

Quantum Chromodynamics in the Exascale Era with the Emergence of Quantum Computing

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The Objective

Imagine being able to predict – with unprecedented accuracy and precision – the structure of the proton and neutron, and the forces between them, directly from the dynamics of quarks and gluons, and then using this information in calculations of the structure and reactions of atomic nuclei and of the properties of dense neutron stars...







Hadrons and Nuclei











Hot and Dense Matter



LHC Quark-Gluon Plasma Temperature RHIC possible critical point Ist-orde phase trans Hadrons Atomic nuclei Neutron stars Baryon density



Nuclei and Nuclear Matter









"Parking-garage" structures in nuclear astrophysics and cellular biophysics D.K. Berry, M.E. Caplan, C.J. Horowitz, Greg Huber, A.S. Schneider. Phys.Rev. C94 (2016) no.5, 055801



Nuclear Physics Scientific Objectives and Applications Rely on High-Performance Computing





Essential, Extensive Collaboration





Necessity is the Mother of Invention





Mid-scale GPU-accelerated Cluster Precursor to Exascale Architectures



QCDSP : 1998 Gordon Bell Prize

HEP-NP collaboration has been essential to NP program



Mission critical, custom logic (testured) for high-pertamance memory access and fast, low-takency off-node communications is combined with standards-based, highly integrated commercial library components.









Exascale Ecosystem for Nuclear Physics

CAPABILITY/CAPACITY RESOURCES VS. HOT/COLD DATA RESOURCES IN 2025 COLD QCD



* Exaflop-system-year refers to the total amount of computation produced by an exascale computer in 1 year.

A single Exascale machine will be immediately oversubscribed by a large factor



Quantum Chromodynamics and NP



Protons and Neutrons

Quarks and Gluons



Quantum Chromodynamics Path Integrals and Lattice QCD

Minkowski Space - probability amplitudes of unit norm

$$Z \propto \int \mathcal{D}A^a_\mu \mathcal{D}\overline{q}_i \mathcal{D}q_i \; e^{rac{i}{\hbar}\int d^4x \; \mathcal{L} + \mathcal{L}_{g.f.} + \mathcal{L}_{ ext{ghosts}}}$$

$$\mathcal{L} = \sum_{i=u,d,s,c,b,t} \overline{q}_i \left[i D - m_i \right] q_i - \frac{1}{4} \sum_{a=1,\dots,8} G^a_{\mu\nu} G^{\mu\nu,a}$$

Euclidean Space - probability distribution

$$\langle \hat{\theta} \rangle \sim \int \mathcal{D}\mathcal{U}_{\mu} \ \hat{\theta}[\mathcal{U}_{\mu}] \ \det[\kappa[\mathcal{U}_{\mu}]] \ e^{-S_{YM}}$$

$$\rightarrow \frac{1}{N} \sum_{\text{gluon cfgs}}^{N} \hat{\theta}[\mathcal{U}_{\mu}] \xrightarrow{\text{Gauge fields sampled}} Fermion integrals can be performed analytically}$$

$$11$$



11



Lattice Quantum Chromodynamics - Discretized Euclidean Spacetime



Lattice Spacing : $a << 1/\Lambda \chi$

(Nearly Continuum)

Lattice Volume : $m_{\pi}L >> 2\pi$

(Nearly Infinite Volume)

Extrapolation to a = 0 and $L = \infty$

Systematically remove non-QCD parts of calculation through effective field theories





Recovering SO(3) from H(3)



Hold all physical scales, and the renormalization scale fixed when taking lattice spacing to zero

Survives at quantum level in QCD - smearing is critical so as not to ``see" the UV cubic structure

Multiplicity of irreps of H(3) allow for combinations to approach SO(3) states - both in position space (a) and momentum space (L)





Lattice QCD The Discretized Action

$$U_{\mu}(x) = \exp\left(i\int_{x}^{x+\hat{\mu}} dx' A_{\mu}(x')\right)$$
$$U_{\mu}(x) \rightarrow U_{\mu}'(x) = \Omega(x)U_{\mu}(x)\Omega^{-1}(x+\hat{\mu})$$
$$P_{\mu\nu} = U_{\mu}(x)U_{\nu}(x+\hat{\mu})U_{\mu}^{\dagger}(x+\hat{\nu})U_{\nu}^{\dagger}(x)$$

$$S_{\text{classical}} \equiv -\beta \sum_{x,\mu>\nu} \left\{ \frac{5P_{\mu\nu}}{3} - \frac{R_{\mu\nu} + R_{\nu\mu}}{12} \right\} + \text{const}$$
$$= \int d^4x \sum_{\mu,\nu} \frac{1}{2} \operatorname{Tr} F_{\mu\nu}^2 + \mathcal{O}(a^4).$$

$$S = -\beta \sum_{x,\mu > \nu} \left\{ \frac{5}{3} \frac{P_{\mu\nu}}{u_0^4} - \frac{R_{\mu\nu} + R_{\nu\mu}}{12 \, u_0^6} \right\}$$

