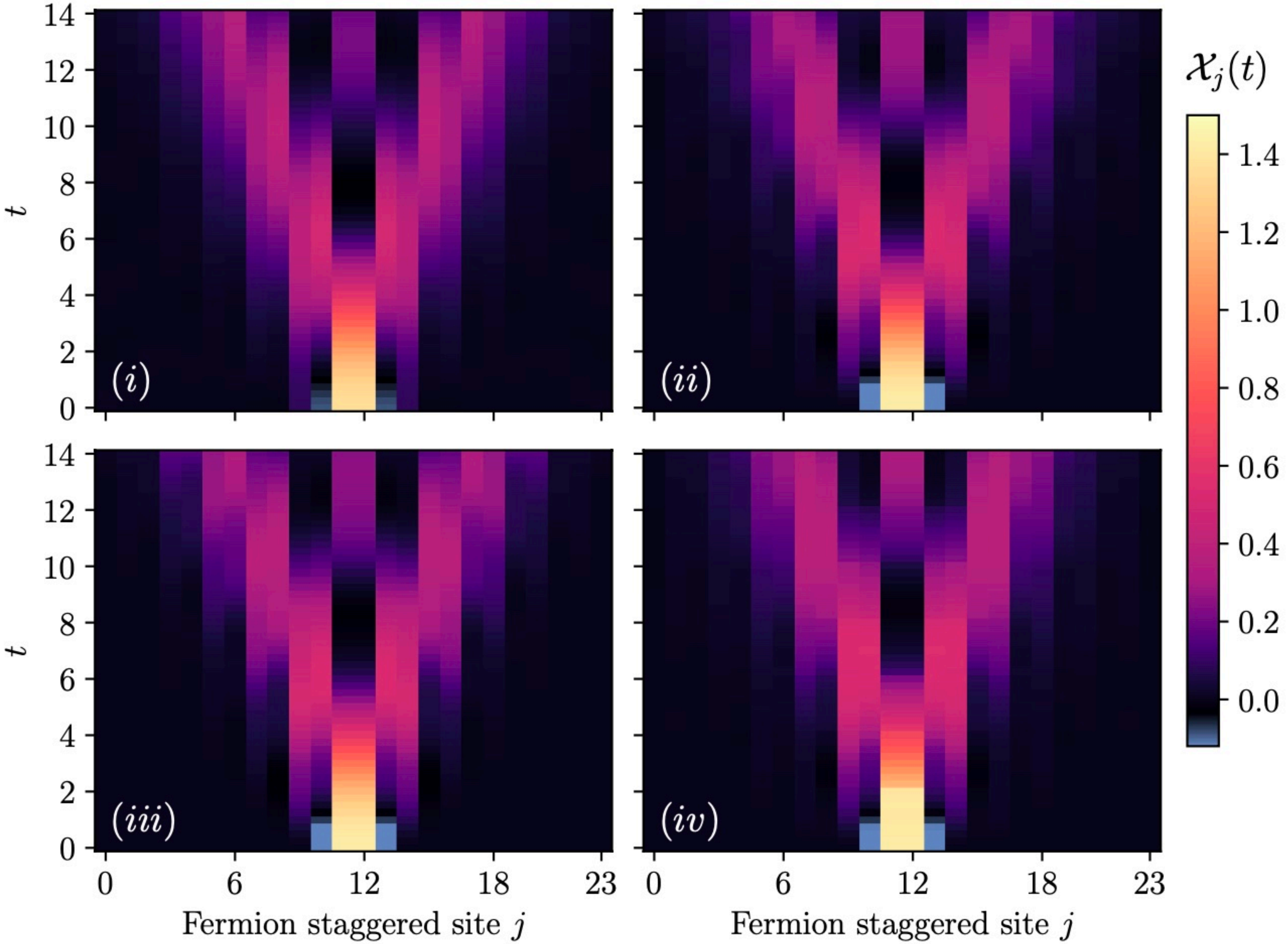
ADAPT-VQE - Sophia Economou et al.

Checking Truncations (HPC)

112 qubits

Exact

2-step SC-Adapt-VQE
Truncated Electric H
Exact evolution



2-step SC-Adapt-VQE
Exact evolution

2-step SC-Adapt-VQE
Truncated Electric H
2nd-order Trotter

Decoherence Renormalization (DR) and Operator DR

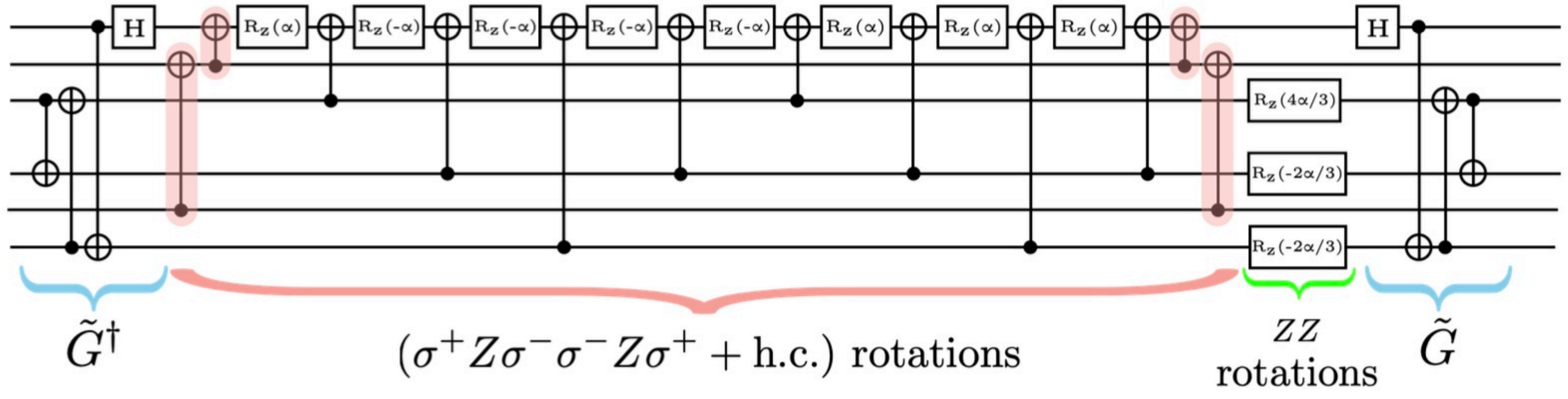
- a disruptive algorithm advance

Workflow

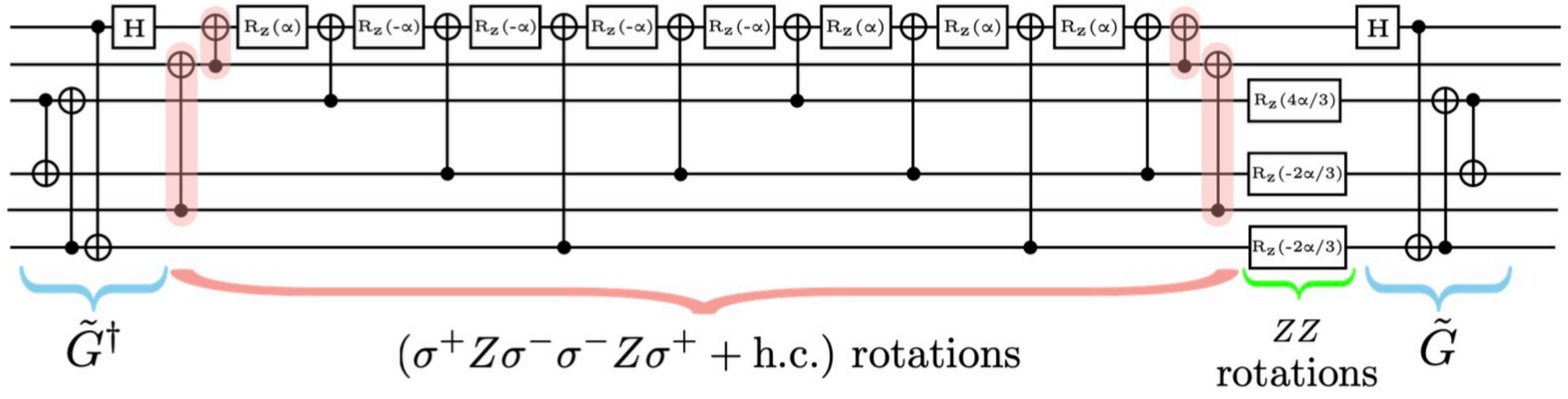
The device is approaching a classical, depolarized set of qubits as time goes by.

