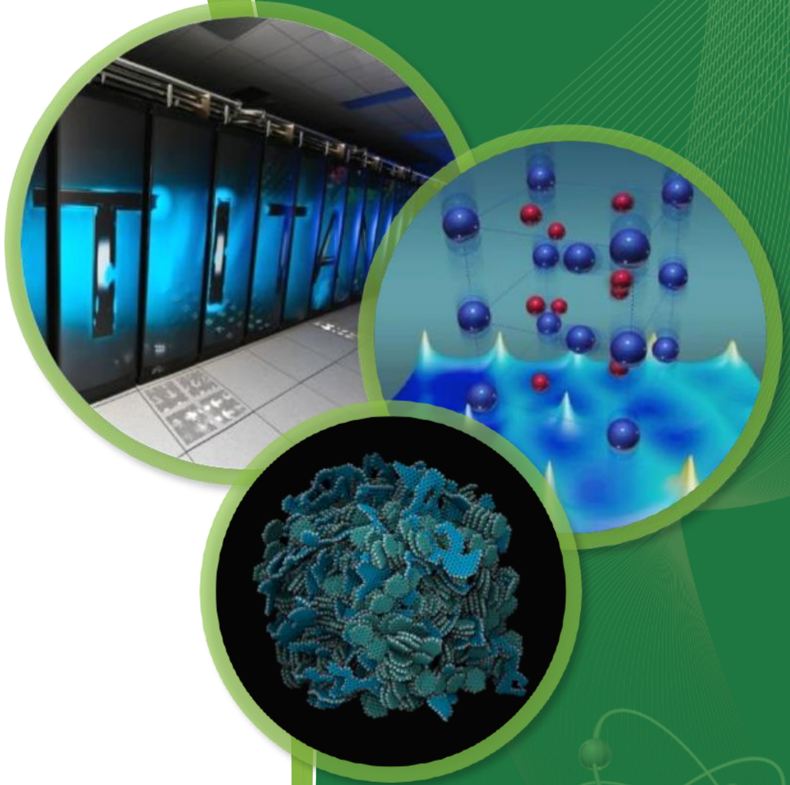
Quantum Computing & Scientific Applications at ORNL

