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On the road to quantum simulating QCD

Zohreh Davoudi University of Maryland, College Park The beautiful world of quarks and gluons builds a world of complexities around us...

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...and continues to push the limits of our theoretical, experimental, and computational abilities to this date!

Even simulating a single proton means solving an infinite-body problem! Quantum mechanics and relativity are in play and interactions are strong!

LATTICE QCD: A MULTI-PRONG PROGRAM THAT SIMULATES QCD NON-PERTURBATIVELY





How to define QCD/Standard Model on a finite grid?

How to preserve/recover symmetries, e.g., gauge symmetry, chiral symmetry, rotational symmetry?

How to take infinite-volume and continuum limits? How to quantify systematics?

How to obtain scattering amplitudes?



Theory developments





Hardware implementation, benchmark, and co-development











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Which tasks can be parallelized and which tasks are done in series?

What are the memory requirements and what kind of node connectivity is required?

Can we take advantage of GPUs? Which parts of the computations are more suitable for given architecture? Hardware implementation, benchmark, and co-development PUTTING ALL THESE HEROIC THEORY, ALGORITHM, AND CO-DESIGN EFFORTS TO WORK AND HAVING ACCESS TO HUNDREDS OF MILLION CPU HOURS ON THE LARGEST SUPERCOMPUTERS IN THE U.S. HAS LED TO MANY IMPRESSIVE RESULTS.



Titan supercomputer, Oak Ridge National Laboratory, USA



For a recent review see: ZD, Detmold, Orginos, Parreño, Savage, Shanahan, Wagman, Phys. Rept. 900, 1-74 (2021).



LATTICE QCD IS SUPPORTING A MULTI-BILLION DOLLAR EXPERIMENTAL PROGRAM!



Slide content courtesy of Martin Savage.

LATTICE QCD IS SUPPORTING A MULTI-BILLION DOLLAR EXPERIMENTAL PROGRAM!



THREE FEATURES MAKE LATTICE QCD CALCULATIONS OF NUCLEI HARD:

i) The complexity of systems grows factorially with the number of quarks.

Detmold and Orginos (2013) Detmold and Savage (2010) Doi and Endres (2013)





ii) There is a severe signal-to-noise degradation.

Paris	(1984	l) and	Lepage	(1989)
Wagman	and	Savage	(2017,	2018)

iii) Excitation energies of nuclei are much smaller than the QCD scale.

Beane at al (NPLQCD) (2009) Beane, Detmold, Orginos, Savage (2011) ZD (2018) Briceno, Dudek and Young (2018)



i) Studies of nuclear isotopes, dense matter, and phase diagram of QCD...both with lattice QCD and with *ab initio* nuclear many-body methods.

Path integral formulation:

$$e^{-S[U,q,\bar{q}]}$$

with a complex action:

$$\mathcal{L}_{\text{QCD}} \to \mathcal{L}_{\text{QCD}} - i\mu \sum_{f} \bar{q}_{f} \gamma^{0} q_{f}$$



ii) Real-time dynamics of matter in heavy-ion collisions or after Big Bang...

...and a wealth of dynamical response functions, transport properties, hadron distribution functions, and non-equilibrium physics of QCD.

Path integral formulation:



Hamiltonian evolution:

$$U(t) = e^{-iHt}$$



An opportunity to explore new paradigms and new technologies: Turning to quantum simulation

Quantum Information Science and Technology for Nuclear Physics, Beck, Carlson, Davoudi, Formaggio, Quaglioni, Savage, et al, arXiv:2303.00113 [nucl-ex].

Quantum Simulation for High Energy Physics, Bauer, ZD et al, arXiv:2204.03381 [quant-ph], *PRX Quantum* 4 (2023) 2, 027001.

https://www.pechakucha.com/

A RANGE OF QUANTUM SIMULATORS WITH VARING CAPACITY AND CAPABILITY

- Atomic systems (trapped ions, cold atoms, Rydbergs)
- Condensed matter systems (superconducting circuits, dopants in semiconductors such as in Silicon, NV centers in diamond)
- Laser-cooled polar molecules
- Optical quantum computing



HOW SIMILAR TO QUANTUM CHEMISTRY SIMULATIONS?



Image credit: CERN courier

Both bosonic and fermionic DOF are dynamical and coupled, exhibit both global and local (gauge) symmetries, relativistic hence particle number not conserved, vacuum state nontrivial in strongly interacting theories.

