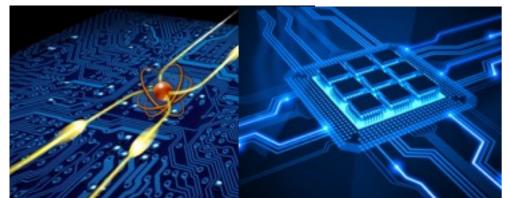




Quantum Chromodynamics in the Exascale Era with the Emergence of Quantum Computing

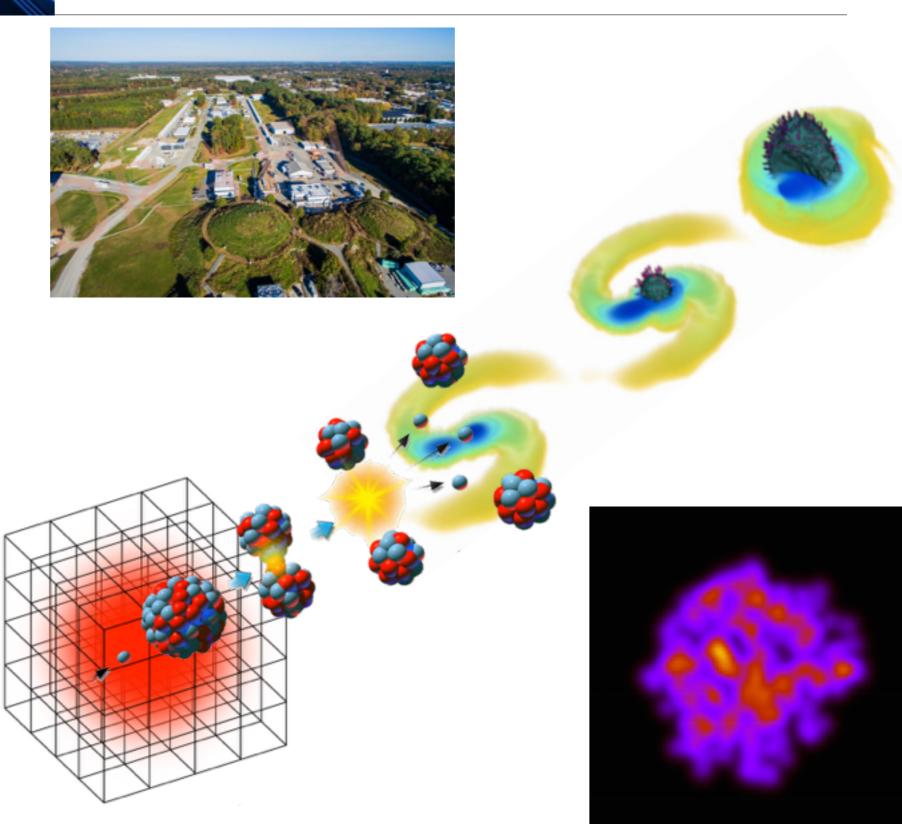
INSTITUTE for

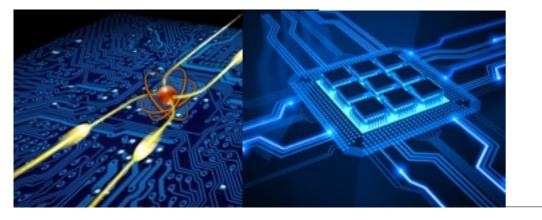
Martin J Savage



The Objective

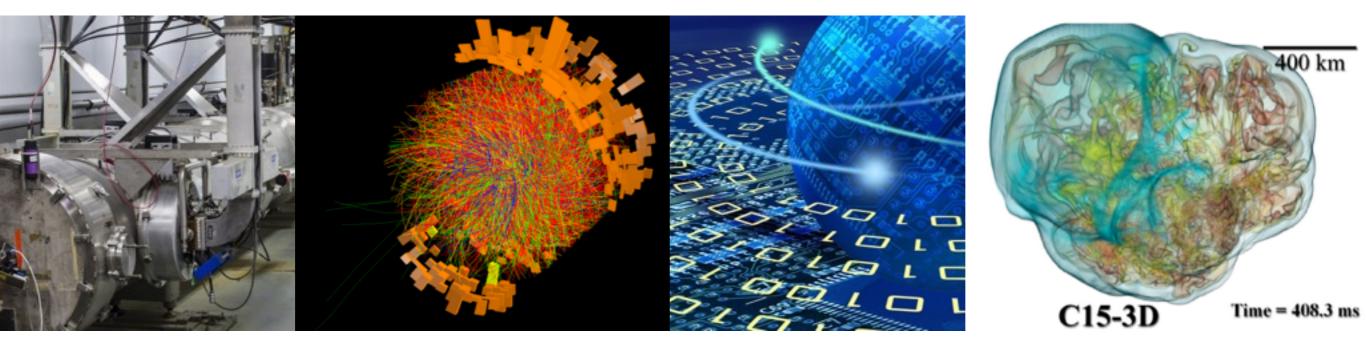
Imagine being able to predict — with unprecedented accuracy and precision — the structure of the proton and neutron, and the forces between them, directly from the dynamics of quarks and gluons, and then using this information in calculations of the structure and reactions of atomic nuclei and of the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



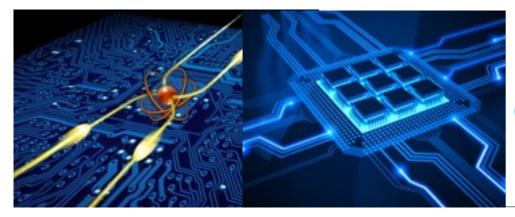


Nuclear Physics Scientific Objectives and Applications Rely on High-Performance Computing

High Performance Computing is essential for NP research program

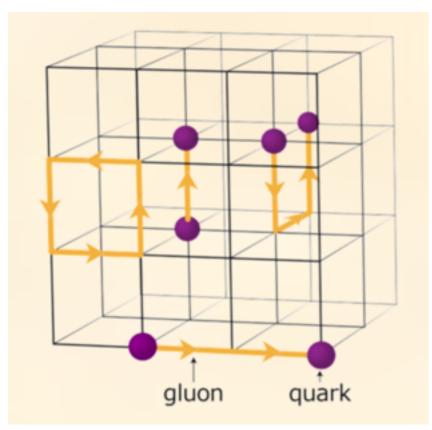


- 1. Design and Optimization of the vibrant NP experimental program ~\$1.2 Bn enterprise for construction+operations, ~4000 users
- 2. Acquisition and handling of experimental data
- 3. Large-scale simulations and calculations of emergent complex systems from subatomic to cosmological

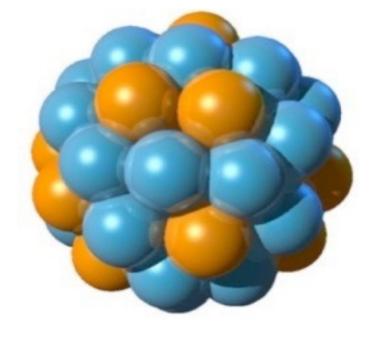


e.g., Hadrons and Nuclei

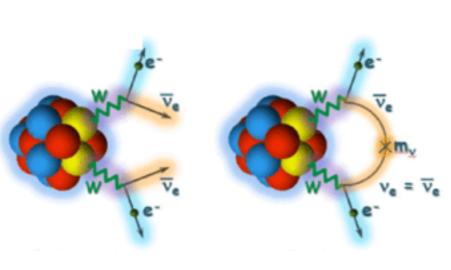


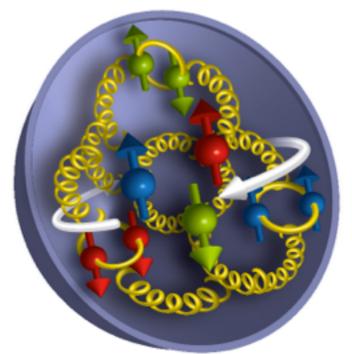


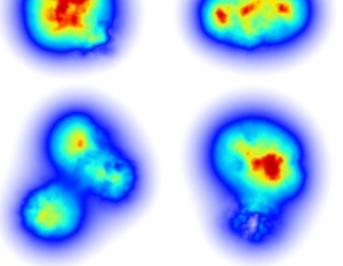
g \q \q



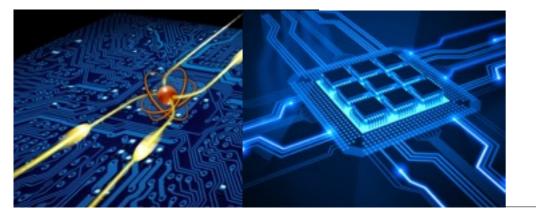
~10% of Leadership Class Computing resources



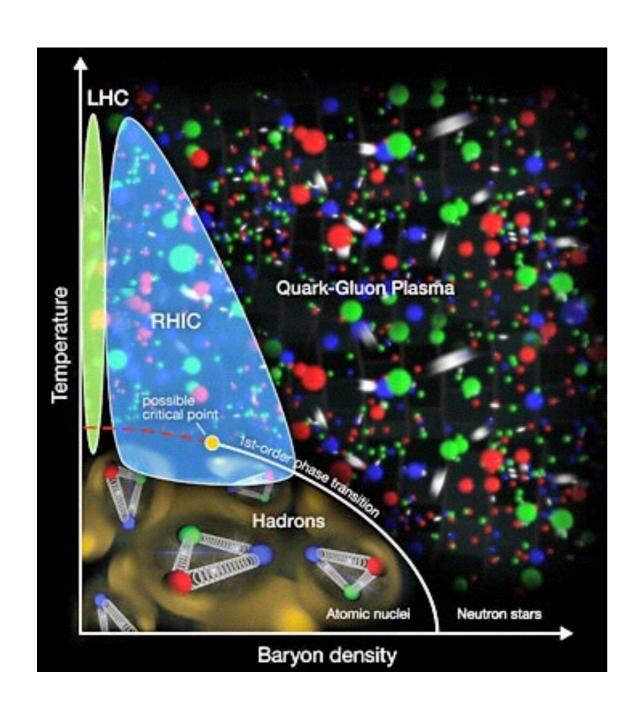


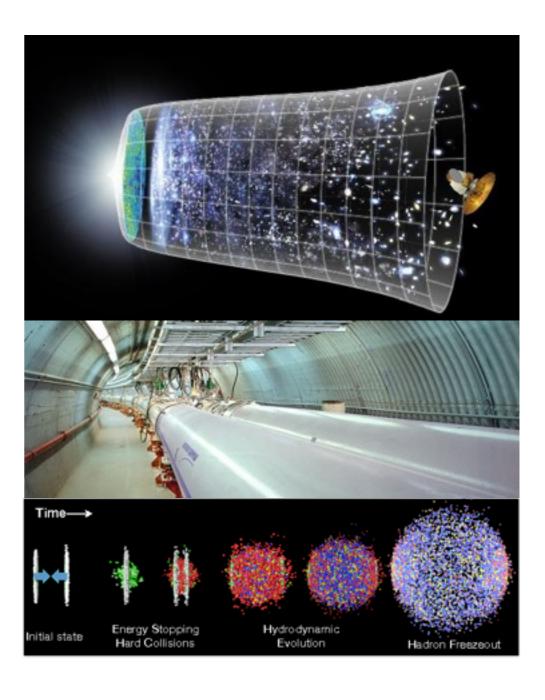


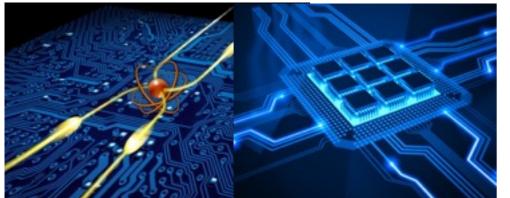
Static quantities with exascale computing reactions and dynamics remain ``difficult"