Pavel Lougovski

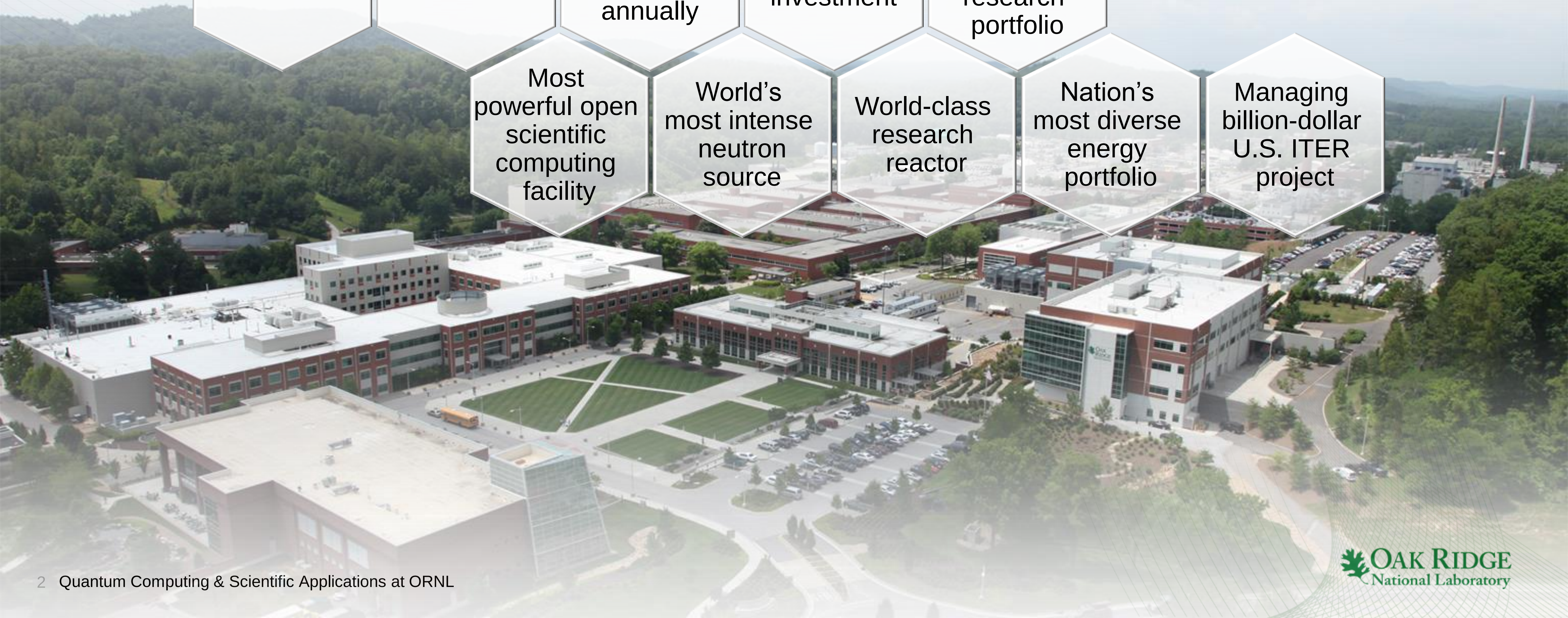
Oak Ridge National Laboratory



ORNL is managed by UT-Battelle
for the US Department of Energy

ORNL at a glance: DOE's largest science and energy laboratory

- $1.65B budget
- 4,400 employees
- 3,000 research guests annually
- $500M modernization investment
- Nation's largest materials research portfolio
- Most powerful open scientific computing facility
- World's most intense neutron source
- World-class research reactor
- Nation's most diverse energy portfolio
- Managing billion-dollar U.S. ITER project



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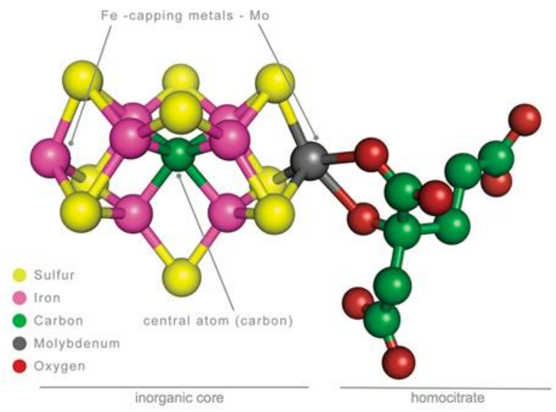
Quantum Computing at ORNL: Applications

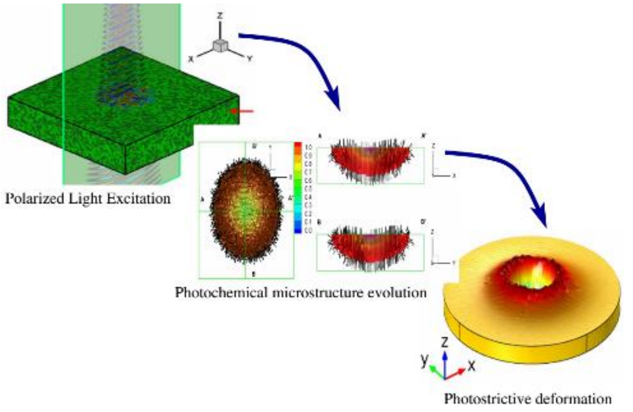
- Scientific discovery and energy security with quantum computing

Physical Sciences: Chemistry, Materials Sciences, Physics



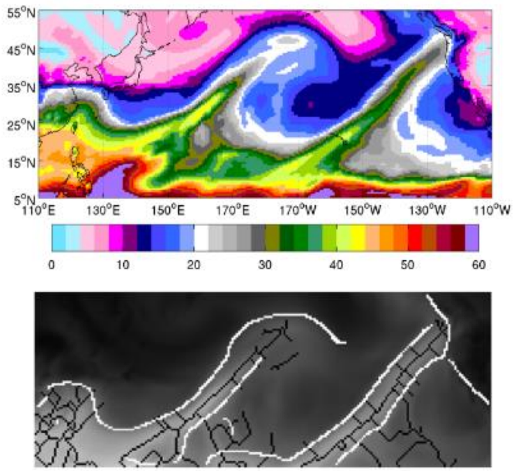
Electronic structure calculations of nitrogenase will support methods for fertilizer production, food security

Applied Sciences: Energy, Medicine, Engineering



Finite-element methods for multi-scale models will support integrated computational materials engineering