Attempts to cast QFT problems in a language closer to quantum chemistry and NR simulations: Kreshchuk, Kirby, Goldstein, Beauchemin, Love, arXiv:2002.04016 [quant-ph], Kreshchuk, Jia, Kirby, Goldstein, Vary, Love, Entropy 2021, 23, 597, Liu, Xin, arXiv:2004.13234 [hep-th], Barata , Mueller, Tarasov, Venugopalan (2020) QUANTUM SIMULATION OF QUANTUM FIELD THEORIES: A MULTI-PRONG EFFORT



QUANTUM SIMULATION OF QUANTUM FIELD THEORIES: A MULTI-PRONG EFFORT



Major focus on my work with my group and collaborators! Apologies for the missing references.



How to formulate QCD in the Hamiltonian language?

What are the efficient formulations? Which bases will be most optimal toward the continuum limit?

How to preserve the symmetries? How much should we care to retain gauge invariance?

How to quantify systematics such as finite volume, discretization, boson truncation, time digitization, etc?

Theory developments

Hamiltonian formalism is a more natural than the path integral formalism for quantum simulation/computation:

Kogut and Susskind formulation:

$$H_{\text{QCD}} = -t \sum_{\langle xy \rangle} s_{xy} \left(\psi_x^{\dagger} U_{xy} \psi_y + \psi_y^{\dagger} U_{xy}^{\dagger} \psi_x \right) + m \sum_x s_x \psi_x^{\dagger} \psi_x + \frac{g^2}{2} \sum_{\langle xy \rangle} \left(L_{xy}^2 + R_{xy}^2 \right) - \frac{1}{4g^2} \sum_{\Box} \text{Tr} \left(U_{\Box} + U_{\Box}^{\dagger} \right).$$

Fermion hopping term
Fermion mass
Energy of color
electric field
Energy of color magnetic field



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Fermion hopping term Fermion Energy of color Energy of color mass electric field magnetic field
Generator of infinitesimal $G_x^a = \psi_x^{i\dagger} \lambda_{ij}^a \psi_x^j + \sum_k \left(L_{x,x+\bar{k}}^a + R_{x-\bar{k},x}^a \right) \implies G_x^i |\psi(\{q_x^{(i)}\})\rangle = q_x^{(i)} |\psi(\{q_x^{(i)}\})\rangle$
Electric Spherical Gaussian surface field lines Gauss's law Inage credit: https://physicsteacher.in/

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mass

Kogut and Susskind formulation:

$$H_{\text{QCD}} = -t \sum_{\langle xy \rangle} s_{xy} \left(\psi_x^{\dagger} U_{xy} \psi_y + \psi_y^{\dagger} U_{xy}^{\dagger} \psi_x \right) + m \sum_x s_x \psi_x^{\dagger} \psi_x + \frac{g^2}{2} \sum_{\langle xy \rangle} \left(L_{xy}^2 + R_{xy}^2 \right) - \frac{1}{4g^2} \sum_{\Box} \text{Tr} \left(U_{\Box} + U_{\Box}^{\dagger} \right).$$

Fermion hopping term Fermion Energy of color Energy of color

Generator of infinitesimal $G_x^a = \psi_x^{i\dagger} \lambda_{ij}^a \psi_x^j + \sum_k \left(L_{x,x+\hat{k}}^a + R_{x-\hat{k},x}^a \right) \implies G_x^i |\psi(\{q_x^{(i)}\})\rangle = q_x^{(i)} |\psi(\{q_x^{(i)}\})\rangle$ gauge transformation

electric field magnetic field







IDEAS TO SUPPRESS LEAKAGE TO UNPHYSICAL SECTOR IN THE SIMULATION



Rev. D 101, 114502 (2020).

SU(3) extension: Kadam,, Raychowdhury, Stryker, arXiv:2212.04490 [hep-lat] (2022).

