Thoughts About The Interface
(By theorists, with Natalie Klco and Alessandro Roggero)

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Thinking about questions such as (analogous to HPC):

If someone gives you access to a quantum device with 1000 physical qubits with a given connectivity, fixed quantum volume, and a maximum of one million “shots” and asks you to compute a SM quantity of impact - what would you do?

- a) 1 or 2 really good logical qubit — probably not
- b) 1000 really poor qubits — probably not
- c) Compute using a different Hamiltonian — maybe
Elements in Talk

- Entanglement
- Collaboration
- Complexity
- Simulating Field Theory
- Advancing QIS
- Co-design
- Co-development
~ 2016 - The Awakening (in the US)

Identified beyond exascale problems in HEP and NP
Real-time, finite density, many-body

Innsbruck demonstration of real-time dynamics in QFT
ORNL calculations of deuteron binding energy

Cloud-accessible quantum devices become available
[Available devices have improved dramatically since]

There had been many pioneering theoretical and algorithm developments related to quantum simulations of QFTs and QMBs for scientific applications (on top of QI advances):
Banuls, Bermudez, Cirac, Jansen, Jordan, Lee, Lewenstein, Muller, Muschik, Preskill, Weise, Zohar, Zoller, many others
Looking for a quantum advantage
Do not scale well using classical computers

- Real-time Minkowski space evolution
  - highly-inelastic processes, fragmentation, S-matrices
  - non-equilibrium systems

- Large Hilbert spaces - quantum field theories, large nuclei

- High-density - potentially mitigate classical sign problem(s)
Targets for Quantum Simulation

 Quantum Field Theories and Symmetries
  • indefinite particle number
  • gauge symmetries (constraints)
  • entangled states

 Real-Time Dynamics
  • parton showers and fragmentation
  • neutrinos in matter
  • early universe
  • phase transitions - matter?
  • non-equilibrium - heavy-ions
  • nuclear reactions
  • neutrino-nucleus interactions

 Matter
  • neutron stars
  • gravity waves?
  • Heavy nuclei
  • chemical potentials
  • entanglement
Amazed by what has been collectively accomplished!
Excellent published works and reviews - I will not be reviewing
Quantum mechanics “works the same” at all scales we have probed

- The promise to simulate systems at one scale with systems at another with fidelity (Feynman, Benioff, Manin and others)

First digital devices became cloud accessible ~ 5 years ago
- increasing selections of qudits+fabrics

How to map systems we want to simulate to the systems we control?
How do we connect the constituents to perform operations?
What do we measure (and want to)?
[most answers are correct at present]
What are the “New” Features Beyond HPC?

Quantum-2 provides access to controllable entanglement and coherence in devices for computation

- Hilbert spaces scaling similar to many-body configuration space
- Real-time evolution is in $\text{BQP}$ (bounded-error requiring polynomial scaling quantum resources)
- "Bounded Errors - theorists and designers can trade-off uncertainties
  - more axes for creativity

Requires us to think "coherently"
Theory to Simulation

Where many of us in this meeting “sit”
How, what?
Depends on available hardware
Relies heavily on QC community
Benefits from our HPC developments

How we (mostly) engage with devices
APIs
Tech companies and in-house
Benefit from our HPC developments

Domain Scientists

Algorithms
Identify problem
Map to qubits and gates

Quantum Software
Express in native gates/connectivity
Compile & compress circuits
Deploy error correction strategy

Control Engineering
Implement Hamiltonian control with E/M fields

Qubit Technology
Interface control fields with qubit system

Quantum Computer Systems for Scientific Discovery, Yuri Alexeev, et al.
P.R.X.Quantum. 2 (2021) 017001, Quantum 2 (2021) 017001 · e-Print: 1912.07577 [quant-ph]
Hardware Development — examples

AMO, Circuit analog simulations
- Optical lattice laser beams
- High-resolution objective
- Mirror 1064 nm window 780 nm
- 16 µm

Digital computations
- e.g. trapped-ions, superconducting qubits
- H: universal gate sets

High-Q Cavities
- e.g. High-Q RF cavities, classically prepare controls to perform quantum operations

H: native to system
- e.g. atoms in optical lattices
- SRF cavities
- BECs

Environments

Quantum devices embedded in HPC environment - Hybrid

— If the system to simulate is (essentially) classical - then use HPC

— basis dependent entanglement — choose efficient basis
— identify quantum “parts” of algorithm, e.g., VQE

Alba, Christine talk
Entanglement - Perspective

In part:

20th Century HEP - QFT
— “chasing” short-distance fundamental interactions
— nonperturbative lattice QCD using HPC
— modeling gave way to EFTs - leading order separable

20th Century NP - QMB systems
— “handling” short-distance (phenomenological) repulsion
— ended NT for a few years! Re-invigorated by RG and EFT from HEP
— quantum many-body computations using HPC
— modeling gave way to EFTs

21st Century HEP+NP - QFT+QMB systems
— quantum correlations and non-locality using/for quantum simulation and quantum computing
What are the potential roles of entanglement?