Data Sciences: Applied Math, Analytics, Artificial Intelligence,



Machine learning methods will support data analytics and artificial intelligence for situational awareness

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Quantum Computing at ORNL: Organization & Funding

- **Quantum Computing Institute**
  - Translational research for scientific applications, quantum computing user community
- **Quantum Information Science Group**
  - Subject matter experts in quantum computing, communication, and sensing
- **Quantum Computing Materials and Interfaces (FY16-18)**
  - LDRD initiative to develop new capabilities in material science for quantum computing
- **DOE ASCR Early Career Award in Quantum Computing (FY16-21)**
  - Quantum software infrastructure and performance analysis using modeling and simulation
- **DOE ASCR Quantum Algorithms Team (FY17-20)**
  - Applications development for chemistry, nuclear physics, and machine learning domains
- **DOE ASCR Quantum Testbed Pathfinder (FY17-22)**
  - Software-hardware codesign of quantum computing systems for scientific applications
- **Multiple Strategic Partnership Projects**

Quantum Computing Institute

- **We focus on translational research of quantum systems and applications**
  - Identify priorities, end users, stakeholders
  - Address near-term technology stack through multi-disciplinary collaborations
- **We build partnerships with external stakeholders and collaborators**
  - Enable support with quantum hardware, software, and expert resources
- **We engage the community through education and user support**
  - Build the future workforce
  - Communications and events

Quantum Computing User Community

- We are providing state-of-the-art quantum computing resources to the user community through strategic partnerships, collaborations, and on-site resources

Quantum Computing Institute
Oak Ridge National Laboratory

Universities

Industry

Government

D-Wave The Quantum Computing Company™

IBM

Google

IONQ

rigetti

Atos

OLCF Oak Ridge Leadership Computing Facility

Oak Ridge National Laboratory | Center for Nanophase Materials Sciences

SNS Spallation Neutron Source

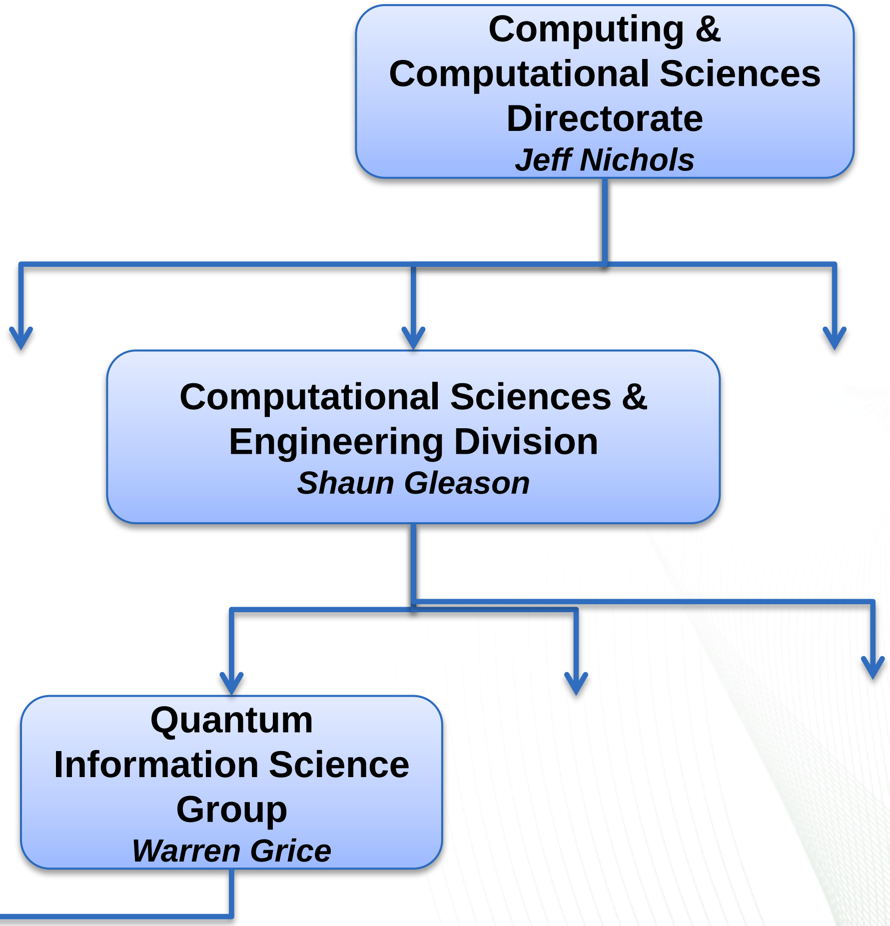
Quantum Information Science Group in ORNL Organization