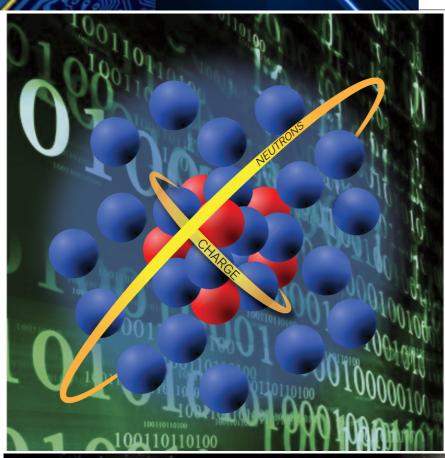
Hot and Dense Matter



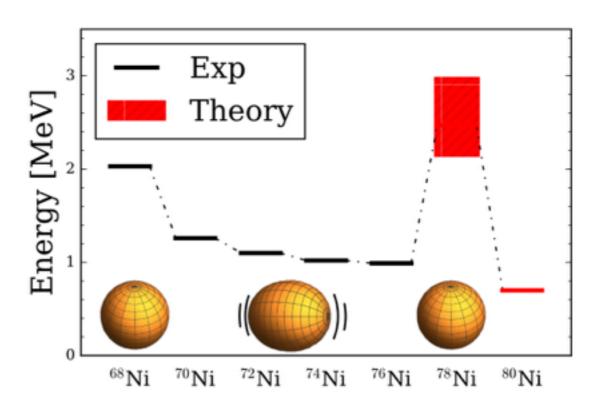


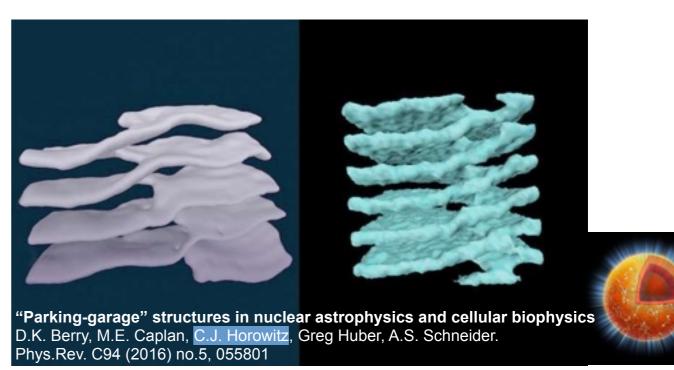


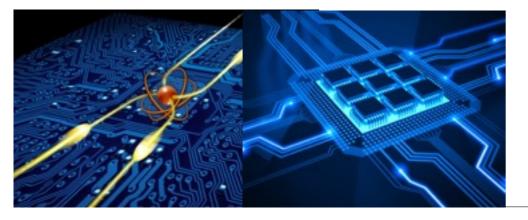
Nuclei and Nuclear Matter



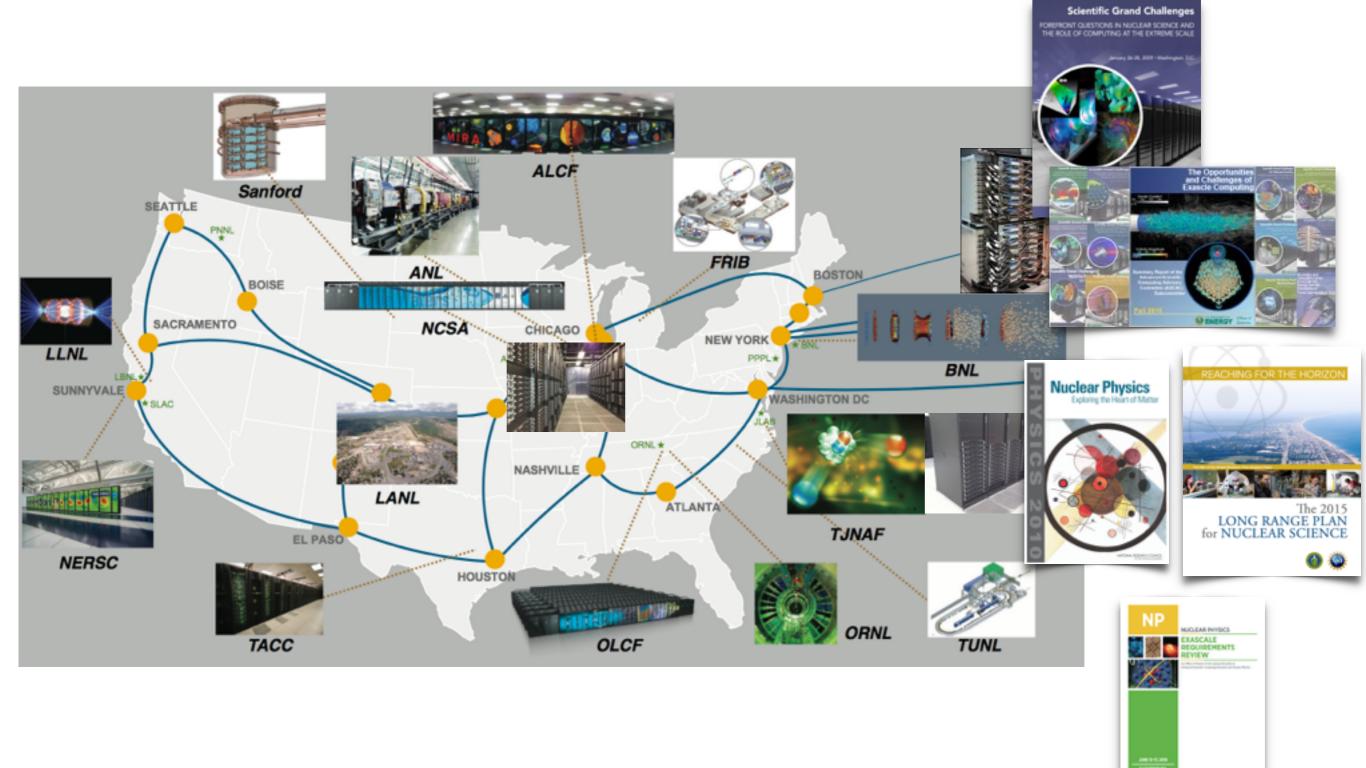


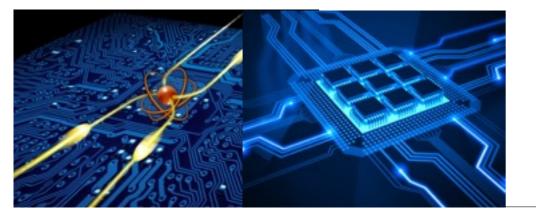






Nuclear Physics Scientific Objectives and Applications Rely on High-Performance Computing

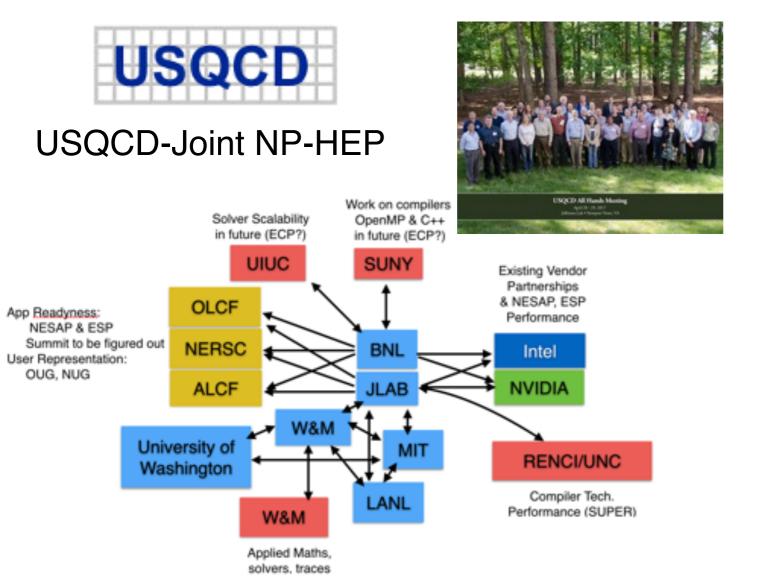


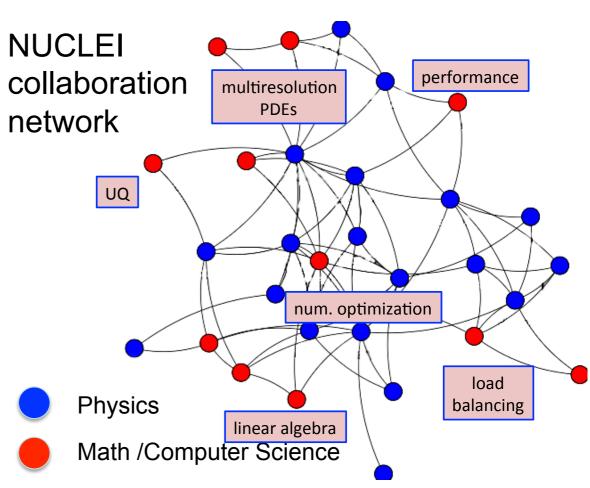


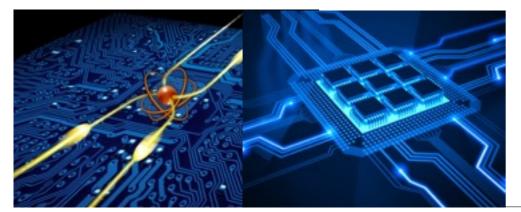
Essential, Extensive Collaboration







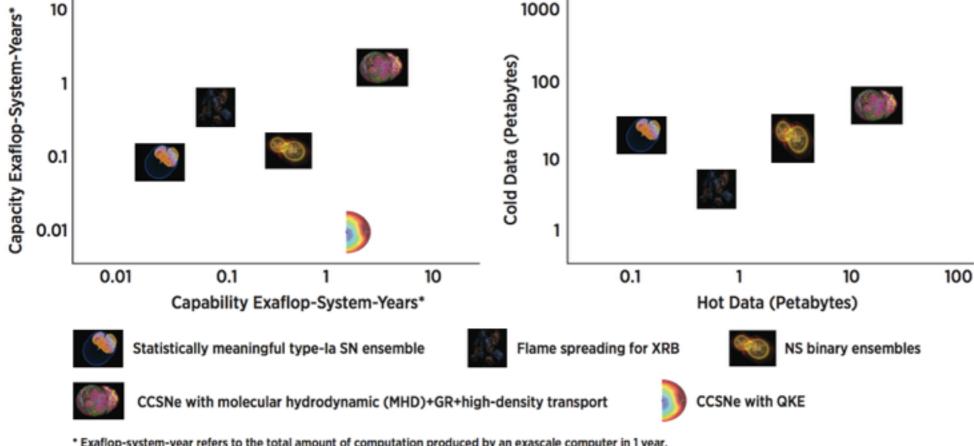




Exascale Ecosystem for Nuclear Physics

Solve computational problems of extreme complexity and magnitude across a very wide range of physical scales.

CAPABILITY/CAPACITY RESOURCES VS. HOT/COLD DATA RESOURCES IN 2025 NUCLEAR ASTROPHYSICS



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



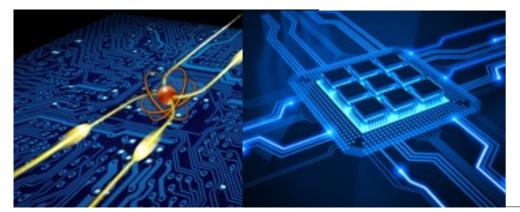
Multi Exascale need in NP alone, >10x in the US

Exascale machine will be oversubscribed by a large factor

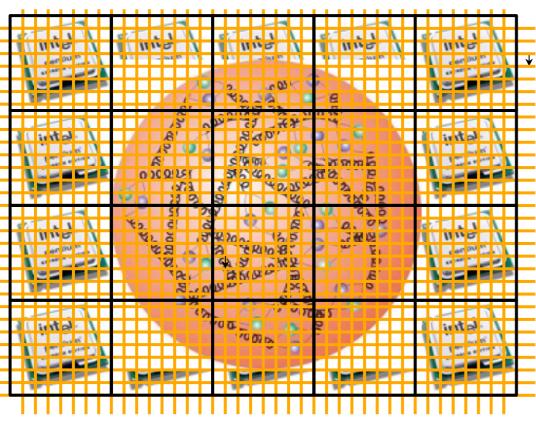








Lattice Quantum Chromodynamics - Discretized Euclidean Spacetime



Lattice Spacing:

a $<< 1/\Lambda \chi$

(Nearly Continuum)

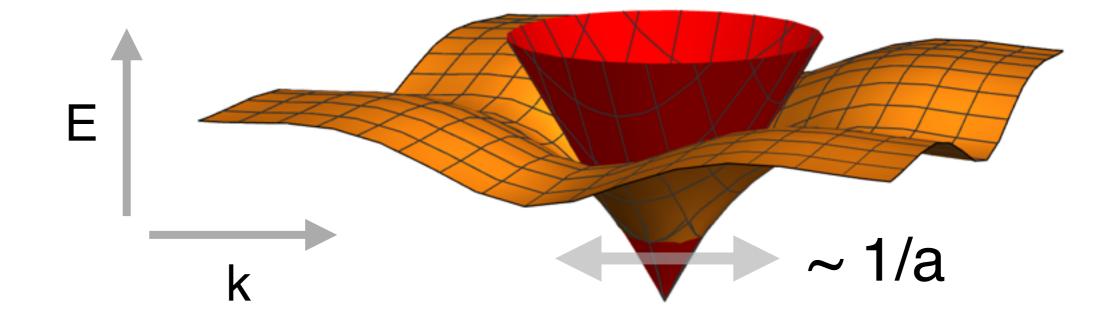
Lattice Volume:

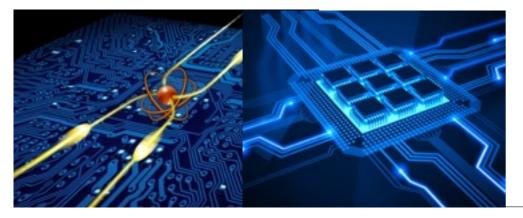
 $m_{\pi}L >> 2\pi$

(Nearly Infinite Volume)