Quantum gauge action tadpole improved









Lattice QCD The Quark Masses



N_f	m_u	m_d	m_u/m_d
2 + 1	2.16(9)(7)	4.68(14)(7)	0.46(2)(2)
2	2.40(23)	4.80(23)	0.50(4)



 $\overline{\mathrm{MS}}$, $\mu = 2 \ \mathrm{GeV}$



Lattice QCD Sketch of Methodology

Start with a selection of quark+gluon sources and sinks ``designed" to have good overlap onto the low-lying hadronic/nuclear states in the volume.

Iteratively (manually) refine to produce ``best estimates" of QCD states.

Form correlation functions between all combinations

Diagonalize to find the energy eigenvalues and eigenstates (Variational or other)

Post-analyze accordingly

- Luscher's Methods for S-matrix elements,...

I anticipate this sort of refinement of sources and sinks occur before initializing a QC.





Lattice QCD Spectroscopy and GlueX





Lattice QCD **Fundamental Symmetries**



 $\langle d; 3 | A_3^- | pp \rangle / Z_A$







Phys.Rev. D94 (2016) no.5, 054508



Lattice QCD QCD to Nuclear Forces: First Steps





Michael L. Wagman, Frank Winter, Emmanuel Chang, Zohreh Davoudi, William Detmold, Kostas Orginos, Martin J. Savage, Phiala E. Shanahan, arXiv:1706.06550

Finite-Volume Energy Eigenvalues

Unnatural systems with approximate SU(6) and SU(16) Spin-Flavor Symmetries

¹⁶O appears to be unbound - limits of Periodic Table

Must calculate over a range of quark masses to refine nuclear forces



Lattice QCD Mass-Splittings





BMW collab



e.g., Proton Structure Deliverables

Quantities with currently quantifiable uncertainties and goals

Quantity	Current uncertainty	Uncertainty Goal	Impact/Target
g_A	5%	3%→1%	Benchmark of LQCD; Neutrino-nucleus X-secs V _{ud} given high enough precision
L_u, L_d	~20%	5%	Understanding the spin of the proton
g_S,g_T	20%, 7%	10%, 3%	Ultracold neutron experimental searches for BSM interactions in neutron decay
$a_{\pi\pi}^{(I=2)}$	1%	\checkmark	More precise than experiment/phenomenology
$\langle N \overline{s}s N\rangle$	25%	10%	Input for dark matter direct detection experiments; mu2e conversion
$\langle x \rangle$	~15%	5%	Aim for ab initio input to PDFs (USQCD goal)
$\langle r^2 \rangle_p$	~10%	2%	Impact proton radius puzzle
L_1, L_{1A}	20%	5%	pp fusion; next generation neutrino detectors

Most goals achievable achievable in 2021 timeframe



Systems to Explore Quantum Computing Potential

S-matrix elements, equilibrium properties, definite quantum numbers, e.g., 2 neutrons and 1 proton



Time evolution of system with baryon number, isospin, electric charge, strangeness, Currents, viscosity, non-equilibrium dynamics - real-time evolution











Systems to Explore Quantum Computing Potential

S-matrix elements, equilibrium properties, definite quantum numbers, i.e. 2 neutrons and 1 proton

Time evolution of system with baryon number, isospin, electric charge, strangeness, Currents, viscosity, non-equilibrium dynamics - real-time evolution





Systems to Explore Quantum Computing Potential One Baryon and More











Systems to Explore Quantum Computing Potential Combinatorics and Antisymmetry

Large number of quark contractions



Proton : N $^{cont} = 2$ ^{235}U : N $^{cont} = 10^{1494}$

$$N_{\text{cont.}} = u!d!s! \text{ (Naive)}$$
$$= (A+Z)!(2A-Z)!s!$$

Symmetries provide significant reduction

 ${}^{3}\text{He}\ :\ 2880 \rightarrow 93$ Recursion Relations are crucial



Systems to Explore Quantum Computing Potential Finite Density, Chemical Potentials

Time evolution of system with baryon number, isospin, electric charge, strangeness, Currents, viscosity, non-equilibrium dynamics - real-time evolution



 $\langle \hat{\theta} \rangle \sim \int \mathcal{D}\mathcal{U}_{\mu} \ \hat{\theta}[\mathcal{U}_{\mu}] \det[\kappa[\mathcal{U}_{\mu}]] \ e^{-S_{YM}}$ Complex for non-zero chemical potential