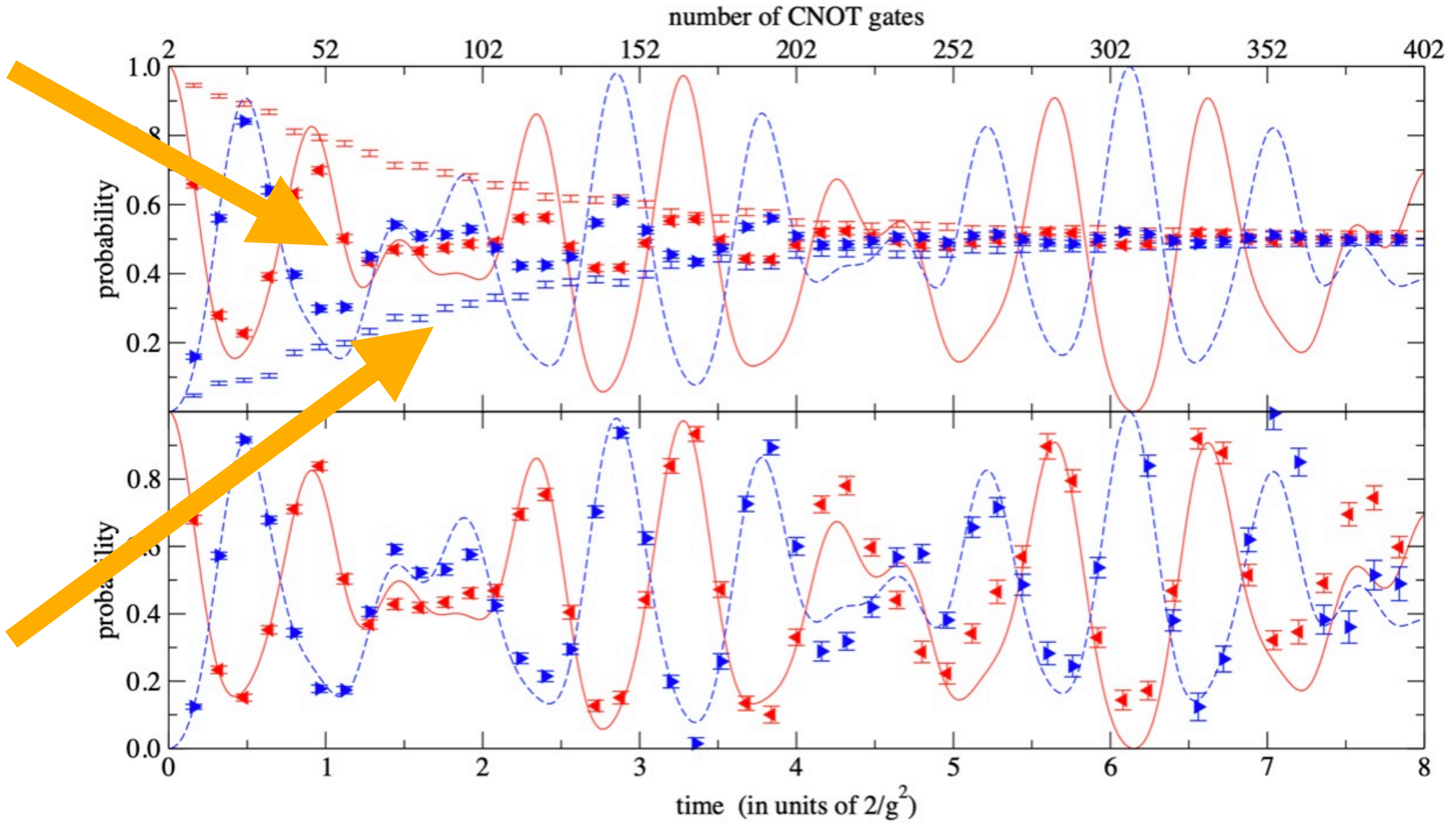
Mitigation methods are essential and effective

“Physics circuit”

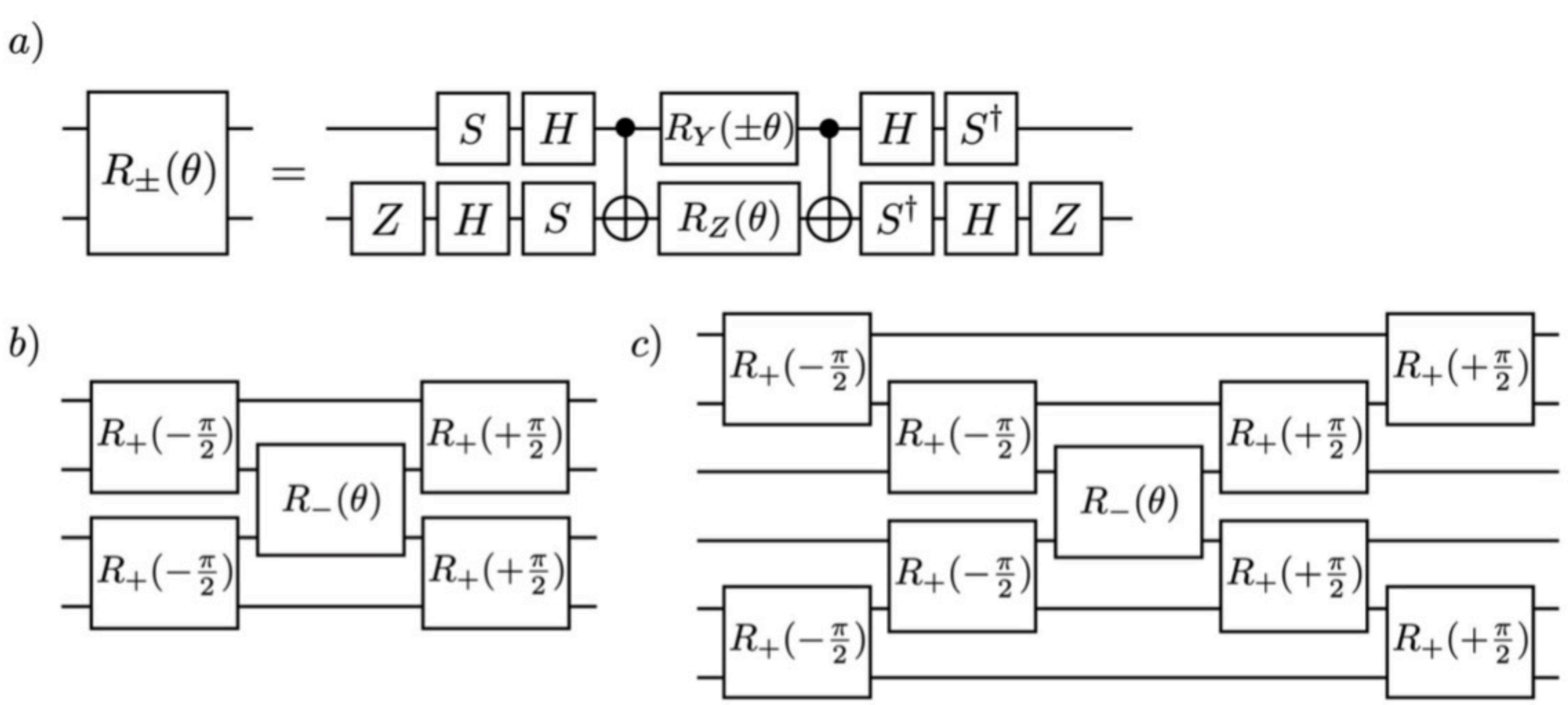


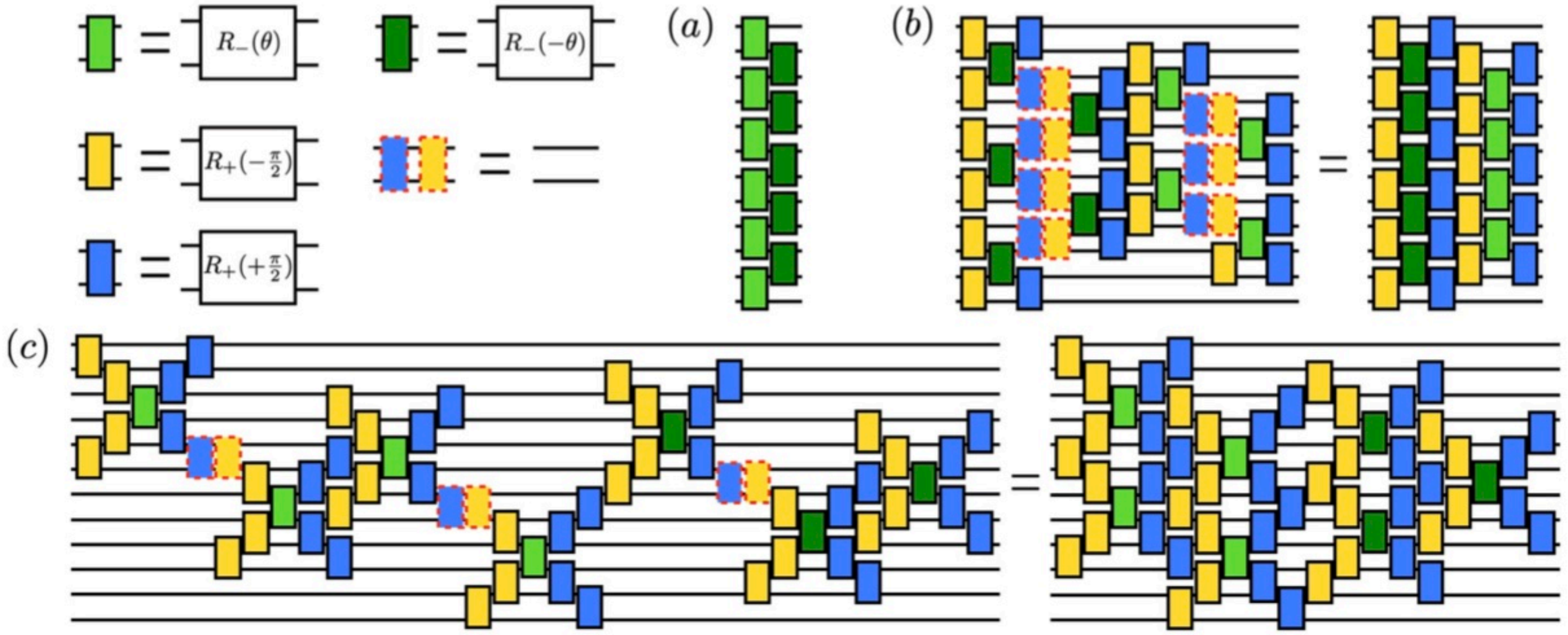
“Mitigation circuit” - all angles set to zero (e.g.)