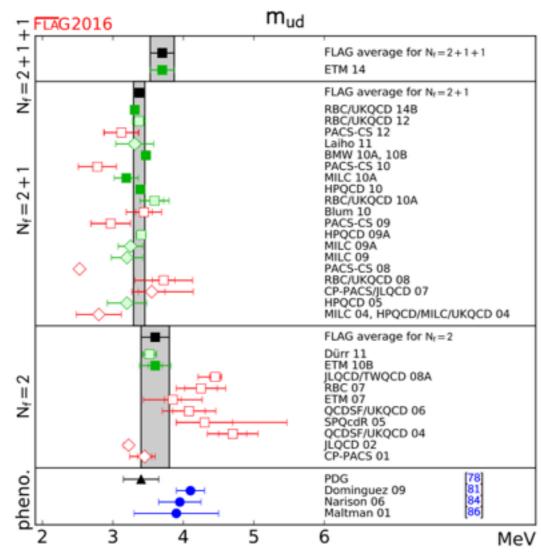
Extrapolation to a=0 and $L=\infty$

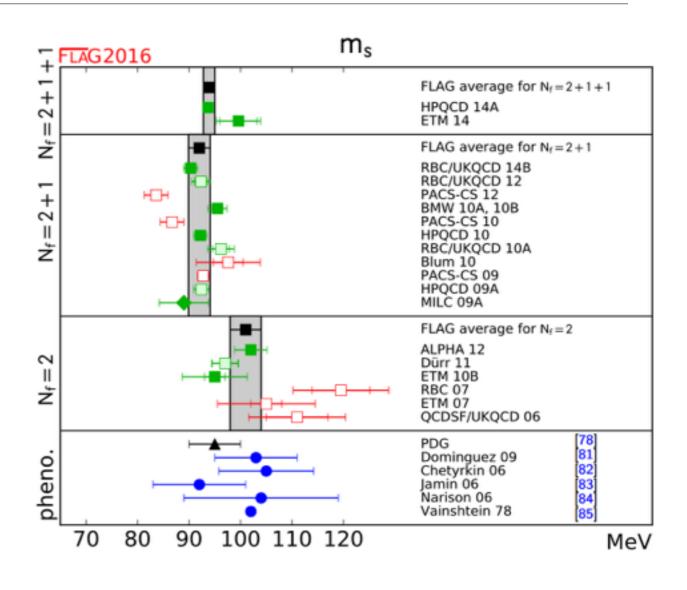
Systematically remove non-QCD parts of calculation through effective field theories





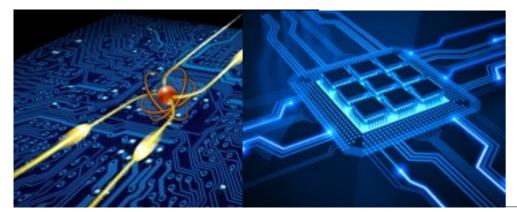
Lattice QCD The Quark Masses



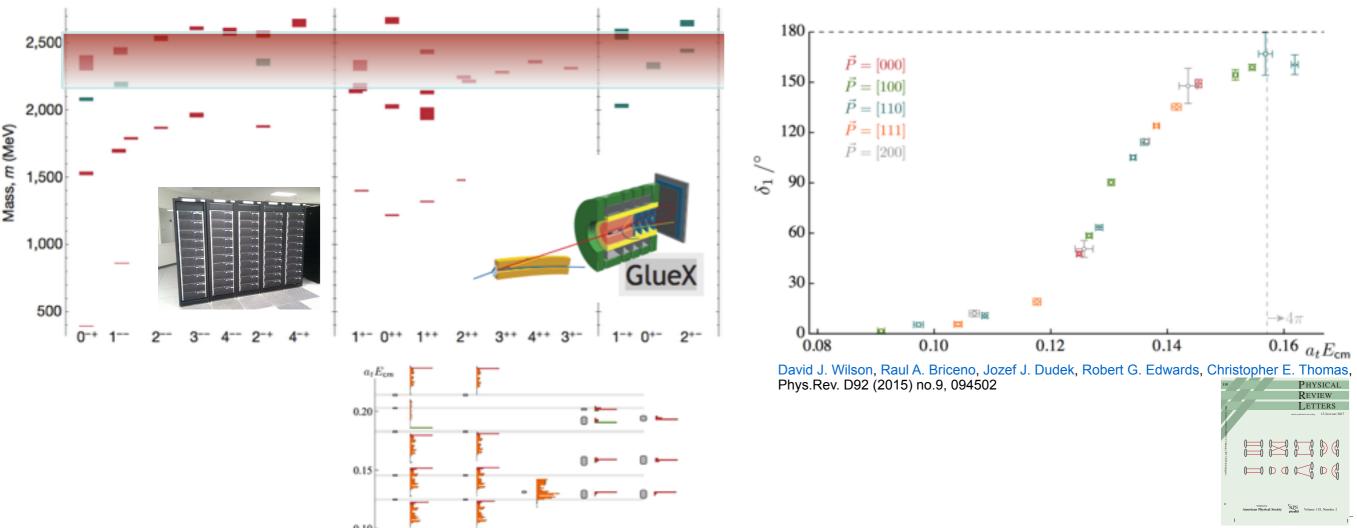


$\overline{N_f}$	m_u	m_d	m_u/m_d		
2+1	2.16(9)(7)	4.68(14)(7)	0.46(2)(2)		
2	2.40(23)	4.80(23)	0.50(4)		

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



Lattice QCD Spectroscopy and GlueX



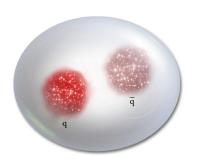
nature

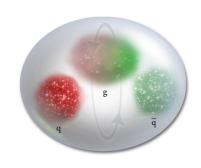
Science in China

 $\pi\pi$ $K\overline{K}$

 $\bar{\psi}\Gamma\psi$

Pattern of states suggest gluonic excitations



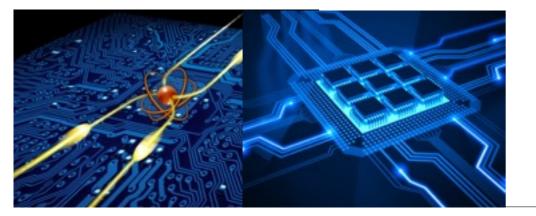


NATURE | REVIEW

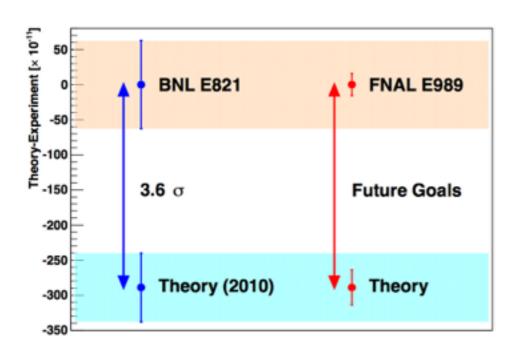
Searching for the rules that govern hadron construction

Matthew R. Shepherd, Jozef J. Dudek & Ryan E. Mitchell

Nature 534, 487-493 (23 June 2016) | doi:10.1038/nature18011



Lattice QCD Fundamental Symmetries



Dave Hertzog, 2016

Figure 1. Comparison of Experiment to Theory at present and expected on completion of future Fermilab E989 and factor of ~ 2 improvements in HVP and HLbL calculations.

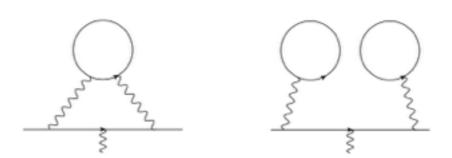
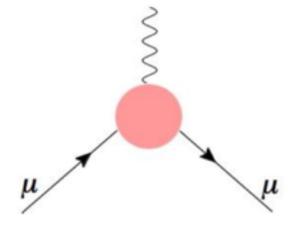
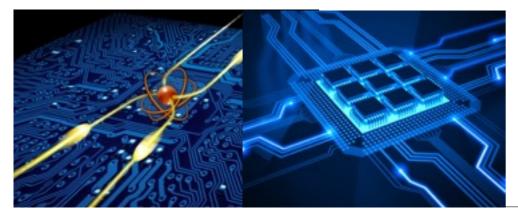


FIG. 1. Quark-connected (left) and quark-disconnected (right) diagram for the calculation of $a_{\mu}^{\rm HVP\ LO}$. We do not draw gluons but consider each diagram to represent all orders in QCD.



Calculation of the hadronic vacuum polarization contribution to the muon anomalous magnetic moment

T. Blum, P.A. Boyle, V. Gülpers, T. Izubuchi, L. Jin, L. Jin, L. Jin, A. C. Jung, A. Jüttner, C. Lehner, A. Portelli, and J.T. Tsang (RBC and UKQCD Collaborations)

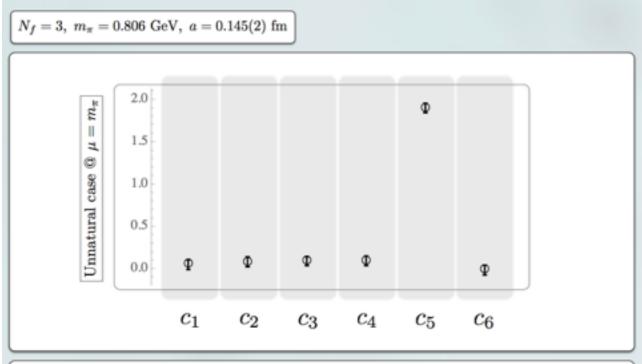


Lattice QCD QCD to Nuclear Forces: First Steps

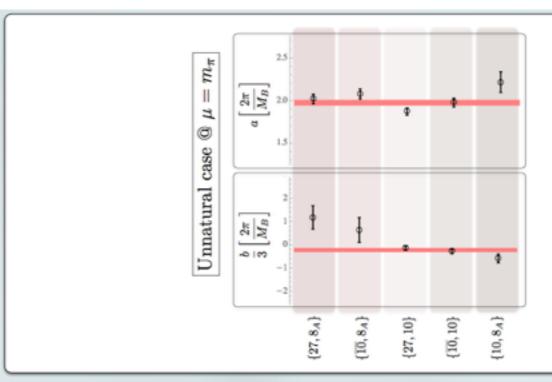


RIKEN Fellow Zohreh Davoudi led this work





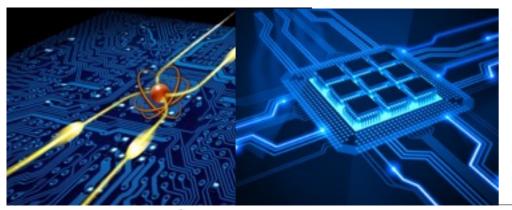
$$\begin{split} \mathcal{L}_{BB}^{(0)} \; &= \; -c_1 \mathrm{Tr}(B_i^\dagger B_i B_j^\dagger B_j) - c_2 \mathrm{Tr}(B_i^\dagger B_j B_j^\dagger B_i) - c_3 \mathrm{Tr}(B_i^\dagger B_j^\dagger B_i B_j) \\ & - c_4 \mathrm{Tr}(B_i^\dagger B_j^\dagger B_j B_i) - \frac{c_5 \mathrm{Tr}(B_i^\dagger B_i) \mathrm{Tr}(B_j^\dagger B_j)}{c_5 \mathrm{Tr}(B_i^\dagger B_i) \mathrm{Tr}(B_j^\dagger B_j)} - c_6 \mathrm{Tr}(B_i^\dagger B_j) \mathrm{Tr}(B_j^\dagger B_i). \end{split}$$