- Organizational principle
- Order parameter
- Insight into structure
- Thermalization
- Geometry
- Simulation design
- Computational complexity
Entanglement - Order Parameters, Structures

Beane, Ehlers

\[ |\Psi\rangle = \alpha_1|\Phi\rangle_1 + \alpha_2|\Phi\rangle_2 + \alpha_3|\Phi\rangle_3 + \ldots + \alpha_k|\Phi\rangle_k + \alpha_{k+1}|\Phi\rangle_{k+1} + \ldots \]

| shell model (LO) \rangle \rangle = | core \rangle \otimes | valence \rangle
Entanglement - Emergent Symmetries

\[ \hat{S}_\sigma = \frac{1}{4} \left( 3e^{i2\delta_3} + e^{i2\delta_1} \right) \hat{1} + \frac{1}{4} \left( e^{i2\delta_3} - e^{i2\delta_1} \right) \hat{\sigma} \cdot \hat{\sigma} \]

\[ \mathcal{E}(\hat{S}_\sigma) = \frac{1}{6} \sin^2 (2(\delta_3 - \delta_1)) \]

Finding GS of n-body system is in **QMA-complete** - generally beyond QC

**SU(4)** for 2 flavors and **SU(16)** for 3 flavors (seen in LQCD calculations)
- more symmetry than large-Nc, [SU(4) and SU(6)]

Emergent approximate symmetries in nuclear systems

Suppressed fluctuations in entanglement

Suppressed sign problems in classical simulations
Entanglement in Simulation - Subtle

Harmonic chains - many really interesting QI works during the last 20 years
Relevant to finite-resource computations

Reznik, many others
Entanglement - Not Always Beyond Classical

Stabilizer states can be entangled and classically evolved efficiently for certain quantum circuits (Gottesman)

e.g., 3-qubit GHZ states circuits with Paulis, H,S and CNOT.

T-gate required for Universal QC, requires beyond classical. (e.g., single qubit rotations)

…. entanglement alone is insufficient to require a quantum device
Mapping and Scaling

Expect that $n$-dof locally interacting for time $T$

requires
$n$-dof evolved through $\sim T$ time steps
for a total of
$\sim nT$ operations. (fermions : $\sim \text{poly}(n)T$)

D-dim systems optimally simulated
with D-dim systems.

E.g., a 2-dim systems of spins will not optimally simulate a 3-dim
system of locally interacting dof.

Implications for 3-d QFT and QMBs .... co-design
i.e., understand how to “simply” scale between system and device
e.g., Exploring Trotterization for Real Time Evolution

Lloyd, Childs, others

\[ \text{e.g., } H = H_a + H_b \]

\[ e^{-i \delta t} H_b e^{-i \delta t} H_a e^{-i \delta t} H_b \ldots \]

\[ e^{-i H t} \left| \Psi \right\rangle \]

Heyl, Hauke, Zoller, Science 2019
Complexity
The scaling of resources required to solve a problem

Scott Aaronson, Sci. Am.

$\text{BQP} = \text{Polynomial scaling quantum resources to achieve a given precision (Bounded Error)}$

$\text{BPP} (\text{Bounded Probabilistic Polynomial})$ in BQP

$\text{g.s. of k-local Hamiltonian}$
(Kempe, Kitaev, Regev)

Interacting Lattice Scalar Field Theory
(Jordan, Krovi, Lee, Preskill)
Quantum Field Theories

- Finite lattice to support the fields
- 3-dim
- Real-time Hamiltonian evolution
- Fields mapped to qubits/qudits
- BCs
- Hybrid - tasks for QPU?

- Different mappings (most “efficient” path to continuum physics?)
  - “qubits arranged” with fermions on sites and gauge fields on links (KS)
  - or continuum fields de-localized. (e.g. quantum link models)
  - truncations/samplings in gauge rotations or irreps
  - and/or Integrate out gauge freedoms
  - and/or Gauss’s law explicit/implicit, error correction to enforce

Truncations, convergence and errors (gauge field, spacetime)
Ultimately, we will need to establish a complete quantification of uncertainties.
Scattering in Scalar Field Theory
-Gold Standard for Algorithmic Design for SM

Quantum Computation of Scattering in Scalar Quantum Field Theories

Stephen P. Jordan,† Keith S. M. Lee,‡§ and John Preskill § *

1. nQ qubits per spatial site, H(3) lattice, digitized field-operator basis
2. Create wavepackets of free theory
3. Adiabatically evolve the system to interacting system
4. Evolve the prepared state forward
5. Adiabatically evolve systems to free theory/introduce localized detectors into the simulation
Remarkable developments in general classical techniques for many-body systems and field theories. Tensor methods.