QIS Group

Ryan Bennink
Phil Evans
Warren Grice
Travis Humble
Ben Lawrie
Pavel Lougovski
Joseph Lukens
Ali Passian
Nicholas Peters
Raphael Pooser

Bing Qi
Brian Williams
Eugene Dumitrescu
Kathleen Hamilton
Fahd Mohiyaddin
Titus Morris
Marouane Salhi
Jason Schaake
Matthew Feldman
Ethan Tucker

11 full-time staff
6 Postdocs
2 Interns



QIS teams

QIS

Quantum Communication

Privacy assurance for data storage & distribution – Nick Peters

Quantum Computing

Scalable algorithms for science, industry, & security – Travis Humble

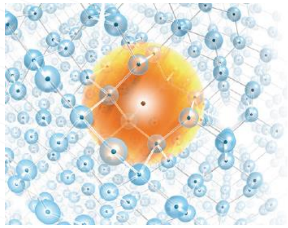
Quantum-Enhanced Sensing

Better data with less time and energy – Raphael Pooser

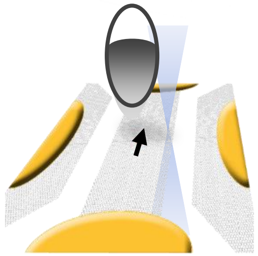
Quantum Computing LDRD Investments

- We are building new capabilities for quantum materials, devices and systems through strategic investments (FY16-18)

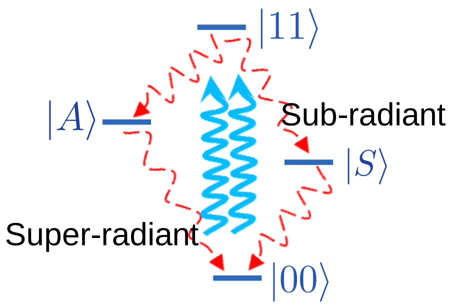
Materials



P & Bi donor in Si (Humble, Lupini)

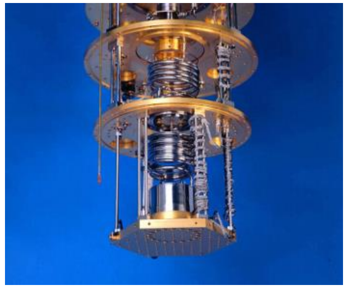


Graphene Qubit (Jesse)

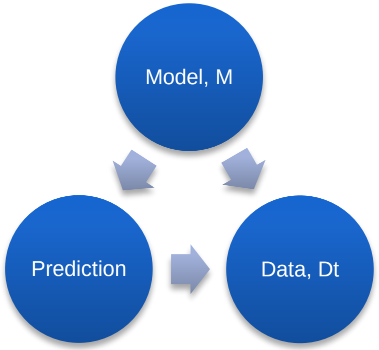


Dissipative QC (Evans)

Devices

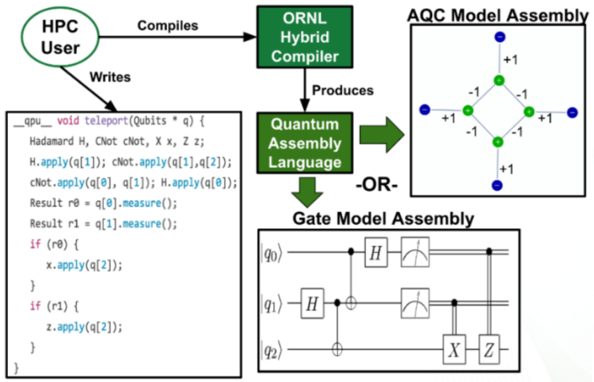


Qubit operations (Peters)