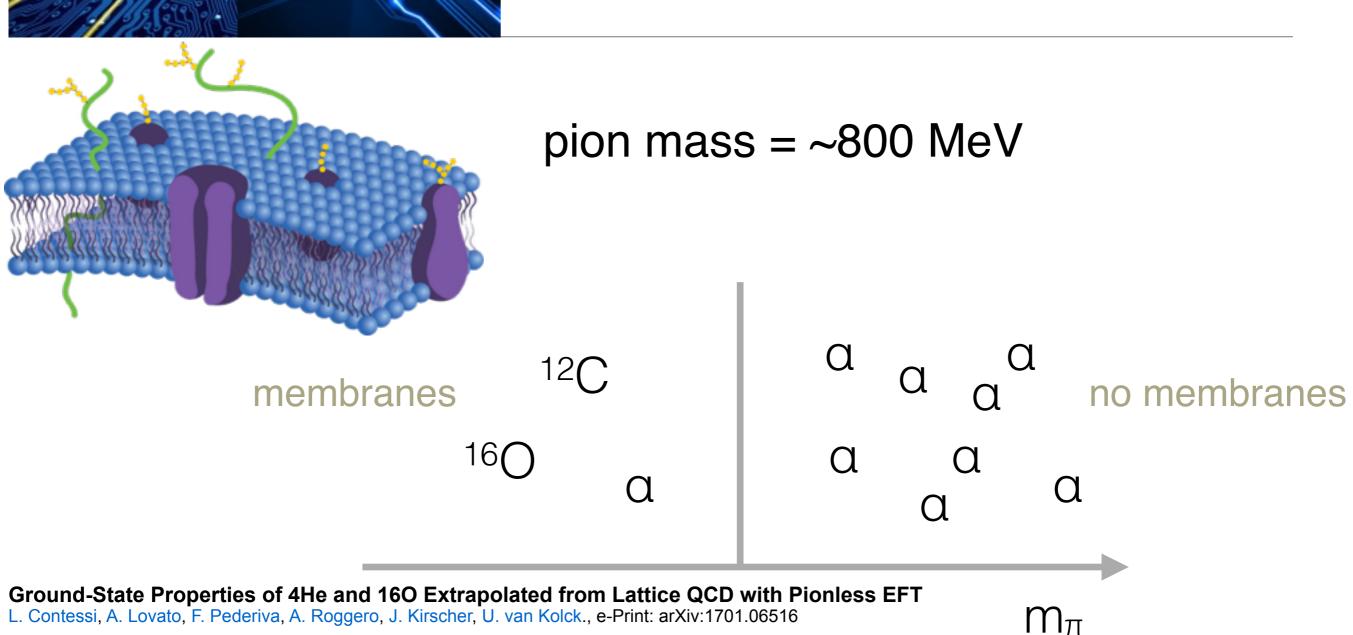
$$\mathcal{L}_{BB}^{(0)} = -a(\Psi_{\mu\nu\rho}^{\dagger}\Psi^{\mu\nu\rho})^2 - b(\Psi_{\mu\nu\sigma}^{\dagger}\Psi^{\mu\nu\tau})(\Psi_{\rho\delta\tau}^{\dagger}\Psi^{\rho\delta\sigma})$$

pionless theory, SU(3) symmetric point

SU(6) spin-flavor symmetry, coefficients indicate very nearly SU(16) symmetry



The Periodic Table at a Pion Mass of ~800 MeV

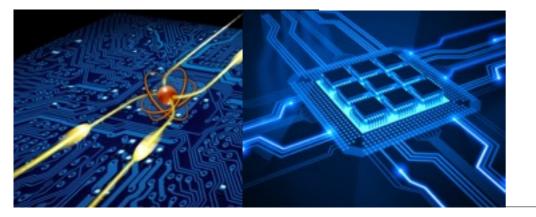


Pion-less effective field theory for atomic nuclei and lattice nuclei

A. Bansal, S. Binder, A. Ekström, G. Hagen, G.R. Jansen, T. Papenbrock. e-Print: arXiv:1712.10246

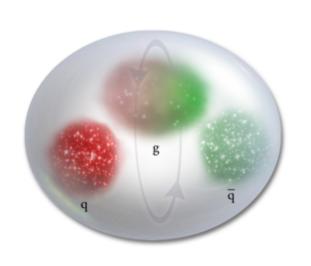
Lattice QCD combined with Nuclear Many-body calculations can explore impact of a significant range of fundamental constants

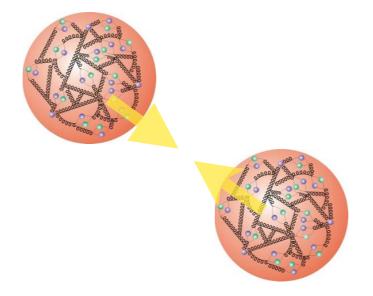
- currently limited by precision of lattice QCD results (determined by compute resources!)



"Features "

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



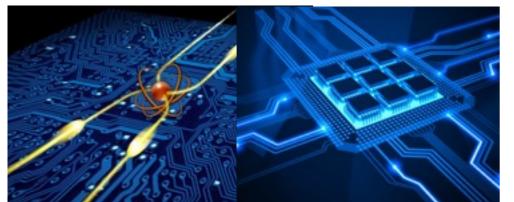




Signal to Noise Problem [Sign Problem]

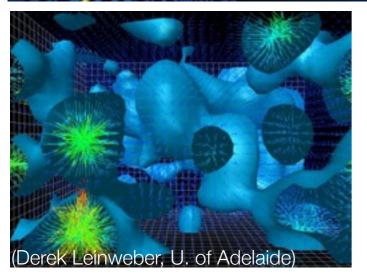
gluon quark

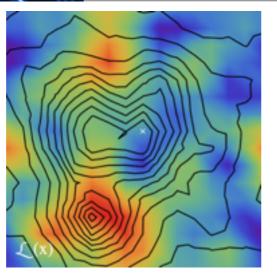
Statistical sampling of the path integral is the limiting element

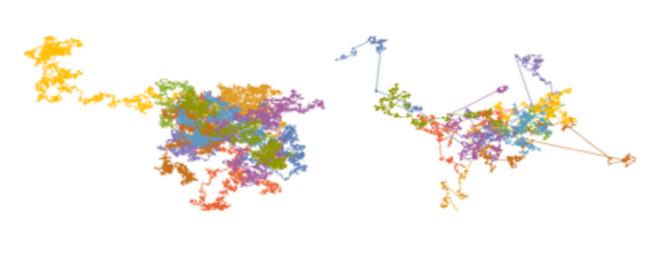


"Features"

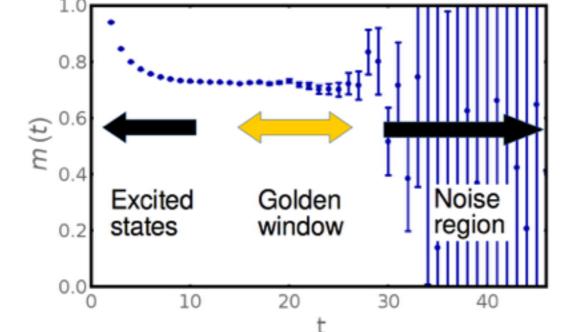
Michael Wagman, PhD Thesis

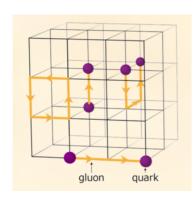


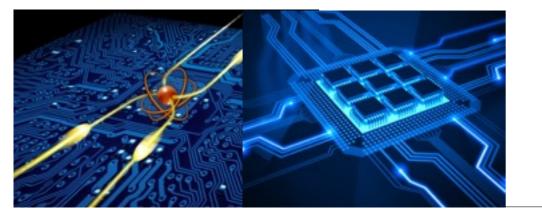




$$C(t) = e^{R(t) + i\theta(t)} \longrightarrow \frac{1}{N} \sum_{U_i} e^{R(t;U_i) + i\theta(t;U_i)}$$

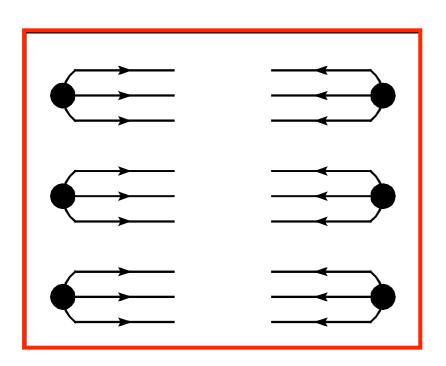






"Features "

Large number of quark contractions

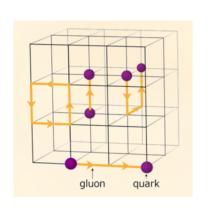


Proton :
$$N^{cont} = 2$$

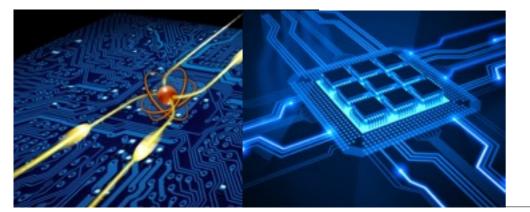
$$^{235}U : N^{cont} = 10^{1494}$$

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

Symmetries provide significant reduction (NPLQCD, PACS - 2010)

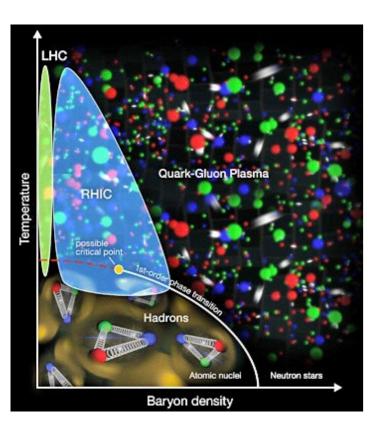


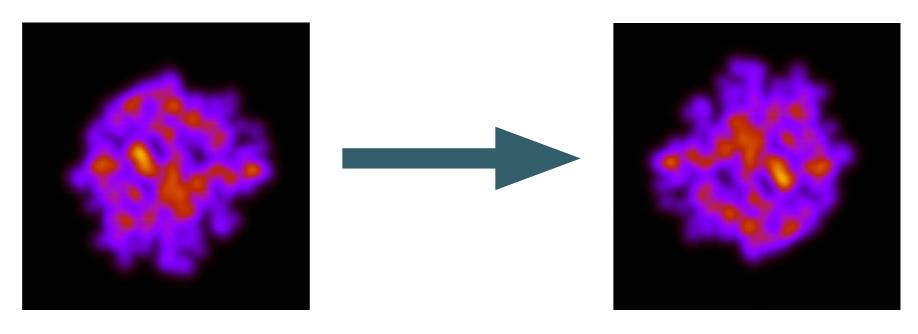
$$^{3}{\rm He} : 2880 \rightarrow 93$$



"Features - Finite Density "

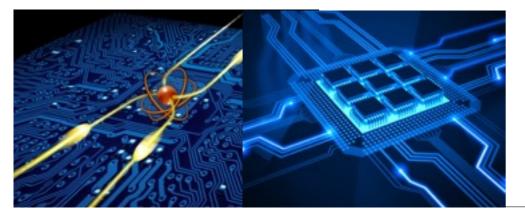
Time evolution of system with baryon number, isospin, electric charge, strangeness, Currents, viscosity, non-equilibrium dynamics - real-time evolution





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

Complex for non-zero chemical potential



"Features "

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

Taylor expansion in μ/T (methodology)

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

with
$$\chi_{i,j,k}^{BQS}(T)=rac{1}{VT^3}\left.rac{\partial^{i+j+k}\ln Z(ec{\mu},T)}{\partial\hat{\mu}_B^i\partial\hat{\mu}_Q^j\partial\hat{\mu}_S^k}
ight|_{ec{\mu}=0}$$
 and $\hat{\mu}=\mu/T$

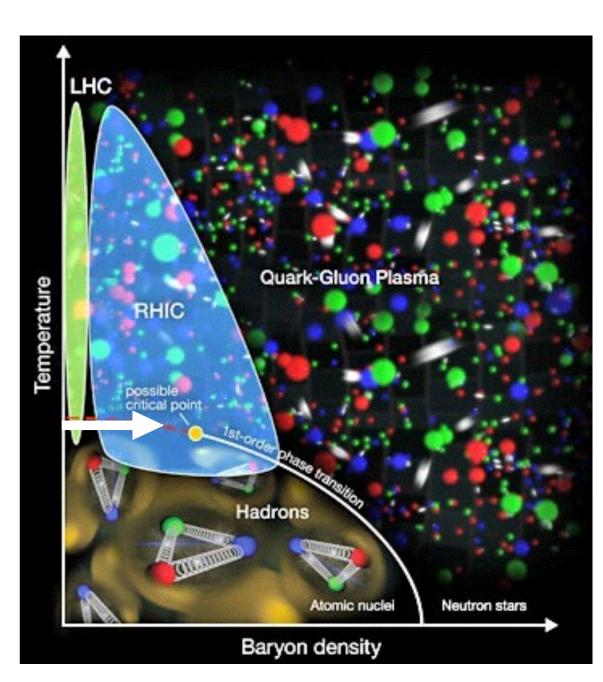
Example:

$$\begin{split} \frac{\partial^2 \ln Z}{\partial \mu^2} &= \left\langle \text{Tr} \left[M^{-1} M'' \right] \right\rangle - \left\langle \text{Tr} \left[M^{-1} M' M^{-1} M' \right] \right\rangle + \left\langle \text{Tr} \left[M^{-1} M' \right]^2 \right\rangle \\ &\simeq \left\langle n^2(x) \bigodot \right\rangle - \left\langle n(x) \bigodot n(y) \right\rangle + \left\langle n(x) \bigodot n(y) \right\rangle \end{split}$$

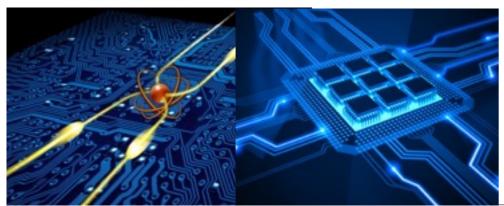
C. Schmidt, SIGN 2017, INT-17-64W, Seattle, WA, USA