IDEAS TO SUPPRESS LEAKAGE TO UNPHYSICAL SECTOR IN THE SIMULATION



Gauge-field theories (Abe	elian and non	-Abelian):
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Group-element representation Zohar et al; Lamm et al Mathu		otential formulation ur, Raychowdhury et al		Loop-String-Hadron basis Raychowdhury, Stryker, Kadam	
Link models, qubitization Chandrasekharan, Wiese et al, Alexandru, Bedaque, et al, Hersch et al.		Fermio Hamer Banuls	nic basis et al; Martinez et al; et al		Bosonic basis Cirac and Zohar
Light-front quantization Loc Kreshchuk, Love, Goldstien, Byr Vary et al.; Ortega Rico at al Cia		cal irreducible representations rnes and Yamamoto; avarella, Klco, and Savage		Manifold lattices Buser et al	
Dual plaquette (magnetic) basis Bender, Zohar et al; Kaplan and Styker; Unmuth- Yockey; Hasse et al; Bauer and Grabowska			Sp Ma	in-dual rep athur et al	presentation
Scalar field theory					
Field basis Jordan, Lee, and Pres	Cont Poos	inuous-vari er, Siopsis	iable basis et al		
Harmonic-oscillator basis Klco and Savage Barata , Mueller, Tarasov, and Venugopalan.					

Algorithmic developments [Digital]

Near- and far-term algorithms with bounded errors and resource requirement for gauge theories?

Can given formulation/encoding reduce qubit and gate resources?

Should we develop gauge-invariant simulation algorithms?

How do we do state preparation and compute observables like scattering amplitudes?

Algorithmic developments [Digital]

Near- and far-term algorithms with bounded errors and resource requirement for gauge theories?

Can given formulation/encoding reduce qubit and gate resources?

Can we develop gauge-invariant simulation algorithms?

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How do we do state preparation and compute observables like scattering amplitudes?





How many qubits and gates are required to achieve accuracy ϵ in a given observables? Are there algorithms that scale optimally?