Explicit symmetry breaking (false vacuum)

\[ H = \sum_{j=1}^{N} \left[ -Z_j Z_{j+1} - gX_j - hZ_j + \lambda \left( X_j Z_{j+1} Z_{j+2} + Z_j Z_{j+1} X_{j+2} \right) \right] \]
But should Complexity be a limitation? …. Not until it is…

Finite resources are not asymptotic.

\[ X^{10} \text{ is worse than } e^{+0.01x} \text{ until } x \approx 9000 \]
\[ 10^6 x \text{ is worse than } e^{+0.01x} \text{ until } x \approx 2000 \]
(Highlighted by quantum chemists - what are the coefficients?)

Complexity class indicates worst case
- can be much easier

The “B” in BQP gives latitude to change theories “a little”

Analogous to BPP and lattice QCD, and MC in general

With a target precision, can use pertubative expansions to potentially change problem difficulty at (tractible) LO. [e.g. includes field truncations]
Examples

1) HQET
   1) 1/M expansion of Hamiltonian about classical trajectories

2) Lattice QCD
   1) Finite volume and lattice spacing effects mitigated by EFT expansions - Symanzik action, ChPT
   2) pQCD matching at lattice scale —- untangled at LO

3) Wigner Symmetry
   1) SU(4) limit - emerges in large-N limit
      1) S-matrix has vanishing entanglement power
         1) classical or highly entangled
         2) no sign problem for MC
      2) Numerically evolve with SU(4) symmetry, then turn on SU(4) breaking

\[ |Q\bar{l}\rangle \sim |Q\rangle \otimes |\bar{l}\rangle \]
A coordinated combination of theory, computation (and experiment) is required

Develop perturbative expansions
  • LO should lie within **BQP** or be “simple configuration” within **QMA**
  • perturbation theory should converge result to below $\epsilon$

Solve a LO Hamiltonian (typically with enhanced symmetry) using a quantum device that gets close, then use a “special-purpose” perturbation theory to reduce systematics. Typically pushes numerical errors to be of NLO, and not LO size.
Quantum Fields for EC

Stabilization of information against errors — the discovery of EC in 1995 (Shor, Knill+Laflamme+Zurek, Aharonv+Ben-Or)

Toric Code (Kitaev)

— both hardware and algorithmic advances

— entangled, topologically ordered ground states of spin systems, with ancillars and (repeated…) application of stabilizers.

— e.g. toric, surface codes, color codes, …
Logical Qubits

— threshold error rate, below which exponential reduction in logical qubit error rate from increasing number of physical qubits.

For our purposes, we are looking to minimize error in simulations of observables of interest.

Aligns well with LQ design, but might also lead to different configurations.
e.g., Yang-Mills, Kogut-Susskind formulation

Color = 1, 3, 8, 6, 6, ....

Gauss’s Law satisfied at each vertex, Color = 1

- Confinement will keep color charges “close” during dynamics - naively easier than EC for 3-dim QED
- Single shot EC in color codes
- Related to self-correcting topologically-ordered GS at finite-T.

Gauss’s Law violated
Considerations for Simulations

- EC thresholds for surface code around 0.5%
- Different problems have different “ε”, and different circuits depths
- Can be mapped differently onto hardware
  - A given hardware configuration (device) of physical qubits may be able to address multiple problems
- Co-developed hardware may be required for given problems
Algorithms, Software Interfacing

Classical Simulation

- Simulations of field theories and strongly-coupled QMB
- Codes developed within community for early special purpose LQCD hardware
- SciDAC (US) brought together domain scientists and AM, CS to optimally develop techniques and software
- Hardware co-developed between Technology Companies, Labs and Universities.
- Effectively advanced our field(s) over many decades

Quantum Simulation

- Technology companies providing “easy” access to devices and light-weight programming languages (with ability to control closer to device)
- Enabled some of the early simulations and “recruited” scientists
- Anticipate coherence in community deep development, parallel and independent efforts for verification purposes.
- Anticipate multiple independent distinct co-design and development (hardware+) activities to address specific scientific requirements.
- IP…. robust and stable science pipeline - within labs and universities
- (Many) domain scientists would like API that is architecture-insensitive
  - robustly compiles onto the hardware target without user changes
Gauge Theory Simulations on Digital Devices