6

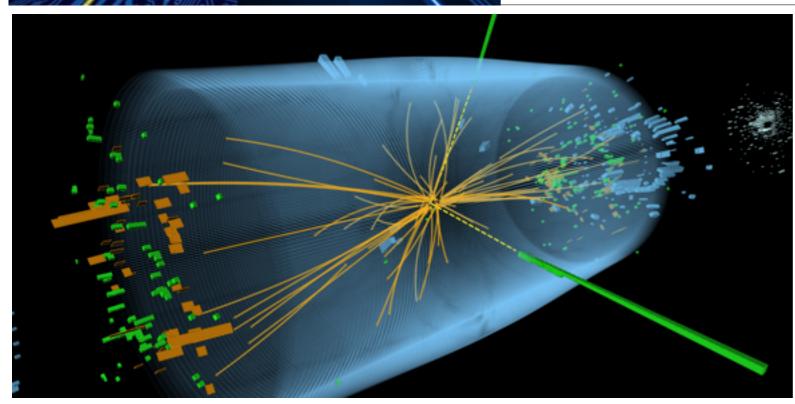




In production - large resource requirements - limits are visible



Fragmentation Vacuum and In-Medium

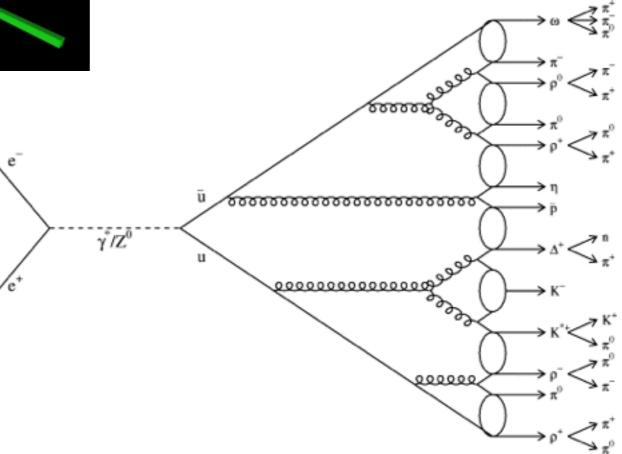


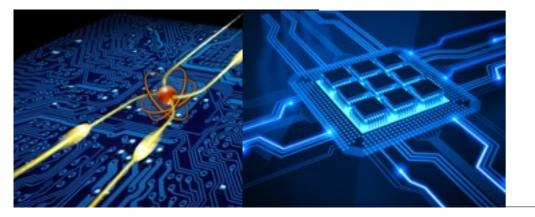
Free-space and in-medium

Diagnostic of state of dense and hot matter

- heavy-ion collisions (e.g., jet quenching)
- finite density and time evolution

Highly-tuned phenomenology and pQCD calculations



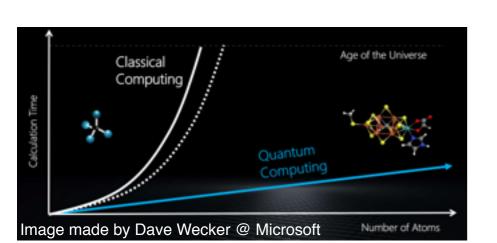


Why Quantum Computing?

The sign problem and the desire for dynamical evolution of QCD systems, requiring *beyond exascale classical computing* resources, lead us to consider the potential of quantum information and computing. [2016-2017]

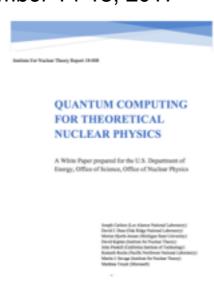


Workshop on Computational Complexity and High Energy Physics
July-31 — August 2, 2017



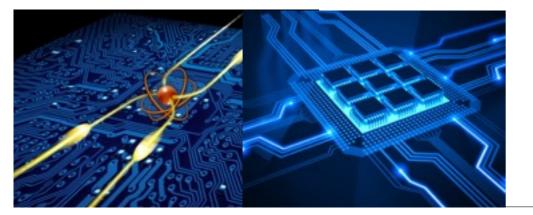


Quantum Computing for Nuclear Physics November 14-15, 2017

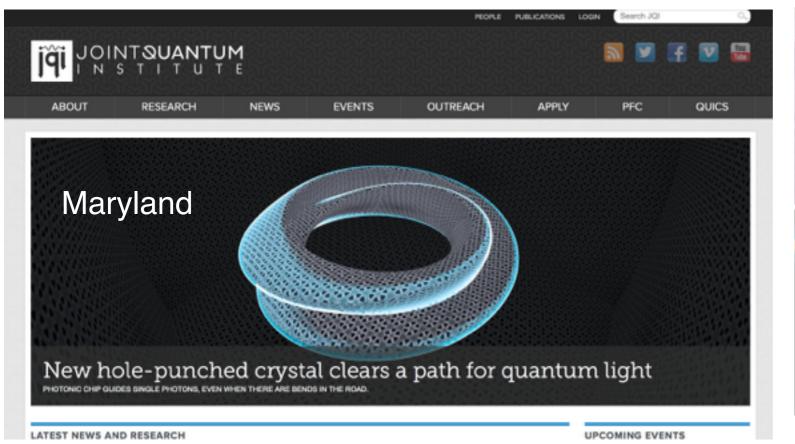


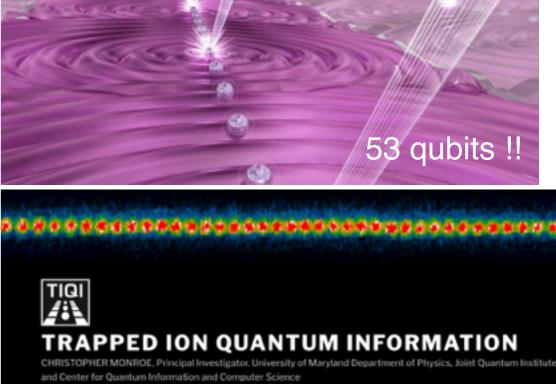


Intersections Between Nuclear Physics and Quantum Information November 14-15, 2017



Quantum Computing





Institute for Quantum Information and Matter, a National Science





Information

by many people & research

| Products & Downloads | Programs & Events ∨ People |

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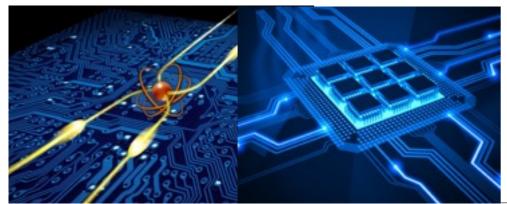
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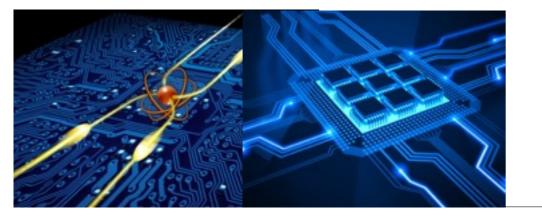
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Microsoft Quantum – Santa Barbara (Station Q)

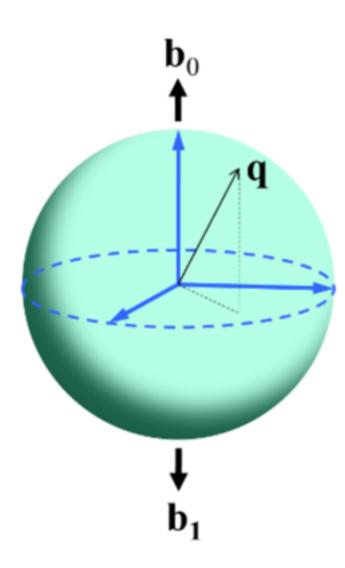


Quantum Computing





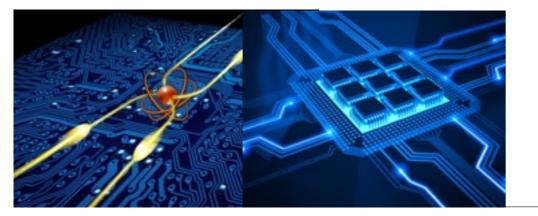
The promise of Quantum Computing



$$|\psi\rangle = a_1|\chi_1\rangle + a_2|\chi_2\rangle + \dots + a_n|\chi_n\rangle + \dots$$

$$H|0\rangle = \frac{1}{\sqrt{2}}|0\rangle + |1\rangle]$$

Parallel Processing of quantum states and information



time=0 for Quantum Computing in Nuclear Physics

Cloud Quantum Computing of an Atomic Nucleus*

E. F. Dumitrescu, A. J. McCaskey, G. Hagen, G. R. Jansen, T. D. Morris, R. C. Pooser, L. D. J. Dean, and P. Lougovski, R. C. Pooser, D. J. Dean, and P. Lougovski,

Computational Sciences and Engineering Division,
Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA
 Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA
 ³Physics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA
 ⁴Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA
 ⁵National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

We report a quantum simulation of the deuteron binding energy on quantum processors accessed via cloud servers. We use a Hamiltonian from pionless effective field theory at leading order. We design a low-depth version of the unitary coupled-cluster ansatz, use the variational quantum eigensolver algorithm, and compute the binding energy to within a few percent. Our work is the first step towards scalable nuclear structure computations on a quantum processor via the cloud, and it sheds light on how to map scientific computing applications onto nascent quantum devices.



http://arxiv.org/abs/1801.03897



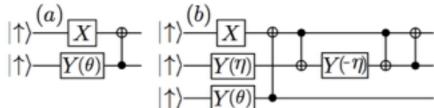
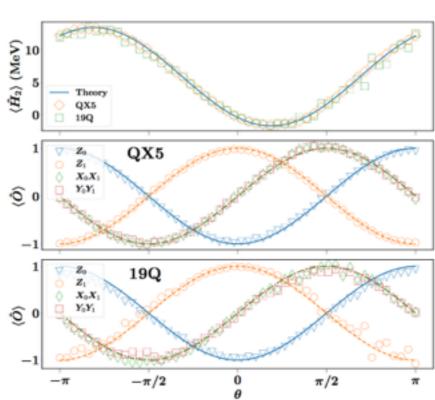


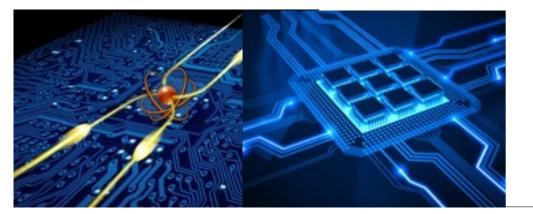
FIG. 1. Low-depth circuits that generate unitary rotations in Eq. (7) (panel a) and Eq. (8) (panel b). Also shown are the single-qubit gates of the Pauli X matrix, the rotation $Y(\theta)$ with angle θ around the Y axis, and the two-qubit CNOT gates.

of a Hamiltonian is to use UCC ansatz in tandem with the VQE algorithm [12, 15, 21]. We adopt this strategy for the Hamiltonians described by Eqs. (4) and (5). We define unitary operators entangling two and three orbitals,

$$U(\theta) \equiv e^{\theta(a_0^{\dagger}a_1 - a_1^{\dagger}a_0)} = e^{i\frac{\theta}{2}(X_0Y_1 - X_1Y_0)},$$
 (7)



See talk by David Dean this morning.