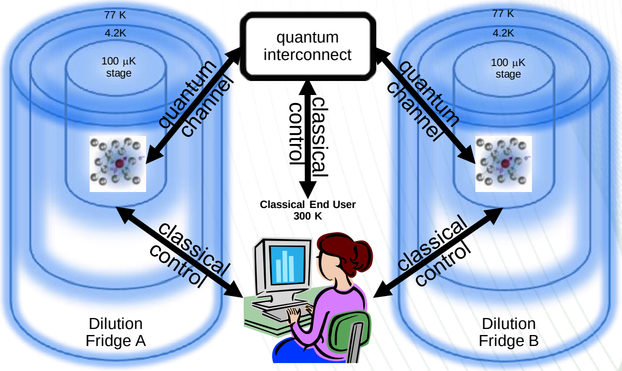


Qubit fidelity modeling (Bennink)

Systems



Qubit Compiler (McCaskey)



Quantum/Classical Interfaces (Lougovski)

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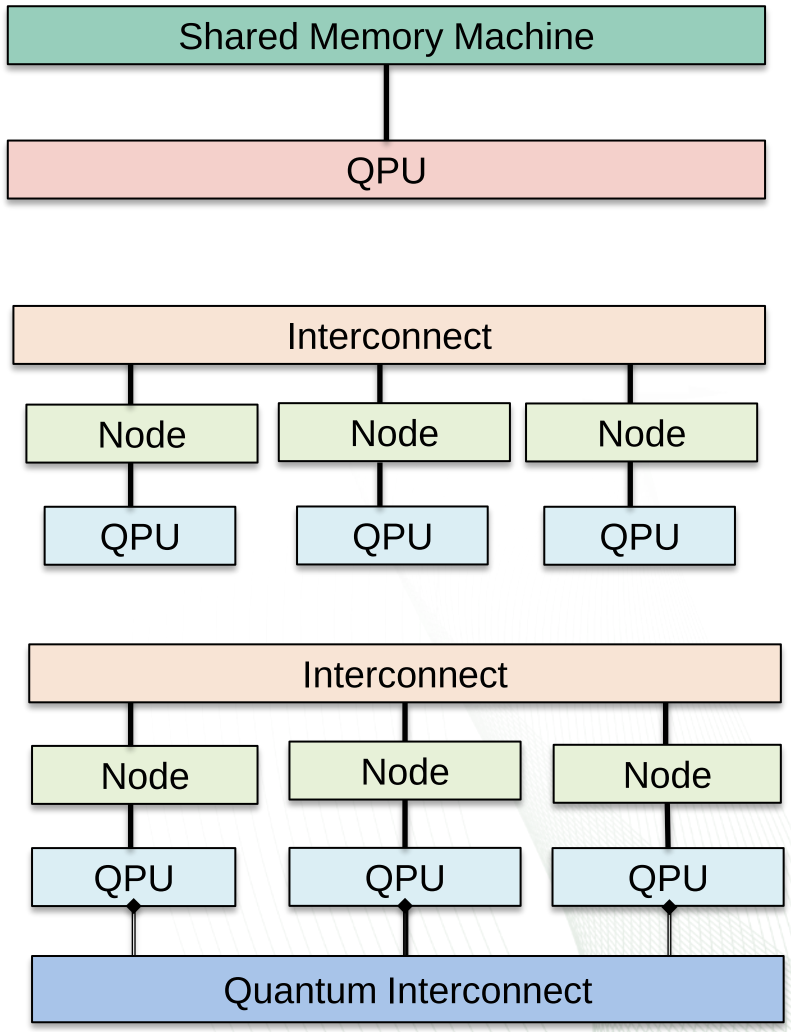
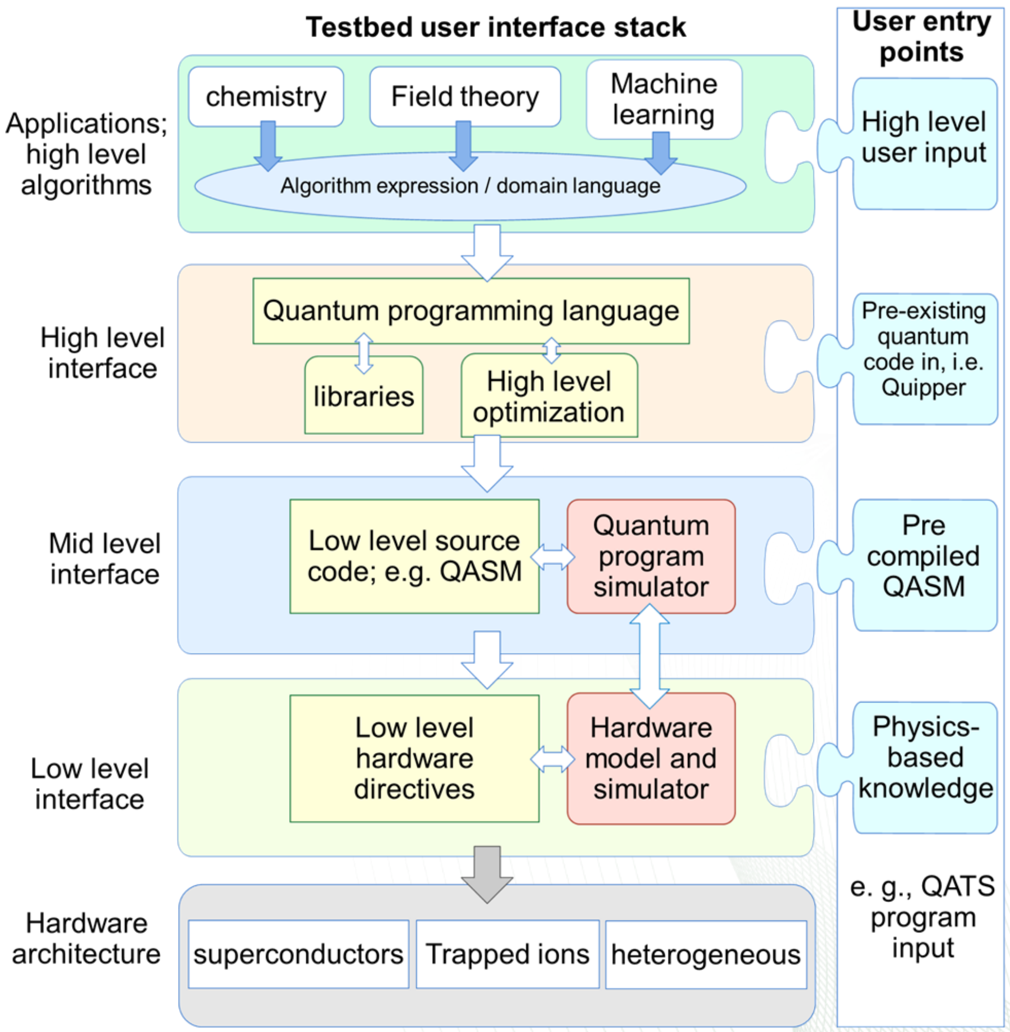
ASCR Early Career Award in Quantum Computing