Ciavarella et al
superconducting

Rahman et al
Annealing

Klco, Stryker et al
superconducting

Kharzeev et al
Classical

Martinez et al
Trapped ions

Klco et al
Trapped ions, Superconducting, Annealing
Toward Quantum Chromodynamics

One of a number of frameworks

\[ \psi(R_1, R_2, R_{L3}) \]

Gauge Invariance

Simulating lattice gauge theories on a quantum computer

Tim Byrnes and Yoshihisa Yamamoto
Phys. Rev. A 73, 022328 – Published 17 February 2006
Including $\mathbf{1}, \mathbf{3}, \overline{\mathbf{3}}, \mathbf{8}$ on each link only

\[
|\psi_1^{(1338;+++)}\rangle = |\chi(1, 1, 1, 1, 1)\rangle ,
\]
\[
|\psi_{2a}^{(1338;+++)}\rangle = \frac{1}{2} \left[ |\chi(3, \overline{3}, 3, 1, 3)\rangle + |\chi(\overline{3}, 3, 3, 1, \overline{3})\rangle + |\chi(1, 3, 1, 3, \overline{3})\rangle + |\chi(1, \overline{3}, 1, \overline{3}, 3)\rangle \right] ,
\]
\[
|\psi_{2b}^{(1338;+++)}\rangle = \frac{1}{\sqrt{2}} \left[ |\chi(3, 1, \overline{3}, 3, 1, \overline{3})\rangle + |\chi(\overline{3}, 1, 3, \overline{3}, 1, 3)\rangle \right] ,
\]
\[
|\psi_3^{(1338;+++)}\rangle = \frac{1}{\sqrt{2}} \left[ |\chi(8, 1, 1, 8, 1, 1)\rangle + |\chi(1, 1, 8, 1, 1, 8)\rangle \right] ,
\]
\[\vdots\]
\[
|\psi_9^{(1338;+++)}\rangle = |\chi(8, 8, 8, 8, 8, 8)\rangle
\]

- 15 basis states (4 qubits)
- Max electric energy $\sim 6 \times 3$
- $8 \otimes 8 \otimes 8$

Keeping states with Casimir above 6-threshold includes only part of that higher-energy space
Local Basis Scales

Building on Byrnes+Yamamoto

- Integrate over gauge space at each vertex (classical - Banuls et al, Klco, Stryer et al)
- Controlled plaquette operators
- **Qudits** seem natural for link registers

\[
\hat{H} = \frac{g^2}{2} \sum_{\text{links}} \hat{E}^2 - \frac{1}{2g^2} \sum_{\Box} (\hat{\Box} + \hat{\Box}^\dagger)
\]
To (partially) address Dorota’s question:

**SU(3) KS - Classical/Quantum Resources**

Trailhead for quantum simulation of SU(3) Yang-Mills lattice gauge theory in the local multiplet basis

Anthony Ciavarella, Natalie Klco, Martin J. Savage


<table>
<thead>
<tr>
<th>$\Lambda_p = \Lambda_q$</th>
<th>dimensions</th>
<th>physical states matrix elements</th>
<th>elements/states</th>
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<tbody>
<tr>
<td>1</td>
<td>(1, 3)</td>
<td>81</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>(1, 3, 8)</td>
<td>529</td>
<td>1.92</td>
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<tr>
<td>2</td>
<td>(1, 3, 8, 6)</td>
<td>5,937</td>
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<td>2</td>
<td>(1, 3, 8, 6, 15)</td>
<td>59,737</td>
<td>7.02</td>
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<tr>
<td>2</td>
<td>(1, 3, 8, 6, 15, 27)</td>
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<td>7.54</td>
</tr>
<tr>
<td>3</td>
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<td>(1, 3, 8, 6, 15, 27, 10, 24)</td>
<td>2,008,297</td>
<td>12.27</td>
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</tbody>
</table>

TABLE III. Properties of the plaquette operator truncated in the local index $(p, q)$ basis and at intermediate truncation organized by dimension. The number of physical states constituting the gauge-invariant basis of the plaquette operator, as well as the number of non-zero matrix elements within the physical subspace are presented. The ratio of these two quantities shown in the right column.

**SU(2):**

 Require a 3-dim resource costing

 Exponential convergence in field space

 Number of singlets $\sim$ Cut-off $\wedge^{(2 \text{nR)}}$
e.g., Neutrinos
• Unique time in (scientific) computing - device capabilities are rapidly increasing
• HEP and NP need quantum simulation capabilities
• Exciting and encouraging early results
• Embrace entanglement - build it in where practical
• Consider techniques/develop EFTs to mitigate complexity
• Collaborate on hardware, theory, algorithms and software
• Explore multiple potential paths forward - quantify/benchmark

Thank you to the Organizers!!!
FIN