Quantum Field Theory with Quantum Computers - Foundational Works

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

 10^4 spatial lattice sites would require 10^5 * D qubits , D=size of register defining value of the field

Quantum Computation of Scattering in Scalar Quantum Field Theories

Stephen P. Jordan, 18 Keith S. M. Lee, 18 and John Preskill 8 *

[†] National Institute of Standards and Technology, Gaithersburg, MD 20899

[‡] University of Pittsburgh, Pittsburgh, PA 15260

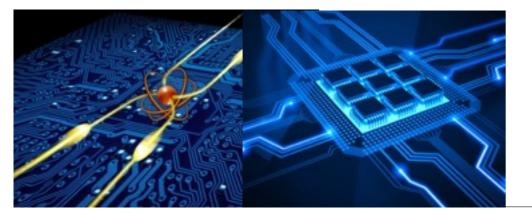
[§] California Institute of Technology, Pasadena, CA 91125

Abstract

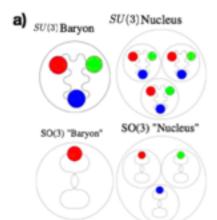
Quantum field theory provides the framework for the most fundamental physical theories to be confirmed experimentally, and has enabled predictions of unprecedented precision. However, calculations of physical observables often require great computational complexity and can generally be performed only 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 Field Theory



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	3-d QCD	1-d SO(3)	2-d SO(3)
gauge symmetry	SU(3)	SO(3)	SO(3)
chiral symmetry	$SU(2)_L \times SU(2)_R$	\mathbb{Z}_2	$\mathbb{Z}_2 \times \mathbb{Z}_2$
flavor symmetry	$SU(2)_{L=R}$	I	\mathbb{Z}_2
baryon symmetry	U(1)	U(1)	U(1)
charge conjugation	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}_2
parity	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}_2

Quantum Link Models and Quantum Simulation of Gauge Theories

Uwe-Jens Wiese

Albert Einstein Center for Fundamental Physics Institute for Theoretical Physics, Bern University



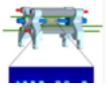
Winter School: Intersections Between QCD and Condensed Matter Schladming, Styria, 2015



European Research Council







SO(3) "Nuclear Physics" with ultracold Gases[☆]

E. Rico^{a,*}, M. Dalmonte^b, P. Zoller^c,
D. Banerjee^{d,e}, M. Bögli^d, P. Stebler^d, U.-J. Wiese^d

^aIKERBASQUE, Basque Foundation for Science, Maria Diaz de Haro 3, E-48013 Bilbao, Spain and Department of Physical Chemistry, University of the Basque Country UPV/EHU, Apartado 644, E-48080 Bilbao, Spain b International Center for Theoretical Physics, 34151 Trieste, Italy
^cInstitute for Theoretical Physics, Innsbruck University, and Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, A-6020 Innsbruck, Austria d Albert Einstein Center for Fundamental Physics, Institute for Theoretical Physics, University of Bern, Sidlerstrasse 5, CH-3012 Bern, Switzerland NIC, DESY, Platanenallee 6, 15738 Zeuthen, Germany

Abstract

Jan

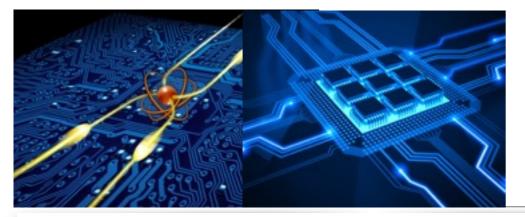
[cond-mat.quant-gas

arXiv:1802.00022v1

An ab initio calculation of nuclear physics from Quantum Chromodynamics (QCD), the fundamental SU(3) gauge theory of the strong interaction, remains an outstanding challenge. Here, we discuss the emergence of key elements of nuclear physics using an SO(3) lattice gauge theory as a toy model for QCD. We show that this model is accessible to state-of-the-art quantum simulation experiments with ultracold atoms in an optical lattice. First, we demonstrate that our model shares characteristic many-body features with QCD, such as the spontaneous breakdown of chiral symmetry, its restoration at finite baryon density, as well as the existence of few-body bound states. Then we show that in the one-dimensional case, the dynamics in the gauge invariant sector can be encoded as a spin $S=\frac{3}{2}$ Heisenberg model, i.e., as quantum magnetism, which has a natural realization with bosonic mixtures in optical lattices, and thus sheds light on the connection between non-Abelian gauge theories and quantum magnetism.

Keywords: ultracold atoms | Lattice gauge theories | Quantum simulation

20



Quantum Field Theory - recent examples

Quantum sensors for the generating functional of interacting quantum field theories

A. Bermudez, 1,2, G. Aarts, and M. Müller

Department of Physics, College of Science, Swansea University, Singleton Park, Swansea SA2 8PP, United Kingdom Instituto de Física Fundamental, IFF-CSIC, Madrid E-28006, Spain

Difficult problems described in terms of interacting quantum fields evolving in real time or out of equilibrium are abound in condensed-matter and high-energy physics. Addressing such problems via controlled experiments in atomic, molecular, and optical physics would be a breakthrough in the field of quantum simil work, we present a quantum-sensing protocol to measure the generating functional of an interfield theory and, with it, all the relevant information about its in or out of equilibrium phenomen.

can be understood as a collective interferometric scheme based on a generalization of the notio sources in quantum field theories, which make it possible to probe the generating functional. W scheme can be realized in crystals of trapped ions acting as analog quantum simulators of self-in quantum field theories.

arXiv:1702.05492 proposed method

Dynamics of entanglement in expanding quantum fields

arXiv:1704.02877

Quantum Simulation of the Abelian-Higgs Lattice Gauge Theory with Ultracold Atoms

Daniel González-Cuadra^{1,2}, Erez Zohar² and J. Ignacio Cirac²

¹ ICFO – The Institute of Photonic Sciences, Av. C.F. Gauss 3, E-08860, Castelldefels (Barcelona), Spain

² Max-Planck-Institut f
ür Quantenoptik, Hans-Kopfermann-Straße 1, D-85748 Garching, Germany

arXiv:1712.09362 [hep-th]

Jürgen Berges, Stefan Floerchinger and Raju Venugopalan

Electron-Phonon Systems on a Universal Quantum Computer

arXiv:1802.07347 [quant-ph]

Alexandru Macridin, Panagiotis Spentzouris, James Amundson, Roni Harnik

Quantum simulation of the universal features of the Polyakov loop

Jin Zhang¹, J. Unmuth-Yockey², A. Bazavov³, S.-W. Tsai¹, and Y. Meurice⁴

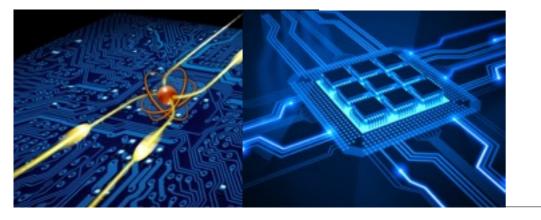
¹ Department of Physics and Astronomy, University of California, Riverside, CA 92521, USA

²Department of Physics, Syracuse University, Syracuse, New York 13244, USA

³, Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan, 48824, USA and

Department of Physics and Astronomy, The University of Iowa, Iowa City, IA 52242, USA

Batavia, Illinois 60510, USA

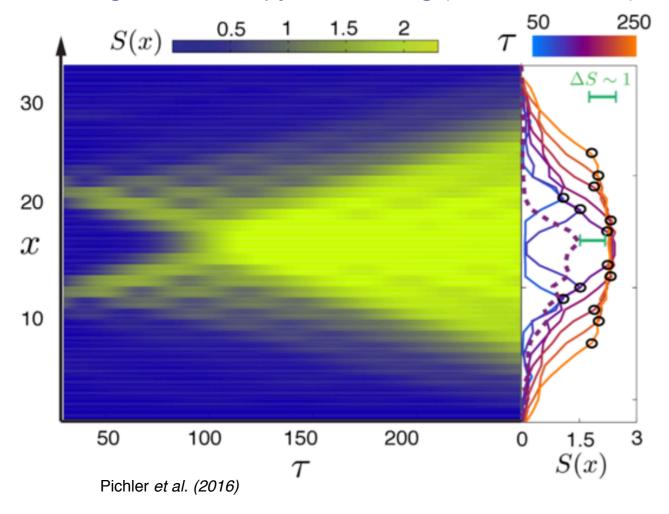


Quantum Field Theory and Quantum Information

Are there new insights into the forces of nature and/or calculational techniques to be had by thinking in terms of quantum information?

Preskill, Swingle, and others

Entanglement entropy in scattering (tensor networks)

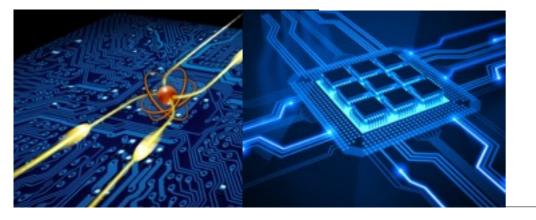


New ways to arrange QCD calculations? New ways to address QCD analytically?

Entanglement in HEP and NP systems is starting to be considered, e.g. fragmentation

Dynamics of entanglement in expanding quantum fields

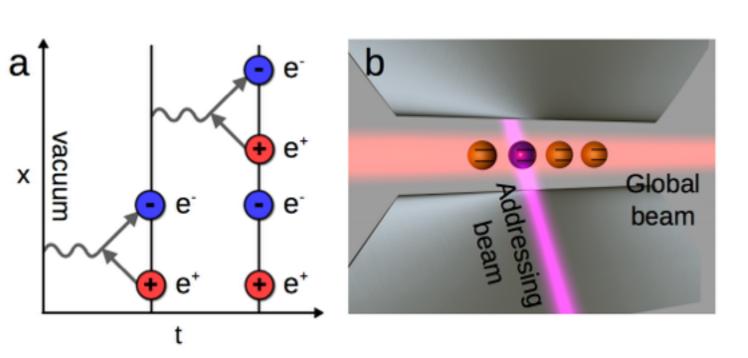
Jürgen Berges, Stefan Floerchinger and Raju Venugopalan

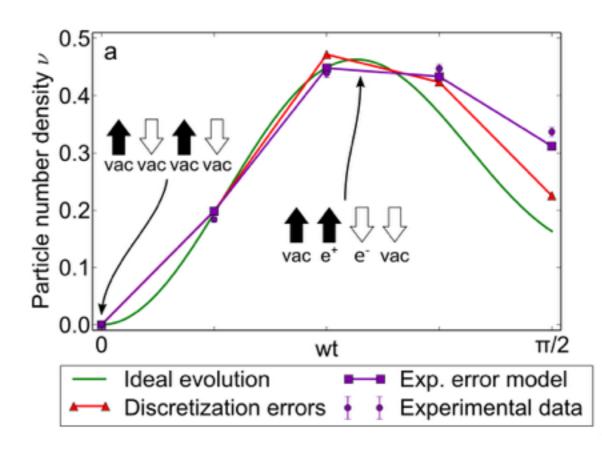


Starting Simple 1+1 Dim QED - Pivotal Paper

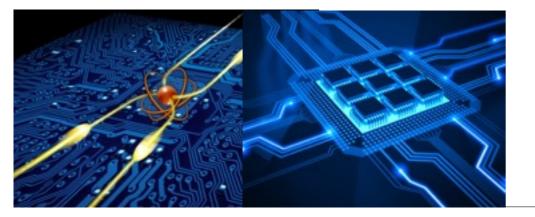
Real-time dynamics of lattice gauge theories with a few-qubit quantum computer

Esteban A. Martinez,^{1,*} Christine Muschik,^{2,3,*} Philipp Schindler,¹ Daniel Nigg,¹ Alexander Erhard,¹ Markus Heyl,^{2,4} Philipp Hauke,^{2,3} Marcello Dalmonte,^{2,3} Thomas Monz,¹ Peter Zoller,^{2,3} and Rainer Blatt^{1,2} (2016)

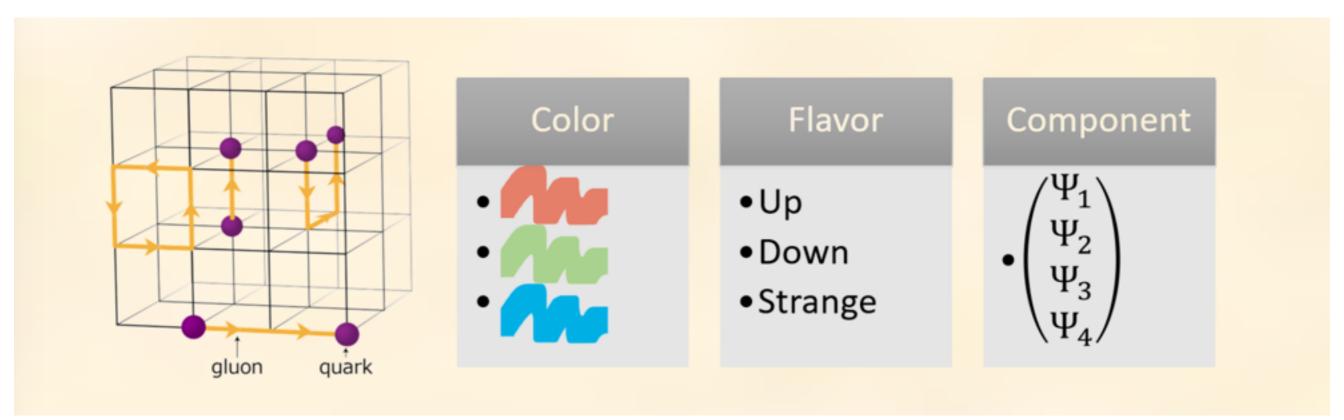




Based upon a string of ⁴⁰Ca⁺ trapped-ion quantum system Simulates 4 qubit system with long-range couplings = 2-spatial-site Schwinger Model > 200 gates per Trotter step

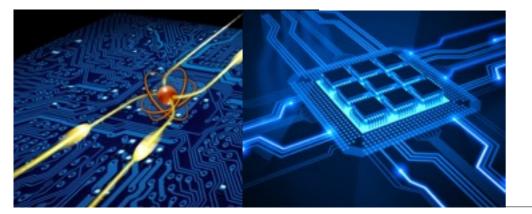


Gauge Field Theories e.g. QCD



Natalie Klco

32³ lattice requires naively > 4 million qubits!