- We are developing long-term capabilities in the design and operation of quantum computing system within DOE HPC facilities.
- The goal of the project is to accelerate existing scientific applications using quantum processors. The approach relies on physics, engineering, and computer science to demonstrate quantum-classical programming and run-time environments for scientific applications.
- ORNL PI Travis Humble
- DOE PM Robinson Pino



ASCR Quantum Testbed Pathfinder (FY17-FY22)

- We are exploring the design and development of quantum computing for scientific applications in chemistry, nuclear physics, and machine learning.
- The team consists of ORNL staff and a consortium of quantum computing stakeholders, including IBM, and IonQ, focused on demonstrating and characterizing application development.
- ORNL PI Raphael Pooser
- DOE PM Claire Crammer



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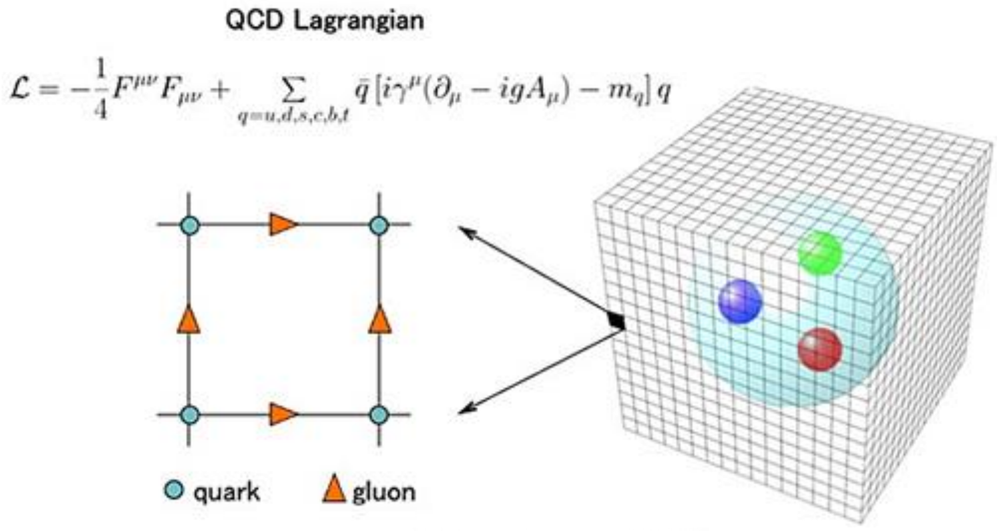
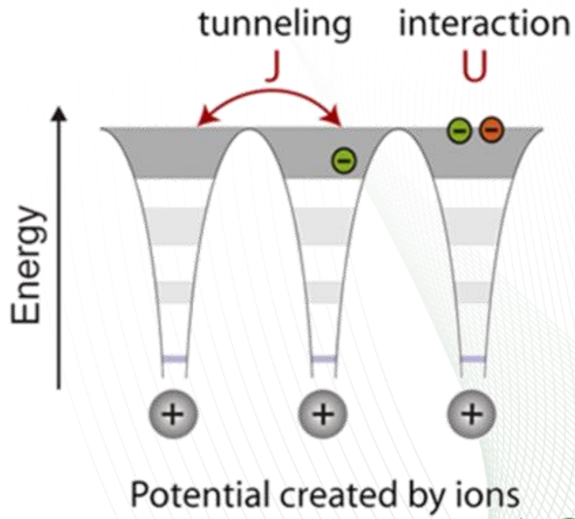
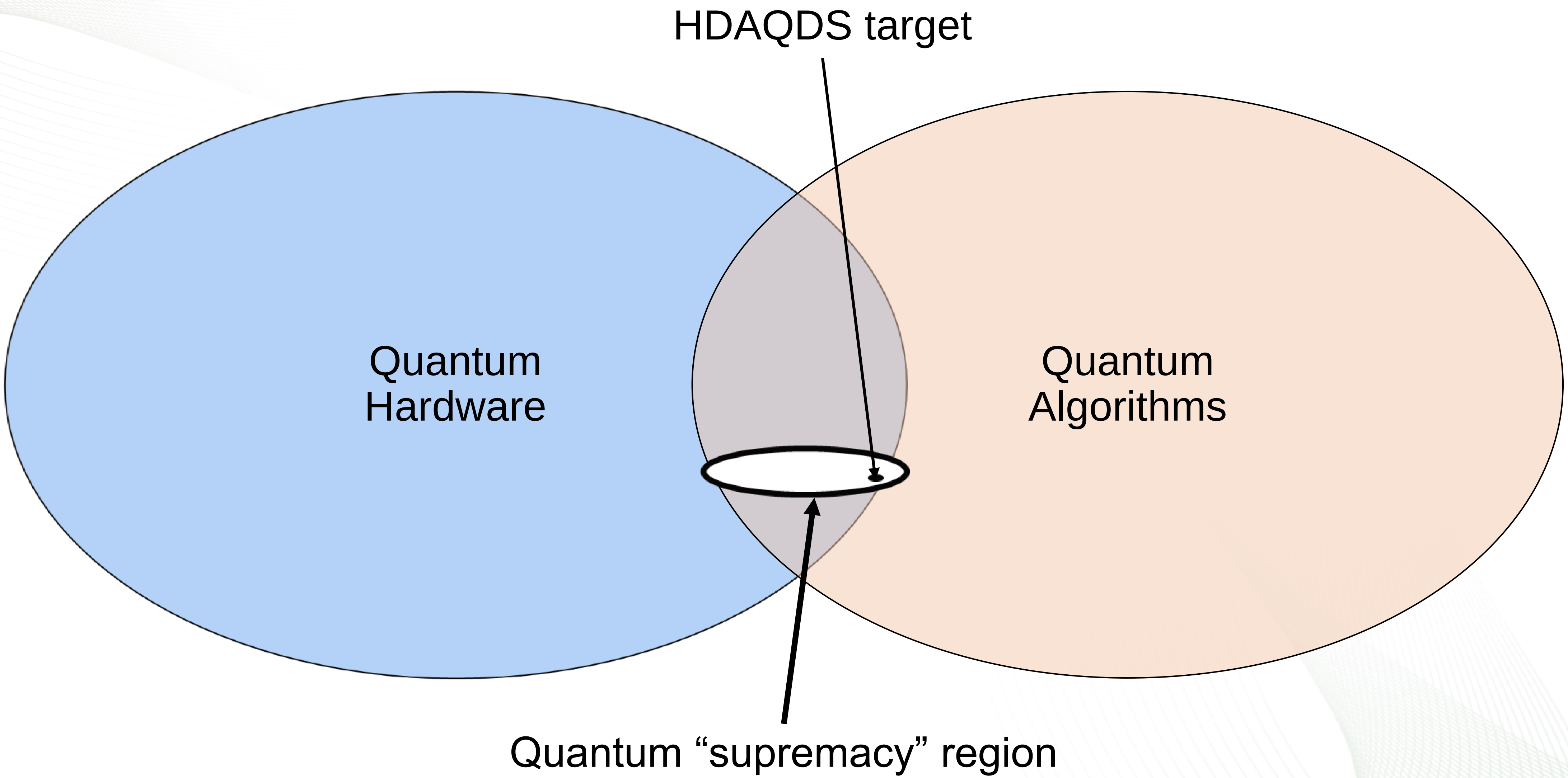
ASCR Quantum Algorithms Team (FY17-FY20)