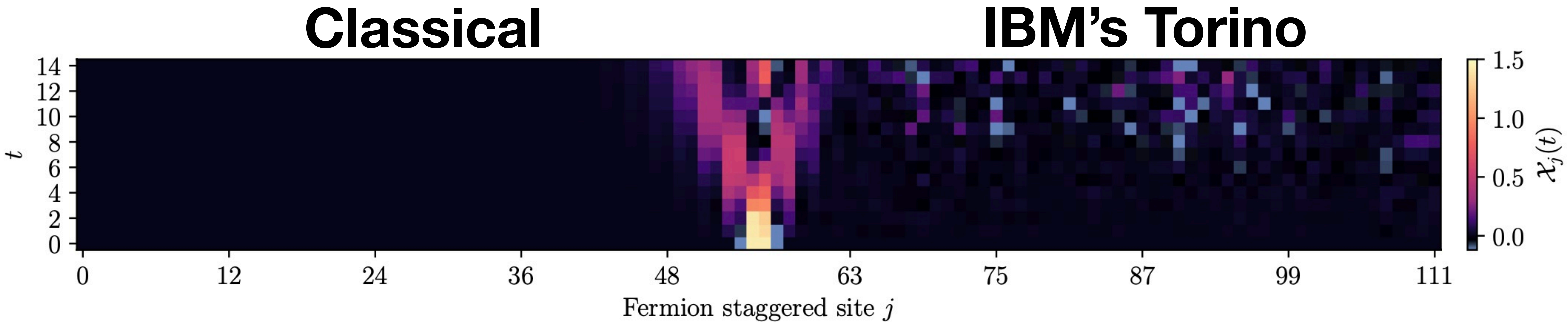
Production using IBM’s Heron Processor Torino

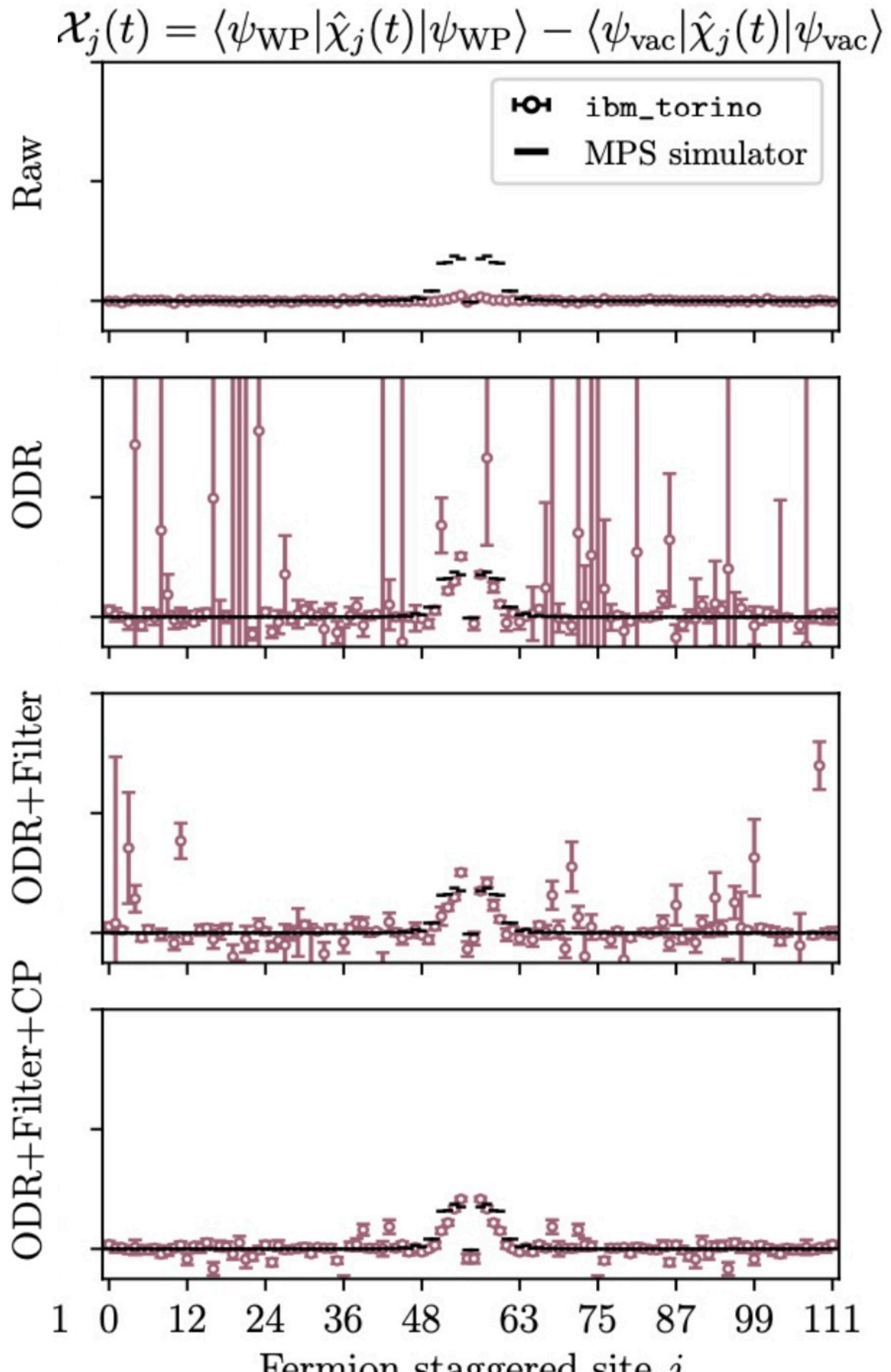




Production highlights

- 14K CNOTs for 14 Trotter steps
- 1.05 Trillion total CNOTs applied
- 154 Million shots
- 112 qubits x 370 depth
- 1 full week of dedicated running





A Case Study

Neutrino Flavor Dynamics

A few groups are focused on this topic. Stimulating new ideas about neutrino entanglement

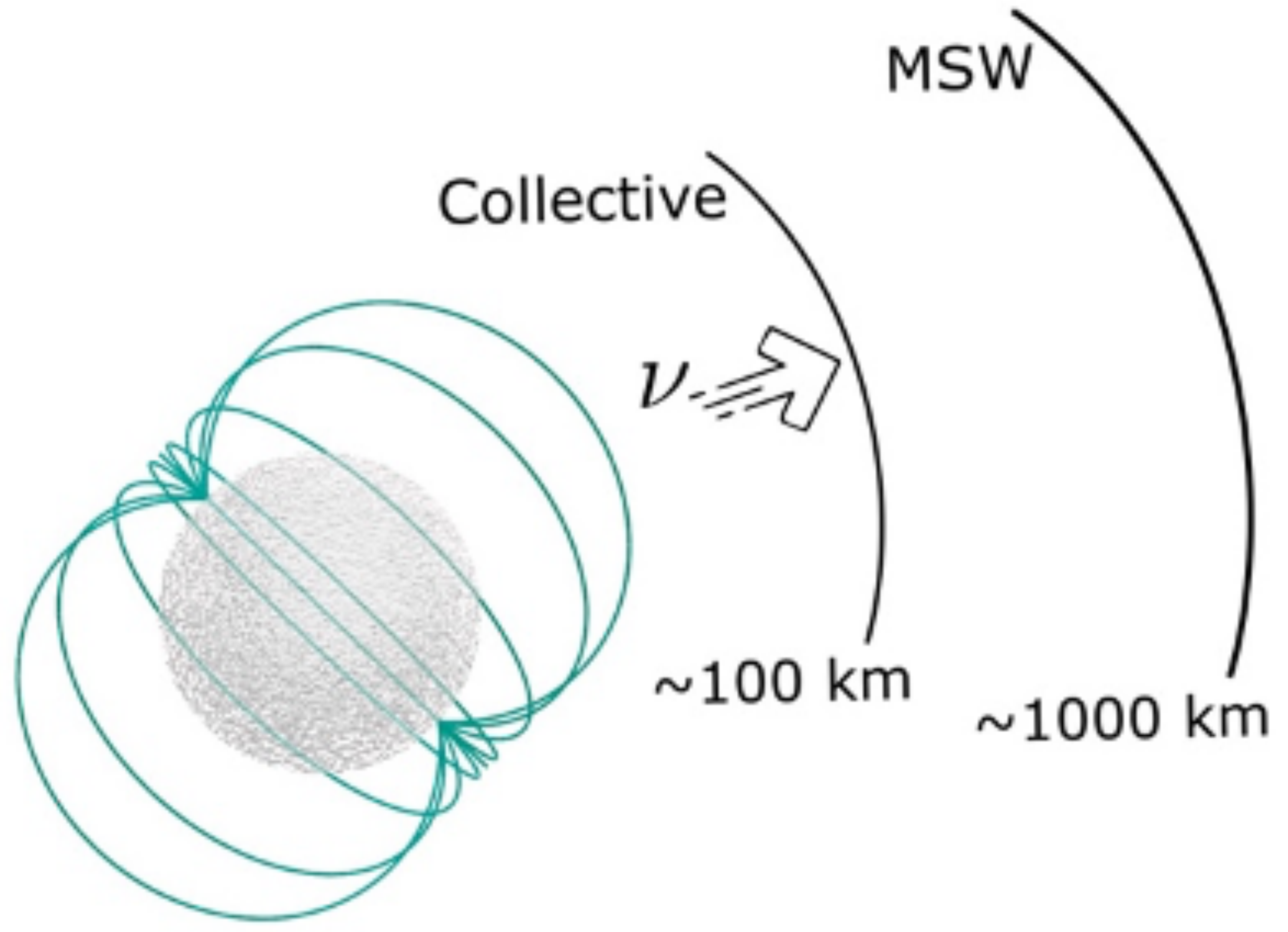
Quantinuum, OLCF, QSC

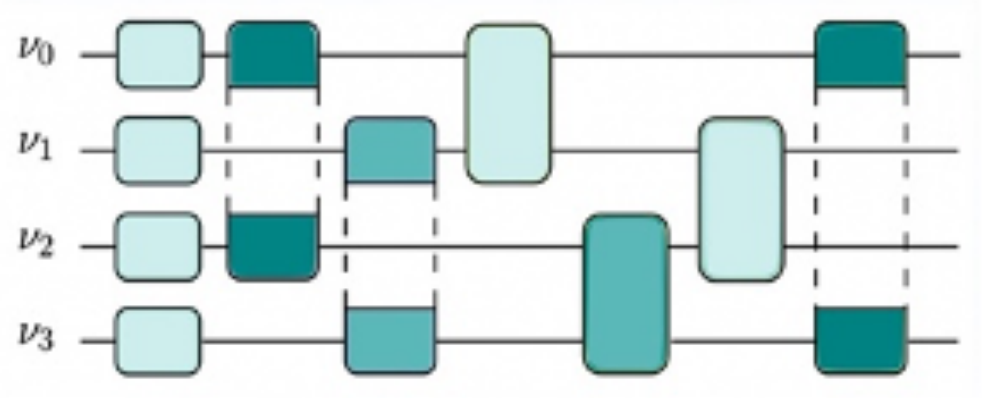
$$H_{FS} = -\sum_{k=1}^{N}\frac{\omega_k}{2}\sigma_k^z + \frac{\mu}{2N}\sum_{i<j}^{N}\mathcal{J}_{ij}\vec{\sigma}_i\cdot\vec{\sigma}_j$$