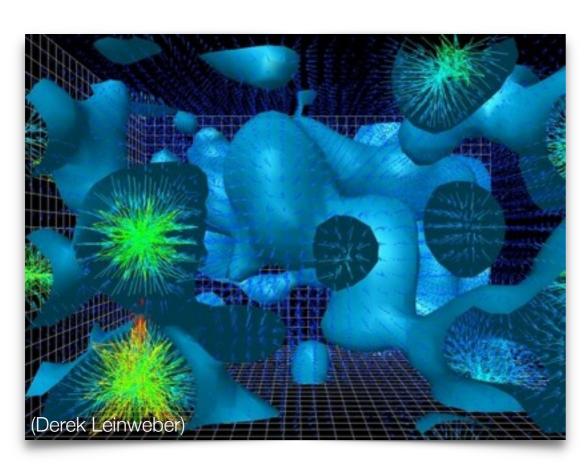


What is the QCD Vacuum : Ea I0>=0 ?

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

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

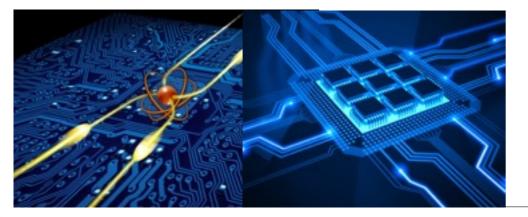
I random > = a I0> + b I(pi pi)> + c I (pi pi pi pi pi) > + + d I (GG) > +



1 vacuum configuration

Probability **e**^{-S}QC

Classical Lattice QCD calculations will likely be required to provide initialization of vacuum. How to do this? What are the algorithms? e.g. parallel of tensor methods in 1-dim? but no explicit fermions,..



QC for QFT Start Simple

Two ORNL-led research teams receive \$10.5 million to advance quantum computing for scientific applications









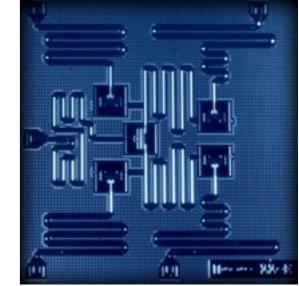
ORNL's Pavel Lougovski (left) and Raphael Pooser will lead research teams working to advance quantum computing for scientific applications. Credit: Oak Ridge National Laboratory, U.S. Dept. of Energy (hi-res image)

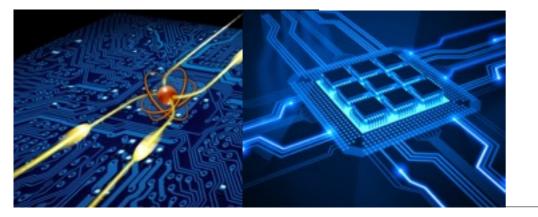
DOE-ASCR

arXiv:1803.03326 [quant-ph]

Heterogeneous Digital-Analog Quantum Dynamics Simulations
Methods and Interfaces for Quantum Acceleration of Scientific Applications

Quantum-Classical Dynamical Calculations of the Schwinger Model using Quantum Computers N. Klco, E.F. Dumitrescu, A.J. McCaskey, T.D. Morris, R.C. Pooser, M. Sanz, E. Solano, P. Lougovski, M.J. Savage.

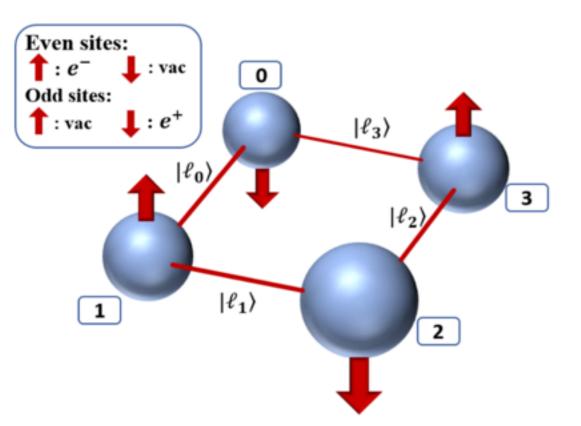


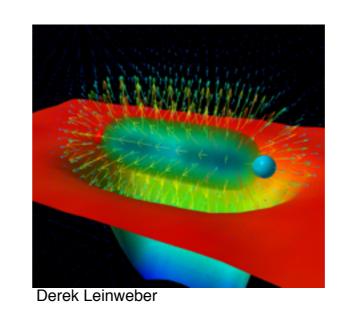


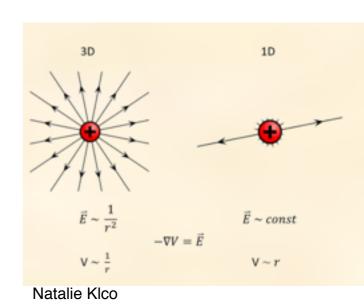
Starting Simple 1+1 Dim QED Construction

$$\mathcal{L} = \overline{\psi} (i \not\!\!\!D - m) \psi - \frac{1}{4} F_{\mu\nu} F^{\mu\nu}$$

- Charge screening, confinement
- · fermion condensate

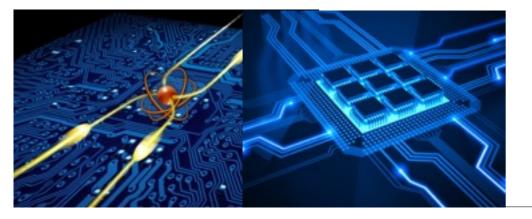




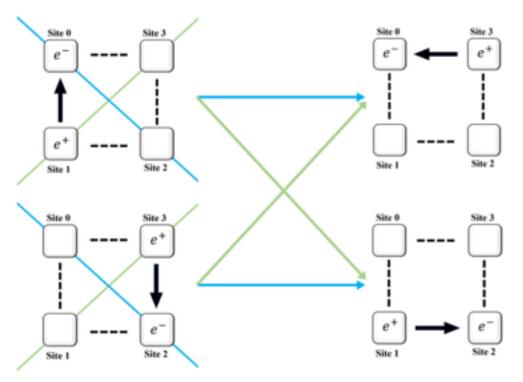


$$\hat{H} = x \sum_{n=0}^{N_{fs}-1} \left(\sigma_n^+ L_n^- \sigma_{n+1}^- + \sigma_{n+1}^+ L_n^+ \sigma_n^- \right) + \sum_{n=0}^{N_{fs}-1} \left(l_n^2 + \frac{\mu}{2} (-)^n \sigma_n^z \right) .$$

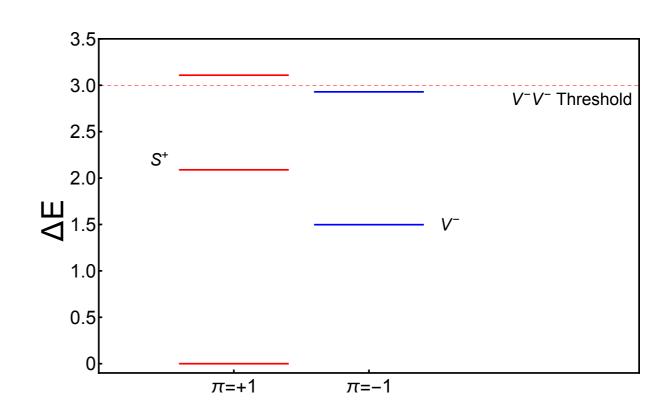
- Clearly, this is just a start far from infinite-volume and continuum limits
- · Will require improved (Symanzik-like) actions, effective field theories, etc



Starting Simple 1+1 Dim QED Symmetries



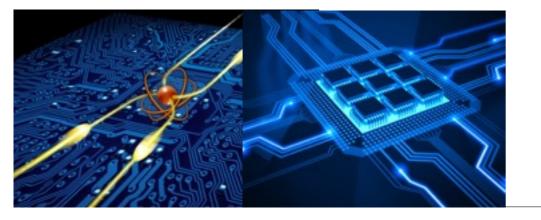
- · Gauss's Law
- (Angular) Momentum
- Parity



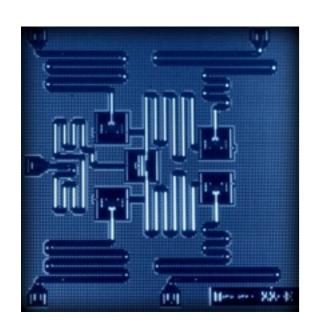
	physical sites	Nq_{lattice}	$D_{ m lattice}$	$D_{ m physical}$	$D_{\mathbf{k}=0}$	D_{even}	D_{odd}	$Nq_{even}^{k=0}$	$Nq_{odd}^{k=0}$
-	1	6	64	5	-	3	2	2	1
	2	12	4.1×10^3	13	9	5	4	3	2
	4	24	1.7×10^7	117	35	19	16	5	4
	6	36	6.9×10^{10}	1,186	210	110	100	7	7
	8	48	2.8×10^{14}	12,389	1,569	801	768	10	10
	10	60	1.2×10^{18}	130,338	13,078	6,593	6,485	13	13
_	12	72	4.7×10^{21}	1,373,466	114,584	57,468	57,116	16	16

Classical pre-processing Can this be done *in situ*?

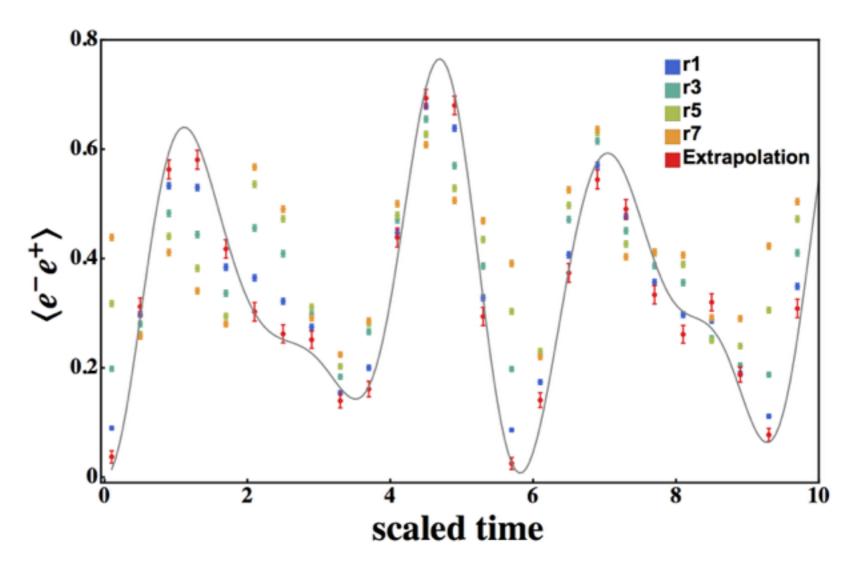
Classical post-processing

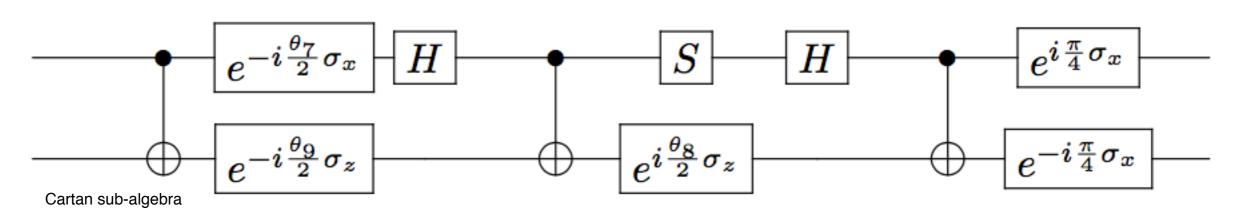


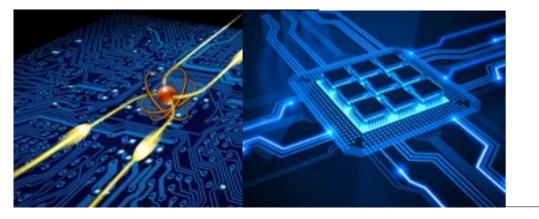
Starting Simple 1+1 Dim QED Living NISQ - IBM Classically Computed U(t)



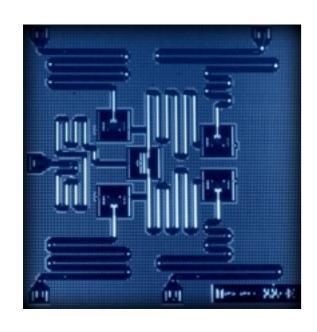
ibmqx2 8K shots per point







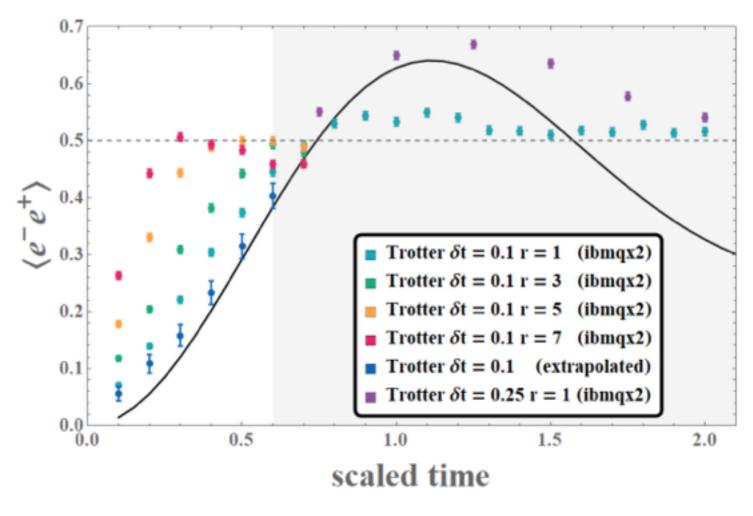
Starting Simple 1+1 Dim QED Living NISQ - IBM Trotter U(t)