Systems to Explore Quantum Computing Potential Finite Density, Chemical Potentials

Time evolution of system with baryon number, isospin, electric charge, strangeness, Currents, viscosity, non-equilibrium dynamics - real-time evolution

6

Taylor expansion in μ/T (methodology)

$$\frac{p(\vec{\mu},T)}{T^4} = \sum_{i,j,k=0}^{\infty} \frac{1}{i!j!k!} \chi^{BQS}_{i,j,k}(T) \left(\frac{\mu_B}{T}\right)^i \left(\frac{\mu_Q}{T}\right)^j \left(\frac{\mu_S}{T}\right)^k$$

$$\text{ with } \left. \chi^{BQS}_{i,j,k}(T) = \frac{1}{VT^3} \left. \frac{\partial^{i+j+k} \ln Z(\vec{\mu},T)}{\partial \hat{\mu}^i_B \partial \hat{\mu}^j_Q \partial \hat{\mu}^k_S} \right|_{\vec{\mu}=0} \text{ and } \hat{\mu} = \mu/T$$

Example:

$$\frac{\partial^2 \ln Z}{\partial \mu^2} = \langle \operatorname{Tr} \left[M^{-1} M'' \right] \rangle - \langle \operatorname{Tr} \left[M^{-1} M' M^{-1} M' \right] \rangle + \left\langle \operatorname{Tr} \left[M^{-1} M' \right]^2 \right\rangle$$
$$\simeq \left\langle n^2(x) \bigoplus \right\rangle - \left\langle n(x) \bigoplus n(y) \right\rangle + \left\langle n(x) \bigoplus n(y) \right\rangle$$

C. Schmidt, SIGN 2017, INT-17-64W, Seattle, WA, USA



In production - large resource requirements - limits are visible



Systems to Explore Quantum Computing Potential Formal Developments

Time evolution of system with baryon number, isospin, electric charge, strangeness, Currents, viscosity, non-equilibrium dynamics - real-time evolution

How to find good deformations ?

Field redefinitions that eliminate or reduce the phase

- Lefschetz Thimbles



real fields $\tilde{\phi}$ parametrize the flowed R^N:

$$S_{eff}[\tilde{\phi}] = S[\phi(\tilde{\phi})] - \log J[\tilde{\phi}]$$

Bedaque, Warrington, ..., Sign 2017, INT

Not yet in large-scale production for QCD - formal algorithm developments



Quantum Field Theory A couple of theory papers that jump out

Simulating lattice gauge theories on a quantum computer

Tim Byrnes^{*} National Institute of Informatics, 2-1-2 Hitotsubashi, Chiyoda-ku, Tokyo 101-8430, Japan

Yoshihisa Yamamoto E. L. Ginzton Laboratory, Stanford University, Stanford, CA 94305 and National Institute of Informatics, 2-1-2 Hitotsubashi, Chiyoda-ku, Tokyo 101-8430, Japan (Dated: February 1, 2008)

We examine the problem of simulating lattice gauge theories on a universal quantum computer. The basic strategy of our approach is to transcribe lattice gauge theories in the Hamiltonian formulation into a Hamiltonian involving only Pauli spin operators such that the simulation can be performed on a quantum computer using only one and two qubit manipulations. We examine three models, the U(1), SU(2), and SU(3) lattice gauge theories which are transcribed into a spin Hamiltonian up to a cutoff in the Hilbert space of the gauge fields on the lattice. The number of qubits required for storing a particular state is found to have a linear dependence with the total number of lattice sites. The number of qubit operations required for performing the time evolution corresponding to the Hamiltonian is found to be between a linear to quadratic function of the number of lattice sites, depending on the arrangement of qubits in the quantum computer. We remark that our results may also be easily generalized to higher SU(N) gauge theories.

Phys.Rev. A73 (2006) 022328

Detailed formalism for 3+1 Hamiltonian Gauge Theory

Discretrized spatial volume - no quarks

10⁴ spatial lattice sites would require 10⁵ * D qubits , D=size of register defining value of the field

Quantum Computation of Scattering in Scalar Quantum Field Theories

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Abstract

Quantum field theory provides the framework for the most fundamental physical theories to be confirmed experimentally, and has enabled predictions of unprecedented precision. However, calculations of physical observables often require great computational complexity and can generally be performed only when the interaction strength is weak. A full understanding of the foundations and rich consequences of quantum field theory remains an outstanding challenge. We develop a quantum algorithm to compute relativistic scattering amplitudes in massive ϕ^4 theory in spacetime of four and fewer dimensions. The algorithm runs in a time that is polynomial in the number of particles, their energy, and the desired precision, and applies at both weak and strong coupling. Thus, it offers exponential speedup over existing classical methods at high precision or strong coupling.