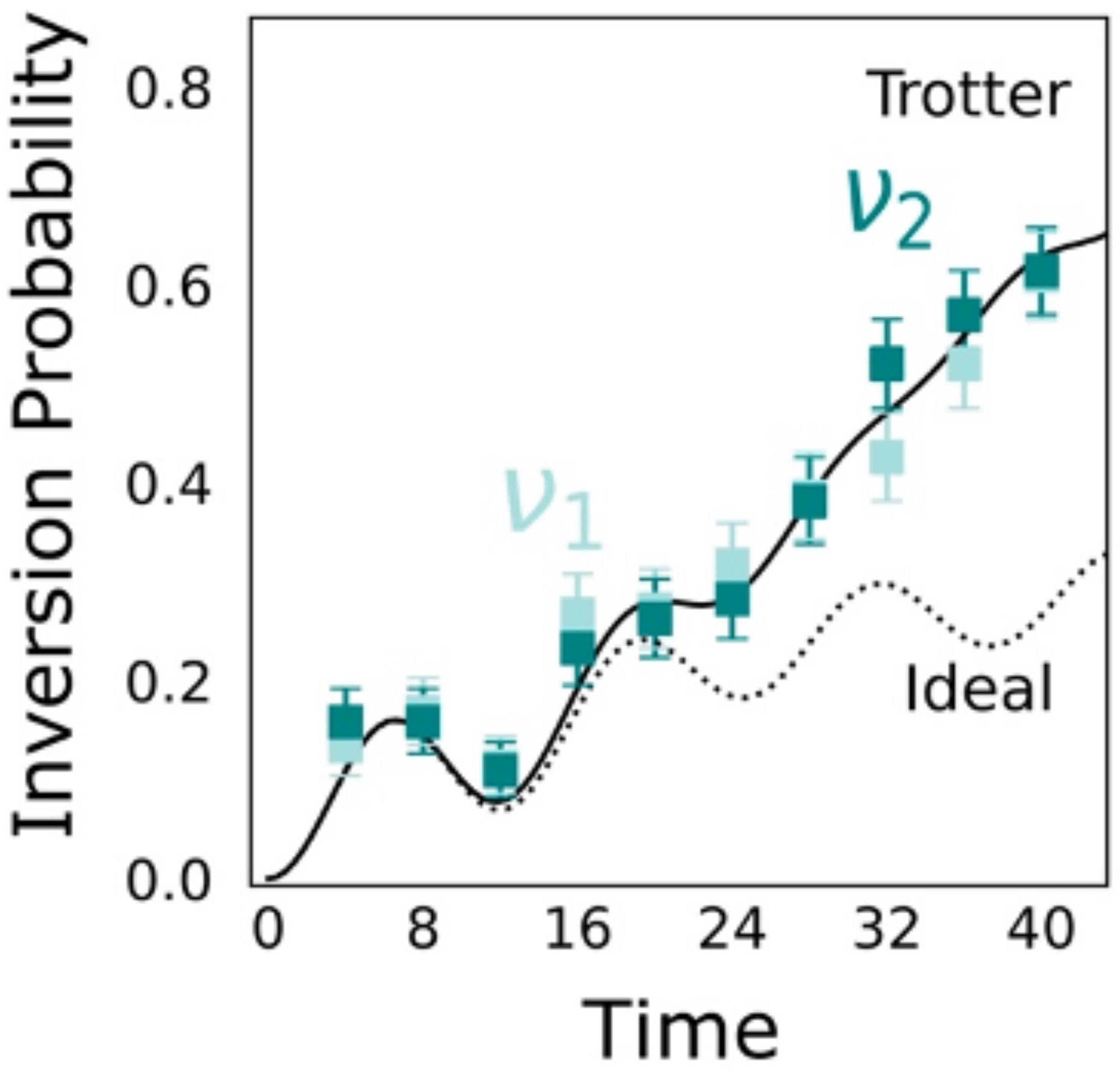
Entanglement

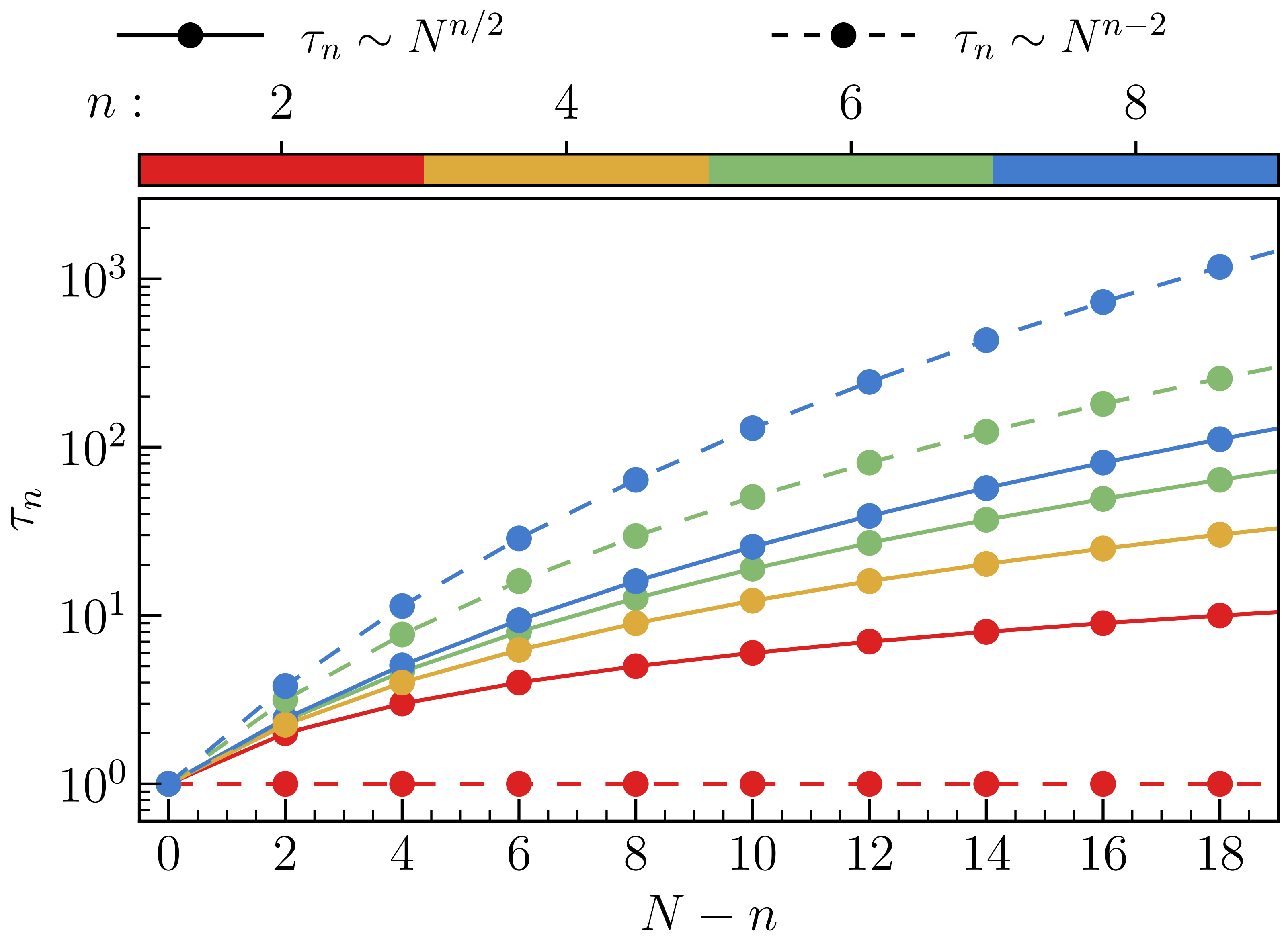
Magic

Trotter, (by-hand) circuit optimization…
qiskit, Mathematica, python, …









Complex systems with hierarchy of length scales, dynamics simulations challenging,
All-to-all connectivity

A Case Study

Transport Properties
Shear Viscosity in 2+1D SU(2)