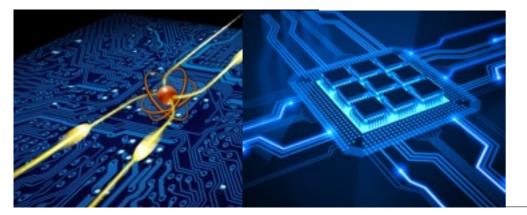
T2 (μs) 55.20 65.10 47.00 35.10 37.60

$$H = \frac{x}{\sqrt{2}} \sigma_x \otimes \sigma_x + \frac{x}{\sqrt{2}} \sigma_y \otimes \sigma_y - \mu \sigma_z \otimes \sigma_z$$
$$+ x \left(1 + \frac{1}{\sqrt{2}} \right) I \otimes \sigma_x - \frac{1}{2} I \otimes \sigma_z$$
$$- (1 + \mu) \sigma_z \otimes I + x \left(1 - \frac{1}{\sqrt{2}} \right) \sigma_z \otimes \sigma_x$$

$$e^{-iHt} = e^{-i\sum_{j} H_{j}t} = \lim_{N_{\text{Trot.}} \to \infty} \left(\prod_{j} e^{-iH_{j}\delta t}\right)^{N_{\text{Trot.}}}$$



3.6 QPU-s and 260 IBM units



Starting Simple 1+1 Dim QED Simple Coding Chroma Vs Python3

```
$Id: HigherLpions_w.cc,v 1.0 SAVAGE Dec 2012 Exp $
    \brief Calculate the Two Pion Phase Shift in higher partial waves
#include "chromabase.h"
#include "util/ft/sftmom.h"
#include "HigherLpions_w.h"
#include <strstream>
#include <string>
namespace Chroma {
/! pion-pion interactions in higher L
  \ingroup hadron

    This routine is specific to Wilson fermions!

   Construct propagators for mesons with "u" and "d" quarks.
  Calculate the correlators for pion (p1) pion (p2) from displaced sources
                             gauge field (Read)
                             quark propagator 1 ( Read )
  \param quark_prop1
                             quark propagator 2 ( Read )
   \param quark_prop2
                             cartesian coordinates of the source ( Read )
   \param src_coord
                             object holds list of momenta and Fourier phases ( Read )
   \param phases
                             xml file object ( Read )
                             group name for xml data ( Read )
   \param xml_group
void PIPIints(const multild<LatticeColorMatrix>& u.
         const LatticePropagator& quark_prop1,
        const LatticePropagator& quark_prop2.
        const multi1d<int>& src_coord1,
        const multi1d<int>& src_coord2,
         const SftMom& phases,
         XMLWriter& xml.
        const string& xml_group)
 START_CODE():
 if ( Ns != 4 || Nc != 3 )( /* Code is specific to Ns=4 and Nc=3. */
   QDPIO::cerr<<"HigherLpions code only works for Nc=3 and Ns=4\n";
    QDP_abort(111) ;
```

Lattice QCD application *chroma* code written by Savage (2012) for NPLQCD, adapted from other *chroma* codes written by Robert Edwards and Balint Joo [JLab, USQCD, SciDAC].

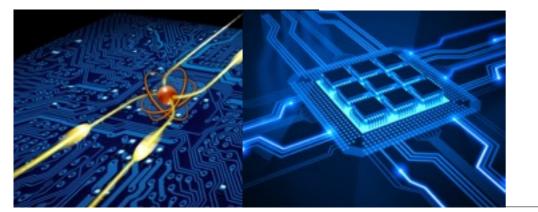
C++

Displaced propagator sources generate hadronic blocks projected onto cubic irreps. to access meson-meson scattering amplitudes in L>0 partial waves.

```
for ii in range(0,len(NTrotter)):
        p0=qp.get_circuit(pidtab[ii])
        ntrott = NTrotter[ii]
        print("Calculating ntrott = ",ii," : = ",ntrott)
       for jjTT in range(0,ntrott):
           print("ii = ",ii," jjTT = ,",jjTT, "ntrott =",ntrott)
# One Trotter Step
# acting with Cartan sub-algebra to describe a1,a2,a3 = h1,h2,h3
            p0.cx(qr[0],qr[1])
            p0.u3(a1,-halfpi,halfpi,qr[0])
            p0.h(qr[0])
            p0.u3(0,0,a3,qr[1])
            p0.cx(qr[0],qr[1])
            p0.s(qr[0])
            p0.h(qr[0])
            p0.u3(0,0,-a2,qr[1])
            p0.cx(qr[0],qr[1])
            p0.u3(-halfpi,-halfpi,halfpi,qr[0])
            p0.u3(halfpi,-halfpi,halfpi,qr[1])
# I x sigmax to describe h4
           p0.u3(a4,-halfpi,halfpi,qr[1])
```

Python3 code written by Savage (2018) to access IBM quantum devices through ``the cloud" (through ORNL). IBM templates and example codes.

Calculates Trotter evolution of +ve parity sector of the 2-spatial-site Schwinger Model.



Summary

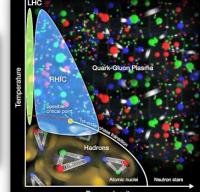


- Exascale conventional computing will provide

 Important finite density systems (including modest) size nuclei) and **dynamics** require exponentially large conventional computing resources.

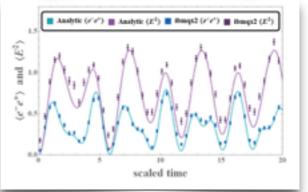
required precision for many experimentally

important quantities in NP and HEP.

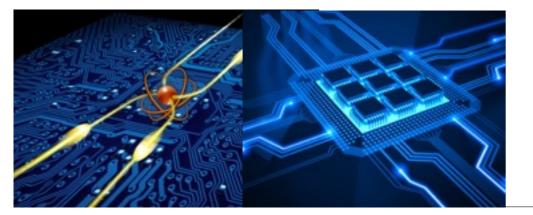


- QFTs on QCs are important for NP and HEP start simple ... explore all architectures
- Workforce development is essential competing with tech. companies for junior scientists is challenging
- NISQ-era coherence times and noise present challenges

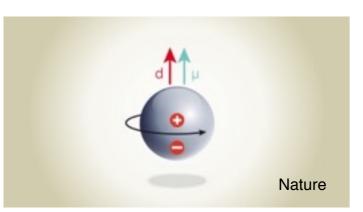


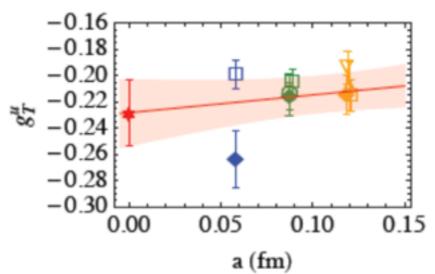


FIN



Lattice QCD Fundamental Symmetries





Low-energy:

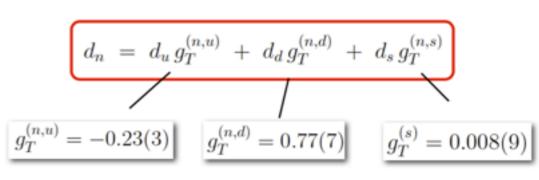
gs,T from lattice

LHC:

√s = 14 TeV

 $L = 10,300 \text{ fb}^{-1}$

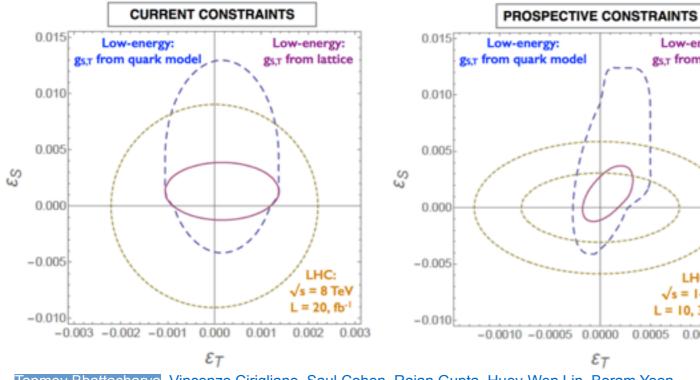
0.0005 0.0010

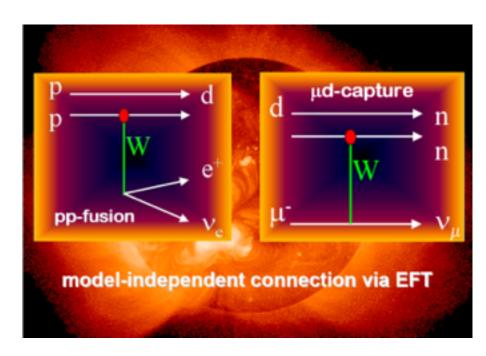


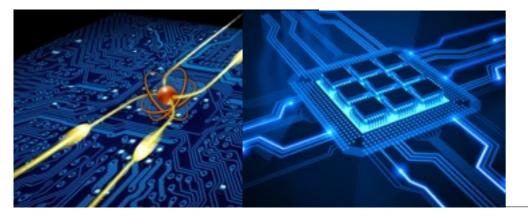
PNDME: Bhattacharya et al PRL 115 (2015) 212002 [1506.04196],

US Lattice Quantum Chromodynamics

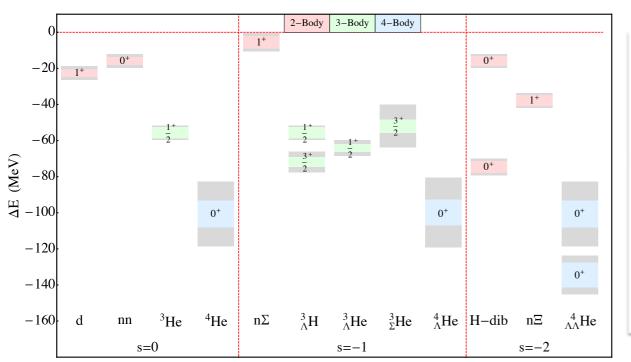
PRD 92 (2015) 114026 [1506.06411]

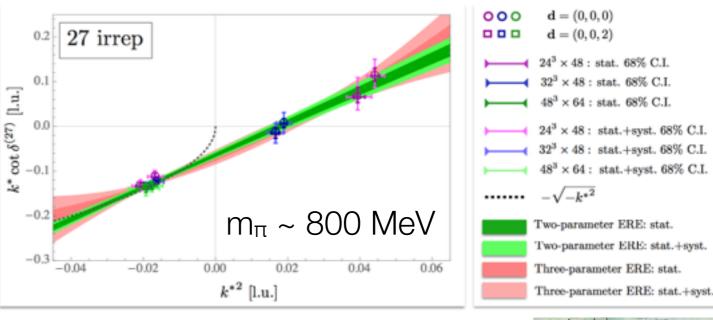


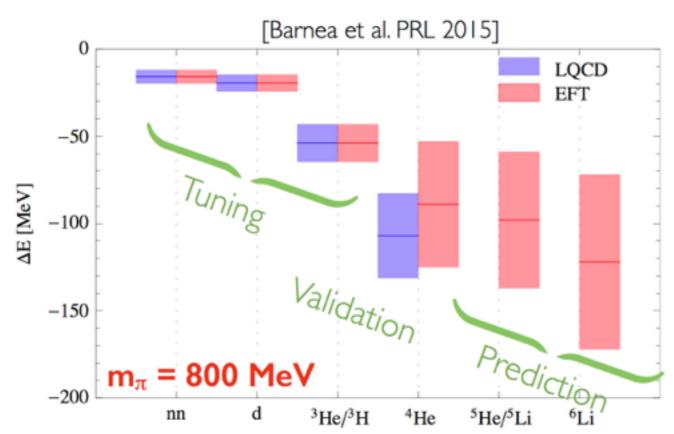




Lattice QCD QCD to Nuclear Forces: First Steps



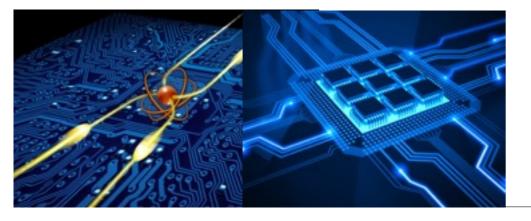




Finite-Volume Energy Eigenvalues

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

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



Exascale Ecosystem for Nuclear Physics

Read, write, manage, analyze, curate, and track data/code of complexity and scale never before encountered





DOE: Data Management Plans