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Important algorithmic progress for U(1), SU(2), and SU(3) theories can be found in:
Shaw, Lougovski, Stryker, Wiebe, Quantum 4, 306 (2020).
Ciavarella, Klco, and Savage, Phys. Rev. D 103, 094501 (2021).
Kan and Nam, arXiv:2107.12769 [quant-ph].
ZD, Shaw (2), and Stryker, arXiv:2212.14030 [hep-lat] (2022).
Gustafson, Lamm, Lovelace, and Musk, arXiv:2208.12309 [quant-ph] (2022).
```

Example: SU(2) gauge theory coupled to matter in 1+1 D with loops, strings, hadrons

ZD, Shaw, and Stryker, General Quantum Algorithms for Hamiltonian Simulation with Applications to a Non-Abelian Lattice Gauge Theory, arXiv:2212.14030 [hep-lat] (2022).





Algorithmic developments [Analog]

Can practical proposals for current hardware be developed?

Can we simulate higherdimensional gauge theories?

Can non-Abelian gauge theories be realized in an analog simulator?

Can we robustly bound the errors in the analog simulation? What quantities are more robust to errors?







ZD, Hafezi, Monroe, Pagano, Seif, Shaw, Phys. Rev. Research, 2, 023015 (2020), arXiv: 1908.03210 [quant-ph].

 \bigcap

See for other ideas: Ciavarella, Caspar, Singh, Savage, Lougovski, arXiv:2207.09438 [quant-ph].

$$H_{\text{eff}} = \sum_{\substack{i,j \\ j < i}} \left[J_{i,j}^{(xx)} \sigma_x^{(i)} \otimes \sigma_x^{(j)} + J_{i,j}^{(yy)} \sigma_y^{(i)} \otimes \sigma_y^{(j)} + J_{i,j}^{(zz)} \sigma_z^{(i)} \otimes \sigma_z^{(j)} \right] - \frac{1}{2} \sum_{i=1}^N B_z^{(i)} \sigma_z^{(i)}$$

$$\boxed{\text{No gates}}$$

$$e^{-iHt}$$

Recent development: N-body interactions: Katz, Centina, Monroe, Phys. Rev. Lett. 129, 063603 (2022). Andrade, ZD, Grass, Hafezi, Pagano, Seif, arXiv:2108.01022 [quant-ph], See also: Bermudez et al, Pays.Rev.A79, 060303 R (2009).

Analog
$$H_{\text{eff}} = \sum_{i} J_{i}^{(\sigma)} \sigma_{z}^{(i)} + \sum_{i,j} J_{i,j}^{(\sigma\sigma)} \sigma_{+}^{(i)} \otimes \sigma_{+}^{(j)} + \sum_{i,j,k} J_{i,j,k}^{(\sigma\sigma\sigma)} \sigma_{+}^{(i)} \otimes \sigma_{+}^{(j)} \otimes \sigma_{+}^{(k)} + \text{h.c.}$$
No gates
$$e^{-iHt}$$



$$H = x \sum_{n=1}^{N-1} \left[\sigma_{+}^{(n)} \sigma_{-}^{(n+1)} + \sigma_{+}^{(n+1)} \sigma_{-}^{(n)} \right] + \sum_{n=1}^{N-1} \left[\epsilon_{0} + \frac{1}{2} \sum_{m=1}^{n} \left(\sigma_{z}^{(m)} + (-1)^{m} \right) \right]^{2} + \frac{\mu}{2} \sum_{n=1}^{N} (-1)^{n} \sigma_{z}^{(n)}$$



ZD, Hafezi, Monroe, Pagano, Seif and Shaw, Phys. Rev. R 2, 023015 (2020).

$$H = x \sum_{n=1}^{N-1} \left[\sigma_{+}^{(n)} \sigma_{-}^{(n+1)} + \sigma_{+}^{(n+1)} \sigma_{-}^{(n)} \right] + \sum_{n=1}^{N-1} \left[\epsilon_{0} + \frac{1}{2} \sum_{m=1}^{n} \left(\sigma_{z}^{(m)} + (-1)^{m} \right) \right]^{2} + \frac{\mu}{2} \sum_{n=1}^{N} (-1)^{n} \sigma_{z}^{(n)}$$



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What is the capability limit of the hardware for gauge-theory simulations so far?

What is the nature of noise in hardware and how can it best be mitigated?

Can we co-develop dedicated systems for gauge-theory simulations?

Can digital and analog ideas be combined to facilitate simulations of field theories?

Implementation, benchmark, and co-development



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IMPLEMENTATIONS ON THE ACTUAL QUANTUM HARDWARE



IMPLEMENTATIONS ON THE ACTUAL QUANTUM HARDWARE



NON-ABELIAN GAUGE THEORIES: HARDWARE IMPLEMENATTION



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$$H = -ix \sum_{n=1}^{N-1} \left[\psi_n^{\dagger} U_n \psi_{n+1} - \text{h.c.} \right] + \sum_{n=1}^{N-1} E_n^2 + \mu \sum_{n=1}^{N} (-1)^n \psi_n^{\dagger} \psi_n$$



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Let us compare the circuit structure of digital and analog-digital cases when gauge DOF are present:

Schwinger model					
	Fermion-gauge interaction	Fermion mass	Electric-field term		
Analog-digital	$\mathcal{O}\left(N ight)$	$\mathcal{O}\left(1 ight)$	$\mathcal{O}(N)$		
Digital	$\mathcal{O}\left(N^2\left(\log\Lambda\right)^2 ight)$	$\mathcal{O}\left(1 ight)$	$\mathcal{O}\left(N\left(\log\Lambda\right)^2 ight)$		