IBM, Quantinuum, OLCF, Local

QITE, Trotter, Twirling, ODR, SPAM, …
qiskit, Mathematica, python, …

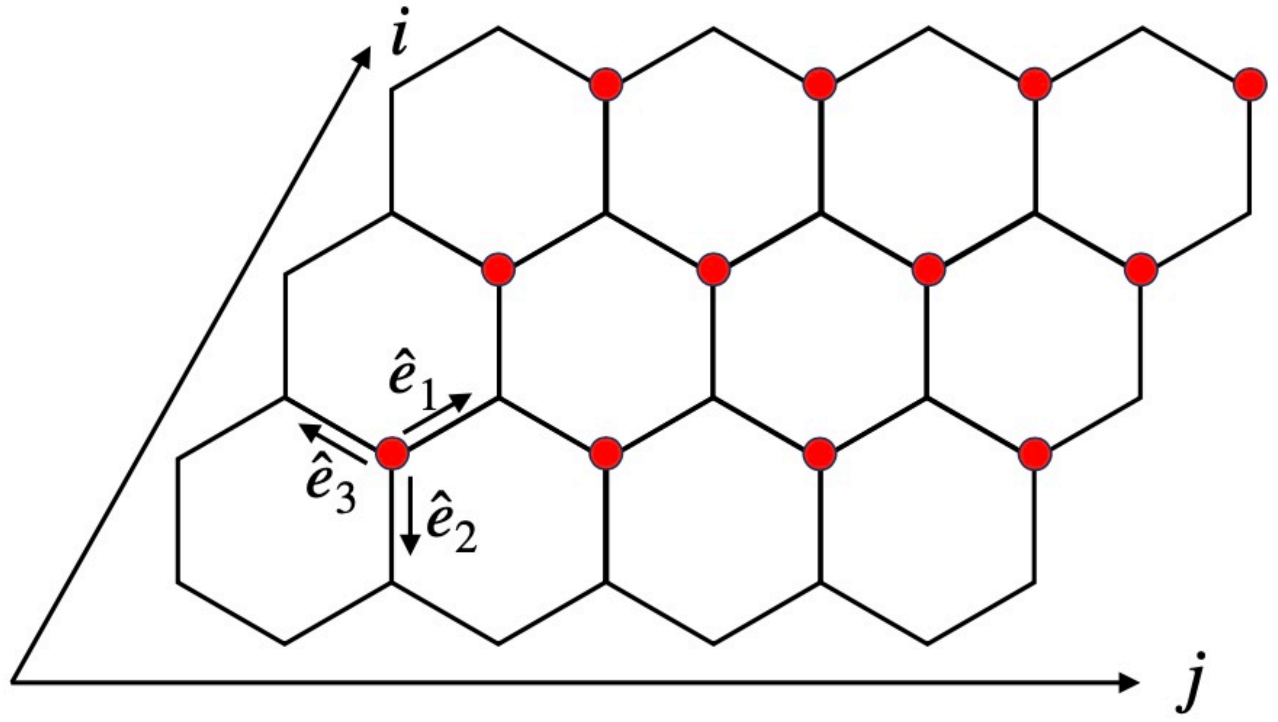
"Tree-level" Kubo formula $\eta = \lim_{\omega \to 0} \frac{\partial}{\partial \omega} G_r^{xy}(\omega)$

Baier, Romatschke, Son, Starinets, Stephanov, 0712.2451

$$G_r^{xy}(\omega) = \int \mathrm{d}t\, e^{i\omega t} G_r^{xy}(t) \equiv \int \mathrm{d}t\, \mathrm{d}^2x\, e^{i\omega t} G_r^{xy}(t, \boldsymbol{x})$$

$$G_r^{xy}(t, \boldsymbol{x}) \equiv \theta(t) \mathrm{Tr}\big([T^{xy}(t, \boldsymbol{x}), T^{xy}(0, \boldsymbol{0})]\rho_T\big)$$

$$T^{\mu\nu} = -\frac{1}{g^2} F^{a\mu\rho} F^{a\nu}{}_{\rho} + \frac{1}{4g^2} \eta^{\mu\nu} F^{a\rho\sigma} F^a_{\rho\sigma}$$



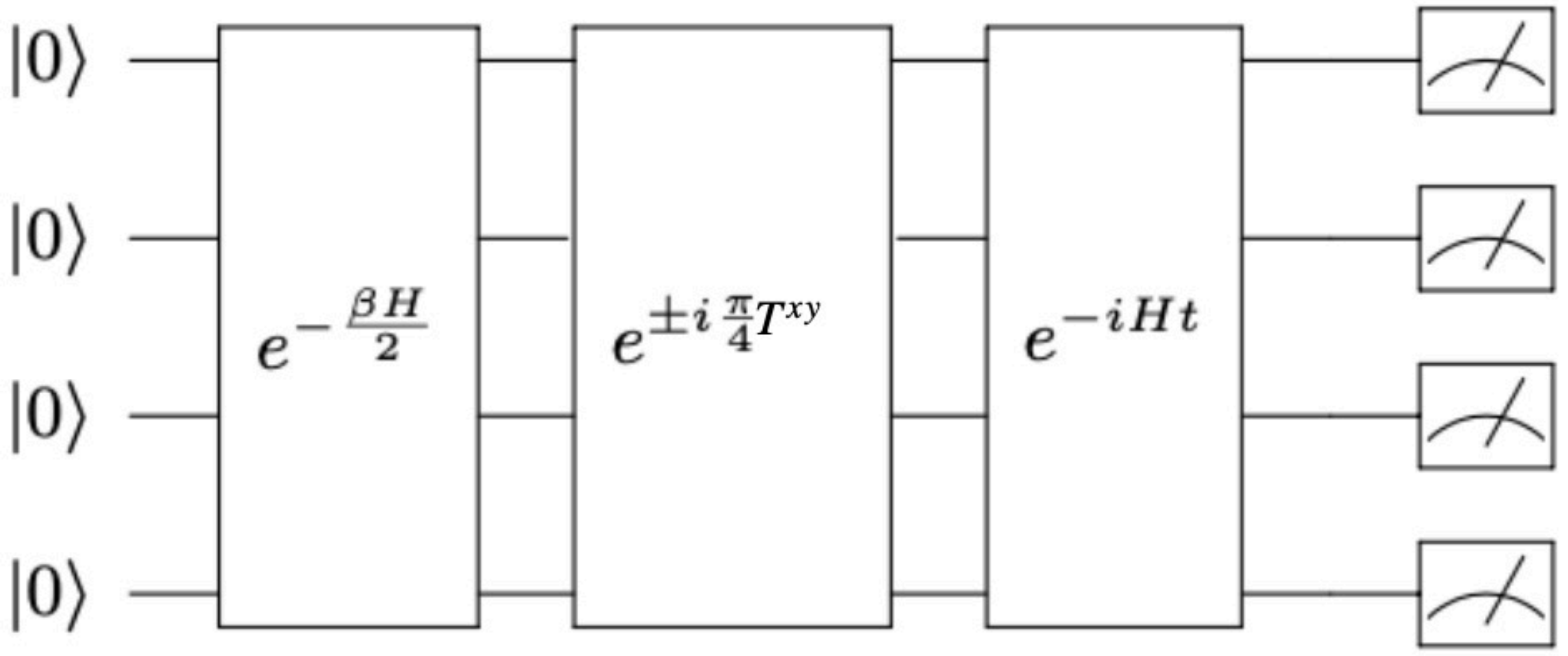
2307.00045
Berndt Mueller and Xiajun Yao

$$H = \frac{3\sqrt{3}g^2}{4} \sum_{\text{links}} E_i^a E_i^a - \frac{4\sqrt{3}}{9g^2a^2} \sum_{\text{plaqs}} \hexagon$$

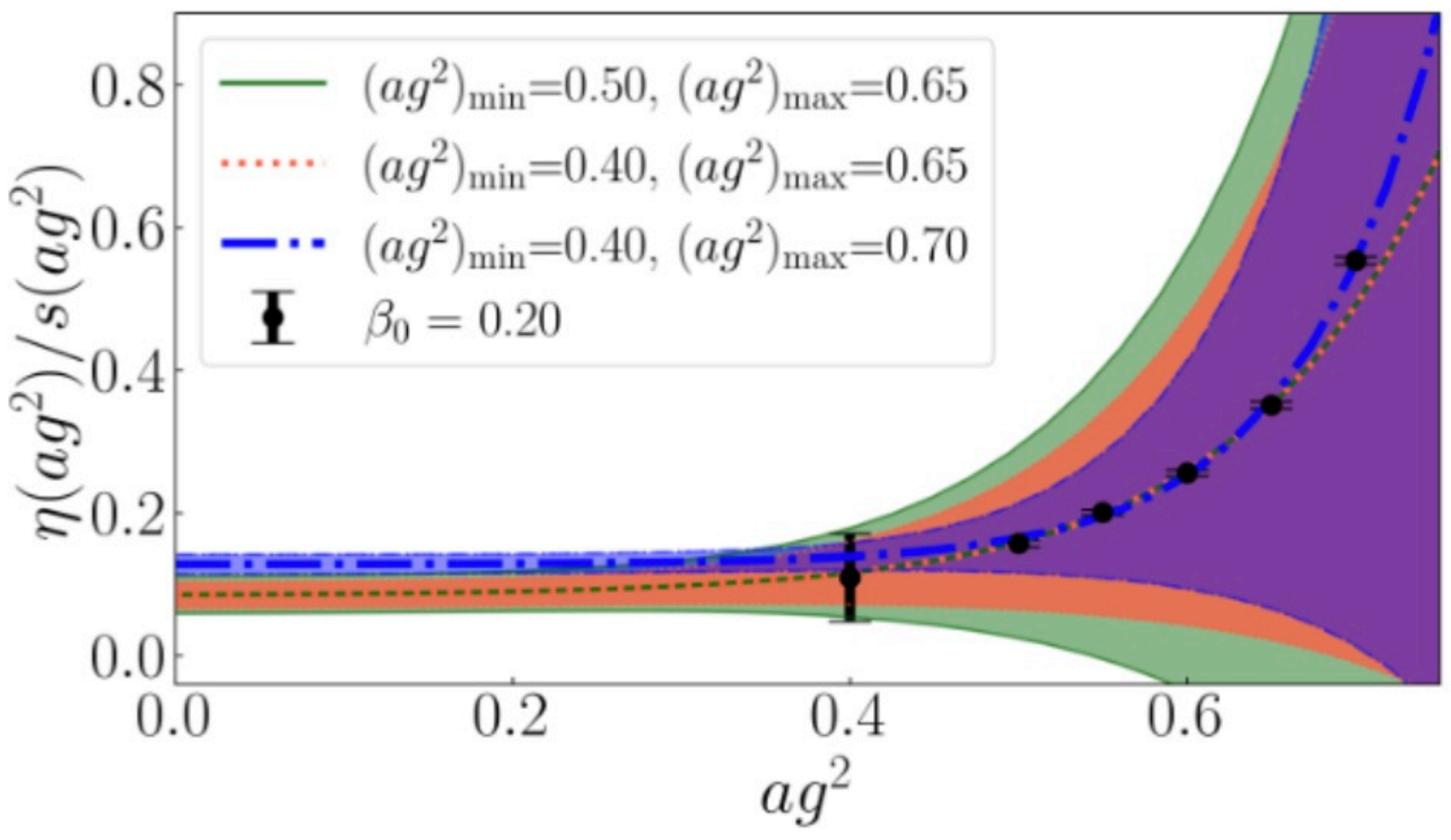
$$T^{xy} = -\frac{g^2}{\sqrt{3}a^2}\big((E_1^a)^2 - (E_3^a)^2\big)$$