Quantum Information and Computation 14, 1014-1080 (2014)

Scalar Field Theory - Hamiltonian is nice



Quantum Chromodynamics Asymptotic States



Asymptotic states of QCD are nonperturbative states of quarks and gluons, and the strong vacuum itself is condensate of quarks and gluons that breaks (approximate) global symmetries of QCD.

Hamiltonian or not or both? Parallel Integrator ?

Maybe start with recovering energy-eigenvalues, and S-matrix elements ala Luscher - classical computing provides optimal spatial sources/sinks ?

Initialization of QC registers - what is the mapping of the problem?



QCD Hamiltonian on a Spatial Lattice

One way to tackle this, might not be the only or best way

+improvements in discretization (clover, etc)+ or actions with good chiral symmetry



What is the Quenched QCD Vacuum : E^a I0>=0 ?

Random fields at each point in spacetime is far from ground state.

- generally all 0++ states will be populated with some amplitude

I random > = a |0> + b |(GG)> + c | (GG)(GG)> +





I random > needs to be ``cooled" to IO>
- repeated ``cuts" after Quantum Fourier Transform ?

In Lattice QCD, first 1000 steps of HMC thermalize

Euclidean-space Lattice QCD will likely be required to provide initialization of vacuum. How to do this ?



What is the Full QCD Vacuum : E^a I0>=0 ?

Random fields at each point in spacetime is far from ground state.

- generally all 0++ states will be populated with some amplitude

I random > = a I0> + b I(pi pi)> + c I (pi pi pi pi) > + + d I (GG) > +





I random > needs to be ``cooled" to I0>
- repeated ``cuts" after Quantum Fourier Transform ?

Euclidean-space Lattice QCD will likely be required to provide initialization of vacuum. How to do this ?



QC for Hamiltonian QCD Naive Estimates of System Register



Gluon Fields:

for each direction (8 real numbers) * (resolution of value of each field)

QC for Hamiltonian QCD Naive Estimates of System Register

Each site has a register of qubits, scales e.g., fully-dynamical QCD with spatial volume u,d,s quarks Number of Qubits = $36 L^3 + 24 L^3 n_{res}$ L=10 and $n_{res}=6$ Number of Qubits $= 180 L^3 = 180 K$ c/w: Quenched QCD L=10 and $n_{res}=6$ Number of Qubits = $24 L^3 n_{res} = 144K$ c/w: Scalar-field Theory: L=10 and n_{res}=6

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Number of Qubits = L^3 n_{res} = 6K
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Lattice spacing and volume extrapolations remain

Some (quasi-random) thoughts

1+1 dim Schwinger model simulated by integrating out gauge fields to leave a spin-model with non-local interactions, (Martinez et al (2016), and others) - caught my attention!

In LQCD with QED : Gauss's law violated by PBCs in LQCD calculations with QED, introduces non-locality, but it is OK as only the zero-mode is removed !

At present, co-design seems essential - developing algorithms for present and near-term QC hardware, as opposed to ``fantasy/wishful thinking" QC hardware.

Resource requirement estimates (qubits, gates, oracles) need to be for the integrated application - i.e. what will it actually take to complete the physics objective.

Physics understanding/techniques and algorithms in NP and HEP may be of benefit to more general QC objectives

The Role of Quantum Computing for QCD in NP (circa 2017 !)

Classical computing is on track to provide sufficient precision for many experimentally important quantities in HEP and NP in the Exascale.

Finite density systems (including modest size nuclei) require exponentially challenging calculations that may be better suited to QCs in the longer-term.

Anticipate that Exascale classical systems will be required to ``precondition''/ map problem onto qubit registers of QC and then read from qubit registers - BUT currently little is known how to use a QC for QCD

QCs may be first used to accelerate parts of classical Lattice QCD calculations.

The next decade will be looked back upon as an important period in QCD in both HEP and NP because of High Performance Computing - possibly accelerated by Quantum Computers.

We speculate that Quantum Computing will be significant in studies of finite-density systems and may be central in achieving important objectives in Nuclear Physics, but significant R+D is required in this area.

The pyramid of classical HPC resources in the exascale is (and will remain) essential.

- QC Algorithms are required for QCD to address
 - systems of nucleons
 - finite density, chemical potentials
 - Hamiltonian evolution
 - Implementing low-energy effective field theories renormalization group techniques, truncated Hilbert space techniques
- Collaborations with QC/QI experts to accomplish the science objectives
- Co-design important

``Standing up" QCD on QCs important for NP and HEP.

The most naive implementation appears costly - but this is just the beginning ...

FIN