Is phonon control experimentally feasible? Yes...at least for small systems so far! ZD, Linke, Pagano, Phys. Rev. Research 3, 043072 (2021).





Debnath et al, Phys. Rev. Lett. 120, 073001 (2018).

Finally a few more examples showcasing progress in hardware implementation of a range of QCD-inspired problems...



A polynomial time quantum final state shower algorithm that accurately models the effects of intermediate spin states similar to those present in electroweak showers.

See also Bepari, Malik, Spannowsky, Williams, Phys. Rev. D 103, 076020 (2021), Williams, Malik, Spannowsky, Bepari, Phys. Rev. D 106 (2022) 056002, Gustafson, Prestel, Spannowsky, Williams, J. High Energ. Phys. 2022, 35 (2022).



PARTON DISTRIBUTION FUNCTIONS, DECAY AMPLITUDES





FIRST STEPS TOWARD SCATTERING IN SPIN SYSTEMS — NUMERICAL SIMULATIONS —



THERMALIZATION AND NON-EQUILIBRIUM PROPERTIES

Thermalization dynamics of U(1) Quantum Link Model in a 71-site analog simulator Gauss's law Zhou et al, Science 377 (a) $3.0 \cdot N = 4$ (2022) 6603. 2.0 Gauge fields Matter fields $\nu(t)$ Energy density (κ) $\hat{H}(m = -0.8\kappa)$ 1.01.0 0.0 (b)20 τ (ms) N = 810.8 2.01.5 $\overbrace{\ell}{}^{(t)}_{1.0}$ 100 Quench evolution time t (ms) 0.50.5 0.0 Stages of thermalization dynamics of Z2 LGT in 2+1 D from entanglement spectrum Mueller, Zache, Ott, Phys. Rev. (a) **State Preparation** Lett. 129, 011601 (2022). $|\tilde{\Omega}\rangle$ $H_0(+m) | \tilde{\Omega} \rangle = E_0 | \tilde{\Omega} \rangle$ Maximization of spreading of entanglement self-simila saturation of Schmidt rank and level repulsion evolution thermal entropy ⊢► 0.1 50 200 e Gap Ratio $\langle r_n \rangle$ 9:0
 0 $\begin{array}{c} 1.00\\ \textbf{Distribution} \ \mathcal{P}(s_n,t)\\ 0.22\\ 0.2$ = 🛛 $\Box \quad \epsilon \cdot t = 0 \text{ (TO)}$ $\Box \quad \epsilon \cdot t \ge 1 \text{ (TO)}$ $\epsilon \cdot t \ge 1 \text{ (RPS)}$ (b) Entr. $|0\rangle - H$ **Average** 0.0 (c)200 100 $|\tilde{\Omega}\rangle$ Q U(t) $\epsilon \cdot t$ 0.00 0 2 3) 0 2 1 Level Spacing s_n Time $\epsilon \cdot t$ Loschmidt echo L(t)

A dynamical phase transition and $(a)_{1.5}$ topological order in lattice N = 4simulator e/m = 0Schwinger model with an IonQ IonQ 1.0quantum computer: $\stackrel{(t)}{T}_{0.5}$ simulator IonQ 0.0 real part $\nu = 2$ **DO --** imag part (b) 0.60.5e/m = 0 $\nu = 0$ 0.4(1) 0.3 $\nu = 2$ 0.2DQP1 0.1 0.0 $n_{
m shots}$ $\nu = 0$ physical 1.0 1.5 2.00.0 0.51.0 2.0 1.5 $t \cdot m$ $t \cdot m$ Mueller, Carolan, Connelly, Dumitrescu, ZD, Mueller, Yeter-Aydeniz, to be released (2022). Basis **Time Evolution** Transformations Hamiltonian evolution $U(t) = e^{-iH(-m)t}$ Quench Diagonal Hamiltonian $m \rightarrow - n$ $e^{-iH_0\delta t}$ $e^{-iH_I\delta t}$ Evolution $\frac{e}{m} > 0$ Π V^{\dagger} $Q = \bigotimes_a Q_a$ State Preparation e^{-iH_0t} e = 0(Fast forwarding) Measurement (c) **Entanglement Tomography** Non-equal Time Observables Random Classical $|0\rangle - H$ neasurement postprocessing $P_U(s)$ $|\tilde{\Omega}\rangle$ Q =U(t) ψ_0 $U^{\dagger}(t)$ ψ_n^{\dagger} U Rényi entropy CUE fidelity Non-equal time correlator $g_a(t)$

FINITE TEMPERATURE AND FINTIE DENSITY PHASE DIAGRAM



QUANTUM ENTANGLEMENT IN HIGH- AND LOW-ENERGY NUCLEAR PHYSICS



We've got a long way to go to get to **QCD** but we know what to do! If one thing we learned from the successful conventional lattice-QCD program is that **theory/ algorithm/experiment** collaborations will be the key. It is even more important in the quantum-computing era since our computers are themselves physical systems!





OTHER COLLABORATORS I AM ENJOYING WORKING WITH IN ONGOING PROJECTS:

Ani Bapat (P) @LBNL

Ron Belyansky (S) @UMD

Elizabeth Bennewitz (S) @UMD

Marko Cetina (F) @Duke

Kate Collins (S) @UMD

Ali Fahimniya (P) @UMD

Lei Feng (P) @Duke

* Navya Gupta (S) @UMD

* Chung-Chun Hsieh (S) @UMD

Or Katz (P) @Duke

Alessio Lerose (P) @U of Geneva

Will Morong (P) @UMD

Alexander Schuckert (P) @UMD

Federica Surace (P) @Caltech

Brayden Ware (P) @UMD

* Christopher White (P) @UMD

Seth Whitsitt (P) @UMD

* Group member

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