2402.04221
Francesco Turro, Anthony Ciavarella and Xiajun Yao

Quantum algorithm for G_r^{xy}



On 4 × 4 lattice w/ $j_{\max} = 0.5$



Future : Source/Sink optimizations

At the Quantum Limit, same as liquid created in heavy-ion collisions

Quantities and Numerical Techniques In Use

Time evolution	< 24 qubits: exact exponentiation of (sparse) matrices via matrix-vector multiplication (EXPOKIT via Krylov methods,…) > 24 qubits: tensor-network approximation (TDVP,…)
Circuit simulation/ verification	< 40 qubits: (noiseless) state-vector simulators (multi-node) < 30 qubits: (noisy) density-matrix simulators (multi-node) > 30-40 qubits: (noiseless) tensor-network approximation (TEBD,…)
Spectrum analysis	< 16 qubits: full spectrum for thermalization studies (exact diagonalization) < 24 qubits: exact low-energy spectrum (ARPACK,…) > 24 qubits: approximate low-energy spectrum (DMRG,…)

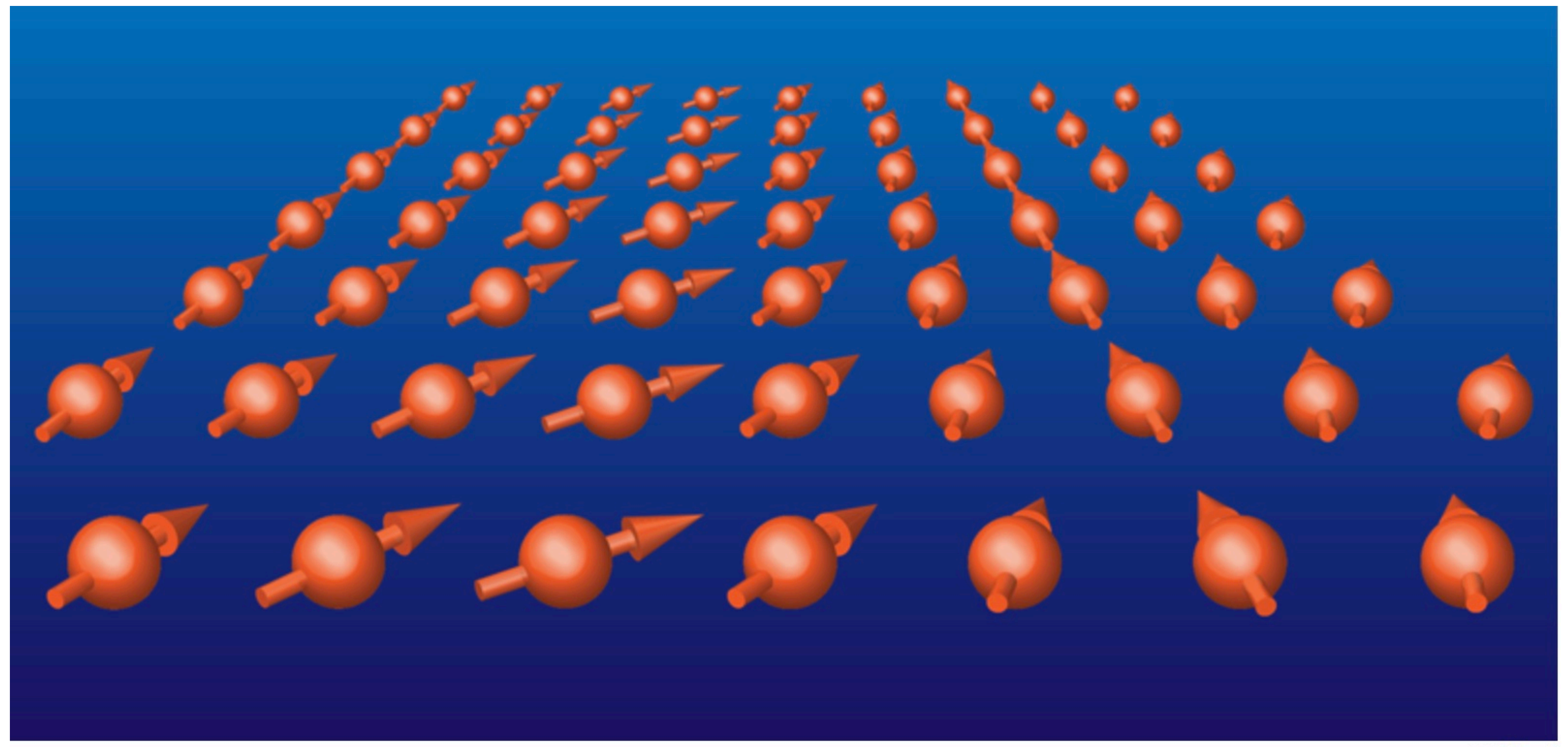
Thanks to Marc Illa

A Case Study

Cold-Atom Systems

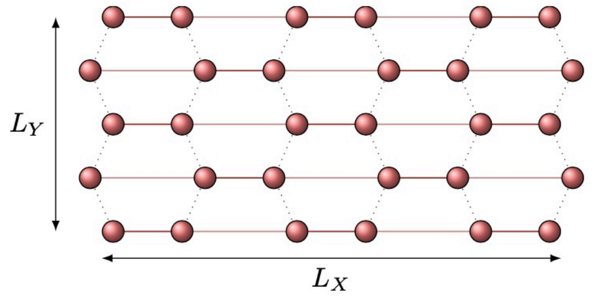

aws

AWS-Quera-IQuS collaboration:
Led to a classical method to solve a sign problem


APS/Alan Stonebraker

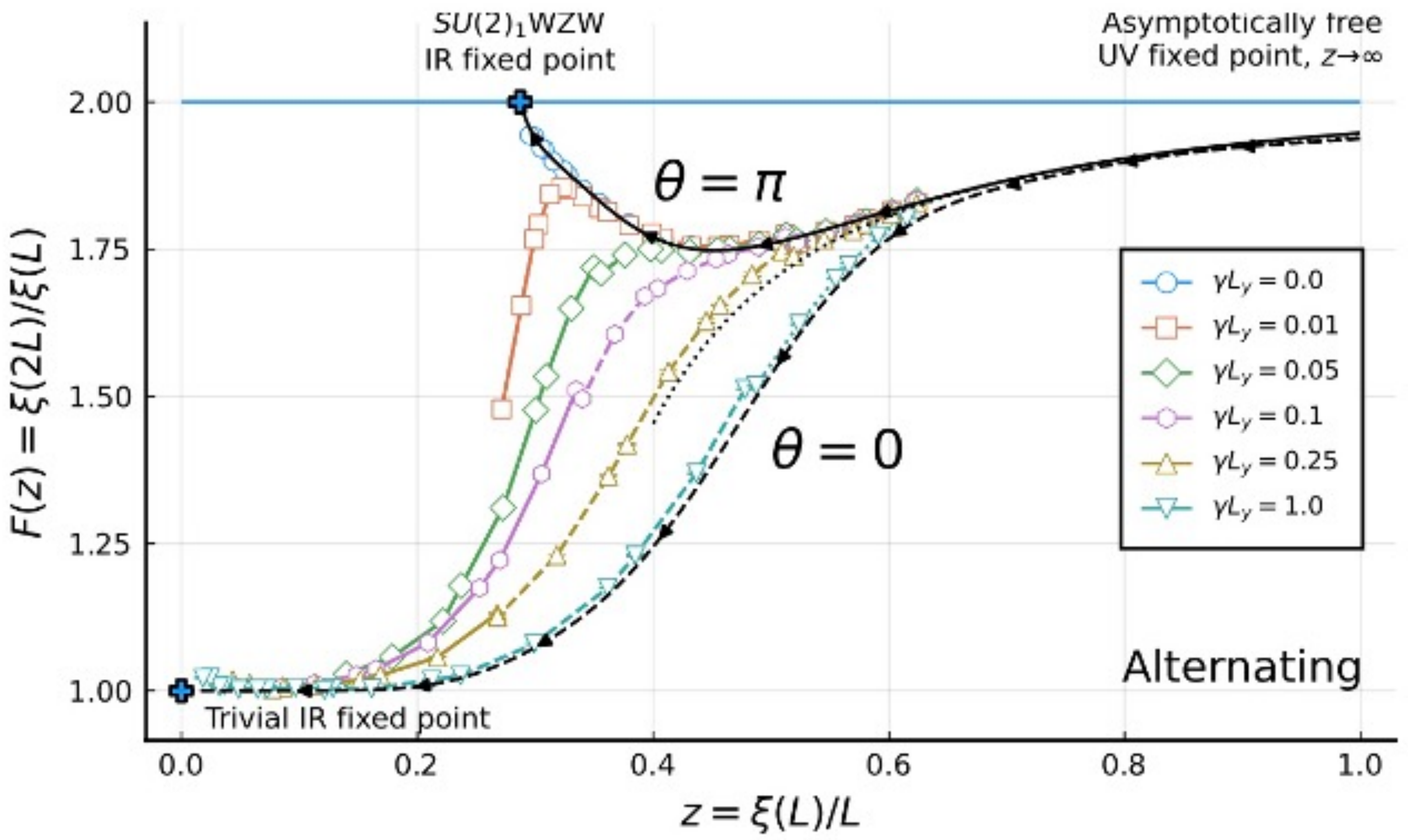
$$S = \frac{1}{2g}\int dt\, dx\, \partial_\mu \vec{\phi}(x,t)\cdot\partial^\mu\vec{\phi}(x,t)$$

$$\hat{H}^D = J_x\sum_{x,y}\vec{S}_{x,y}\cdot\vec{S}_{x+1,y} + J_y\sum_{x,y}\vec{S}_{x,y}\cdot\vec{S}_{x,y+1}$$



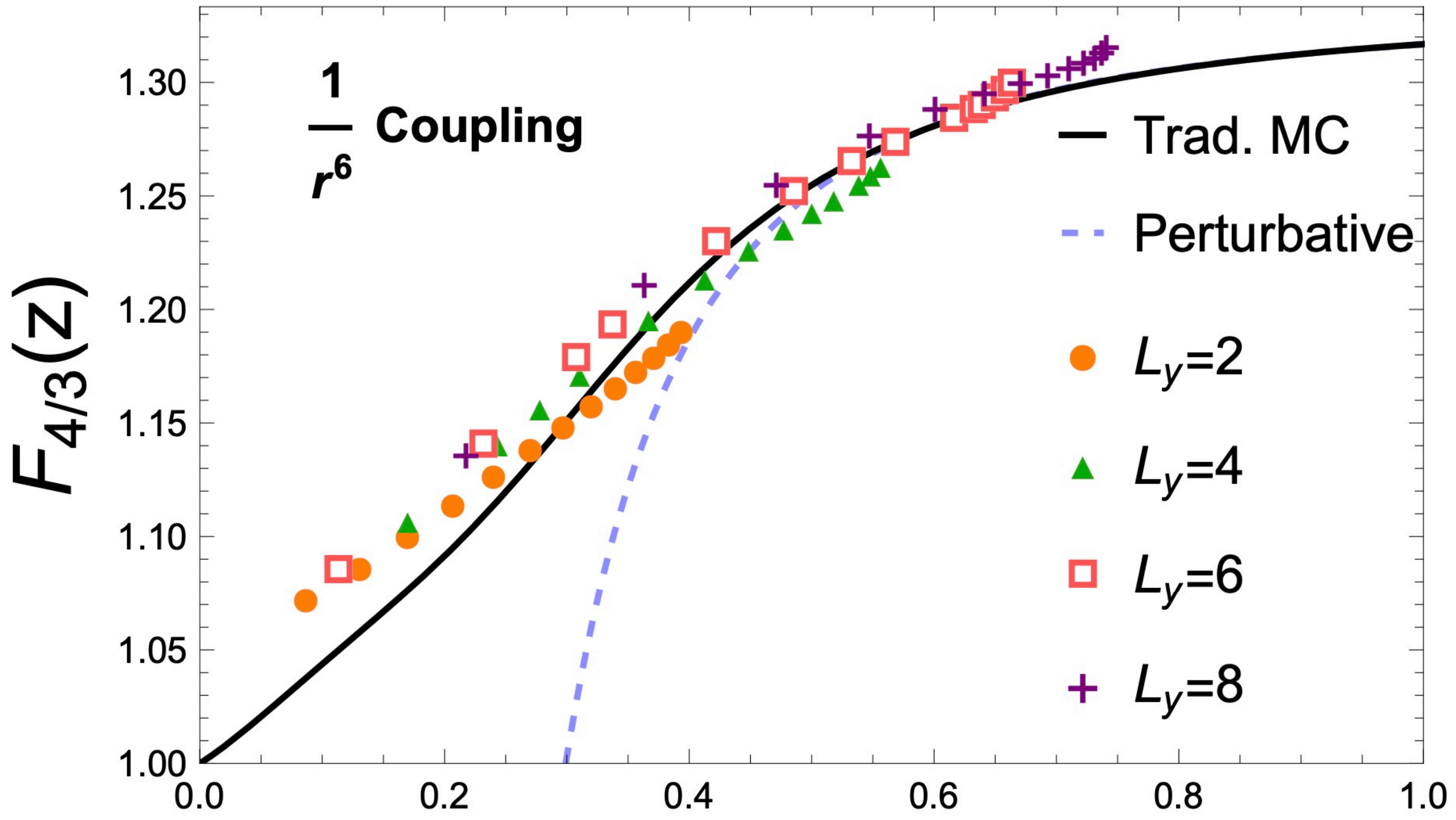
2+1D

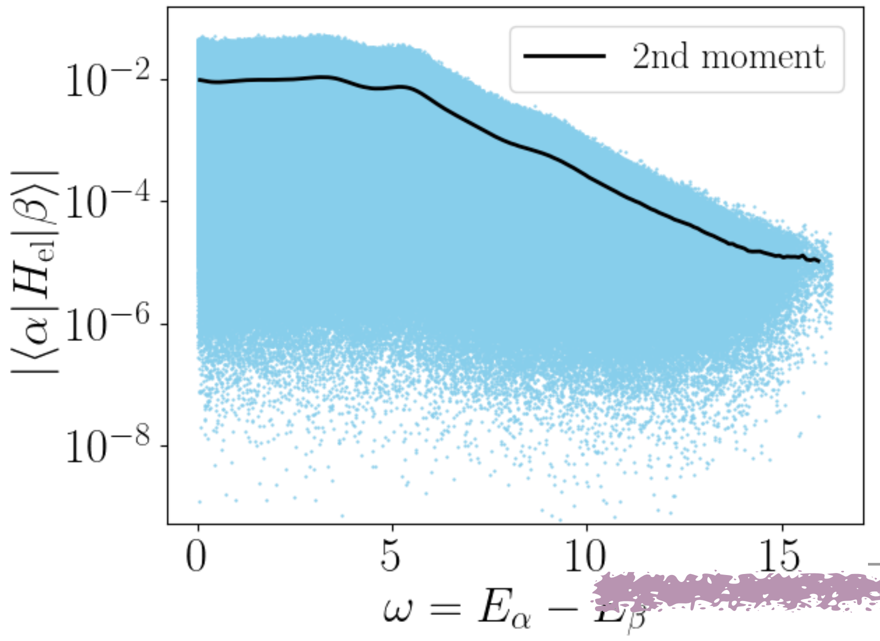
1+1D



Months of 4K core HPC jobs for tuning parameters

Bloqade - extensive tunings using device parameters/uncertainties



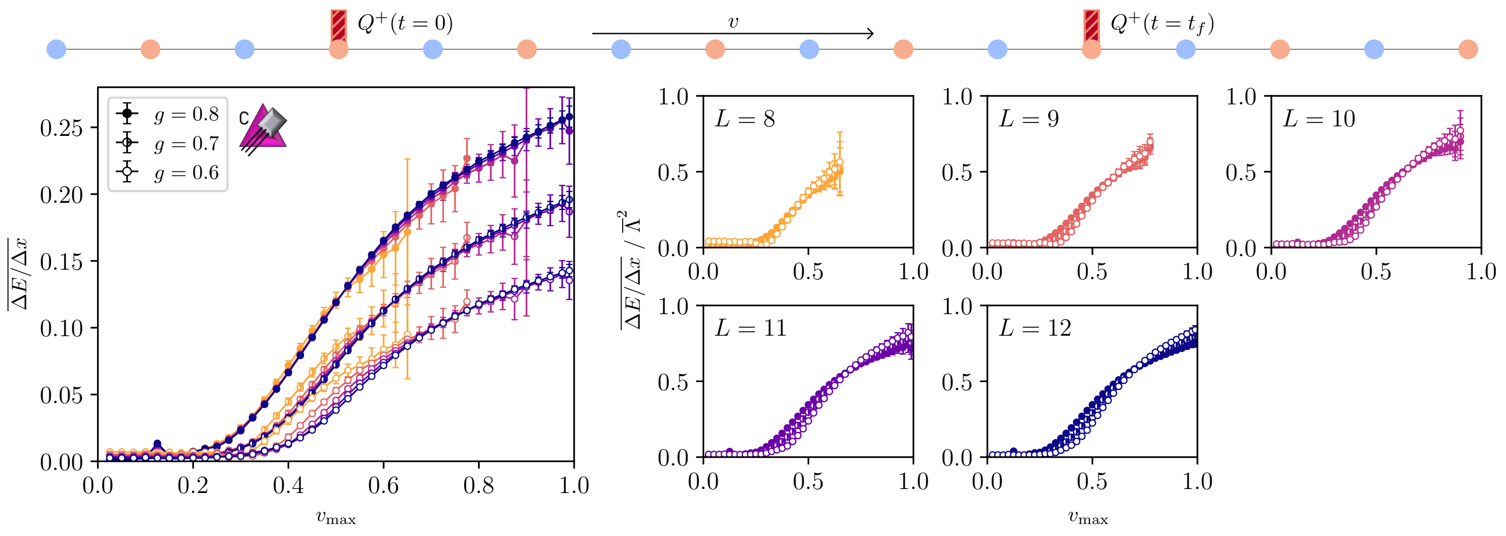


Test ETH IN non-Abelian theories

$$\langle E_\alpha|\mathcal{A}|E_\beta\rangle = \langle\mathcal{A}\rangle_{\rm mc}(E)\delta_{\alpha\beta} + e^{-S(E)/2} f_{\mathcal{A}}(E,\omega)R_{\alpha\beta}$$

ALL eigenstates of Hamiltonian $\sim 10^4 \times 10^4$ and compute matrix elements

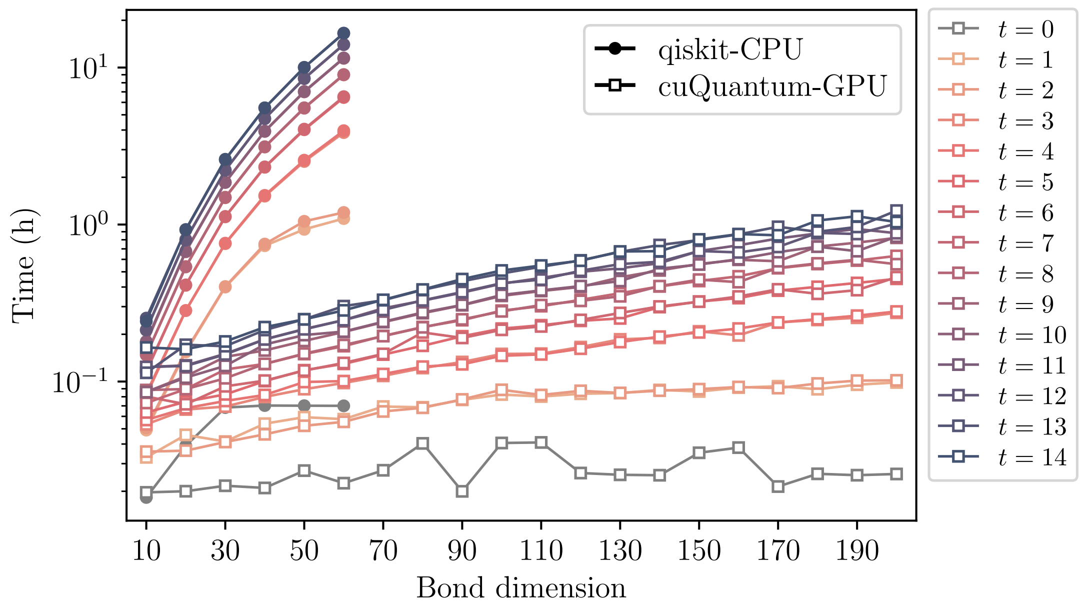
Using python scipy eigen module (1 node), it takes **20 hours**



$$|\psi(t)\rangle = \mathcal{T}\prod_{j=1}^{t/\Delta t} e^{-i\,\Delta t\,\hat{H}(j\,\Delta t)}|\psi(0)\rangle$$

$$\dim(\hat{H}) = 2^{24}\times 2^{24} \approx 10^7\times 10^7$$

For matrix exponentiation, use Expokit algorithm, efficient for sparse matrices (available only with single-node execution, therefore limited by memory on the node)



Verification: Circuits composed of 112 qubits

Maximum depth: 574

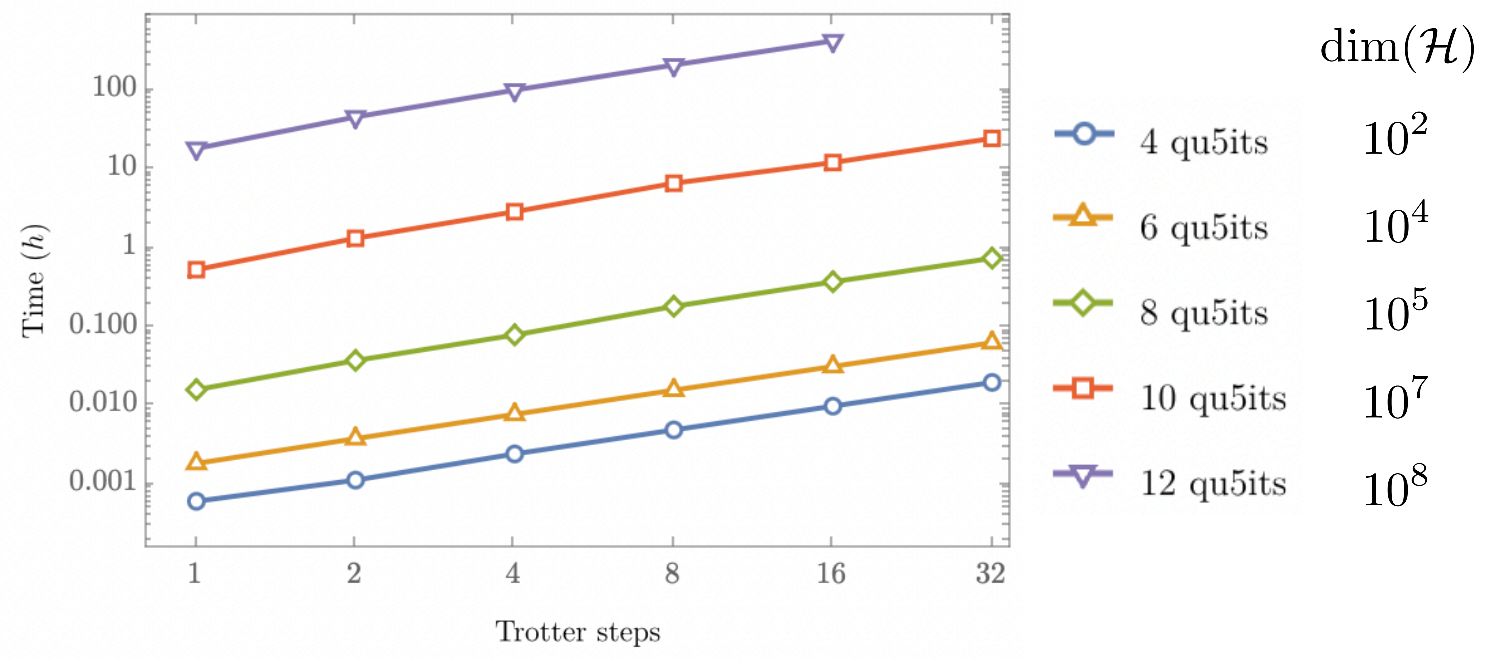
Maximum CNOT depth: 370

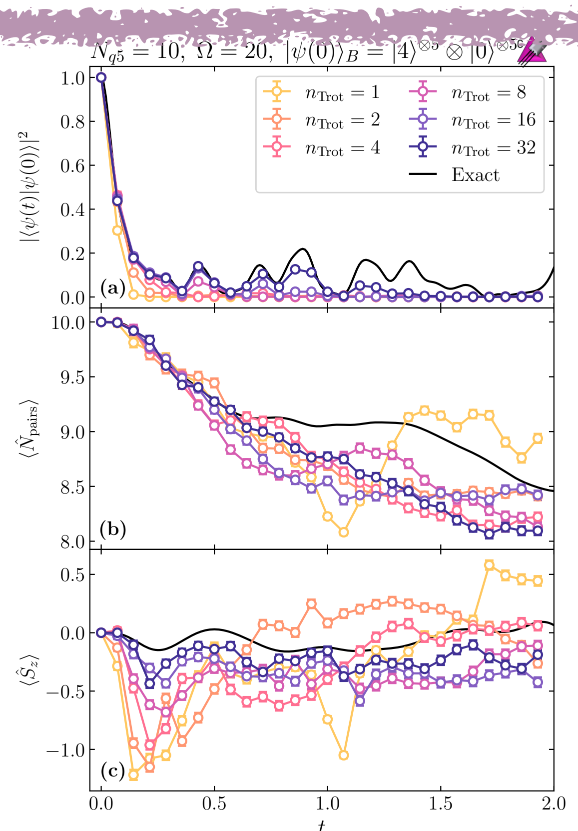
Maximum # gates: 32,016

Maximum # CNOT gates: 13,858

A single NVIDIA RTX A5000, total of **88 GPU hours** (via Open Science Grid Cluster)

Used NVIDIA cuQuantum tensor-network simulator for comparison with results from quantum computer (available with single/multi-GPU execution)





No large-scale qudit circuit simulators available, custom code using google cirq as base (single-node), total of **36 days** on Hyak (UW)

General Comments

While the algorithms and error mitigation strategies are being integrated (by tech companies) into their software stacks in a timely way, NP problems have attributes that require specialized algorithms and optimizations.

Error mitigation is largely tech-company enabled, e.g. IBM. Error-correction is nascent in NP, with a handful of examples in gauge theories (Gauss's law checks etc)

Digital systems now >30 qubits (all-to-all), and 112 qubits (nearest-neighbor) is state-of-the-art

Cold-atom systems >1K atoms, 2D arrangement, two-atom entangling operations (all-to-all)

Need <Pauli strings> , exponentially large number - requires MCMC, ...

Current situation is ``patchwork'' and now requires increased organization for the future

Simulators Required

Digital qubit, qudit simulators at scale - 44-qubit simulation cost $$$$

- Associated HPC resource allocations - synchronize with quantum device access
- Quantum data analysis, error mitigation, etc - moving to larger data
- Requires flexible connectivity and noise models

- Developed a single-node qudit simulator
  - tested performance of another that sits on top of qubit simulator at scale.

Cold-atom simulators - currently limited to about 20 atoms, target >1K but >10K better

- Requires flexibility for rapidly changing device attributes/capabilities, help design next-gen.

IQuS InQubator for Quantum Simulation

IQuS workshops have proven to be effective in QIST-NP integration … leverages INT spacetime

Making progress in developing quantum simulations of important problems.

- techniques have utility in other areas.

Expected future impacts for non-equilibrium dynamics in nuclei and reactions, lattice QCD, neutrinos, hot-dense matter - looking toward QAs

Specialized algorithms are enabling progress, broad interest

Progress requires enhanced flexible simulation capabilities - for available hardware

— both code and algorithm development, and significant HPC resources : organization/structure

Require enhanced access to quantum computers - all architectures. Progress has been spurred by access.