- We are developing near-term applications of quantum computing for solving scientific problems including quantum many-body systems in superconducting materials, lattice QCD, and nuclear physics.
- The team of ORNL staff and subject matter experts from University of Washington and University of Bilbao focuses on demonstrating quantum computation and improving performance through algorithmic design.
- ORNL PI Pavel Lougovski
- DOE PM Ceren Susut





The Landscape



Heterogeneous Digital-Analog Quantum Dynamics Simulations

- Glossary:
  - Heterogeneous – mixed quantum and classical HPC & mixed quantum digital and analog
  - Digital – universal quantum gate set
  - Analog – analog quantum unitaries
  - Dynamics Simulations – e.g., a two-point correlation function

- Focus: Development of digital-analog quantum algorithms for simulating the dynamics of quantum many-body systems (Fermi-Hubbard, Hubbard-Holstein, Lattice QCD) on the near term quantum hardware.
- Partners: University of Washington (Institute for Nuclear Theory),

Evolutionary Approach to Quantum Simulations

Problem: Solve Schrodinger Equation $i\frac{\partial|\psi\rangle}{\partial t} = H|\psi\rangle$

$$|\psi(t)\rangle = U|\psi(0)\rangle; U = e^{-iHt}$$

system dynamics U $\cong$ subsystem dynamics U_1 …… subsystem dynamics U_M

Classical HPC

- Memory limited. Exponential growth in simulation size with the number of particles

Quantum Simulations → Digital Quantum, Analog Quantum

Digital Quantum

- Map simulation onto qubits
- Polynomial scaling in circuit area (# qubits x # quantum gates)
- Unfortunately # of gates is fairly large ~ 10^5

Analog Quantum

- Requires controlled many body quantum systems (as hard to build as a quantum computer)

Variational Approach to Quantum Simulations

Problem: Find the ground state of a many-body Hamitonian

Classical Answer: Minimize energy functional

$$\varepsilon[\Psi] = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi \mid \Psi \rangle}$$

Example: Coupled Cluster ansatz

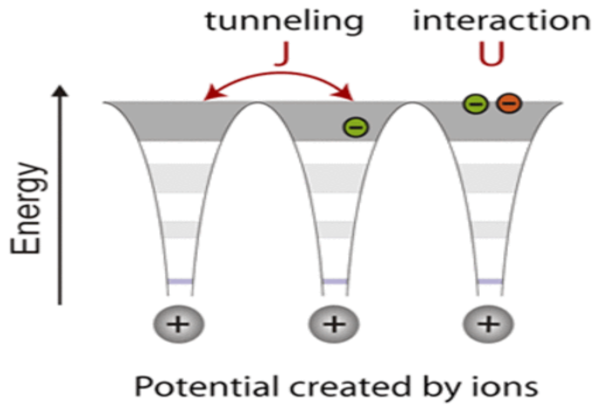
$$|\Psi\rangle = e^{T} |\Phi_0\rangle$$

$$T = T_1 + T_2 + T_3 + \cdots$$

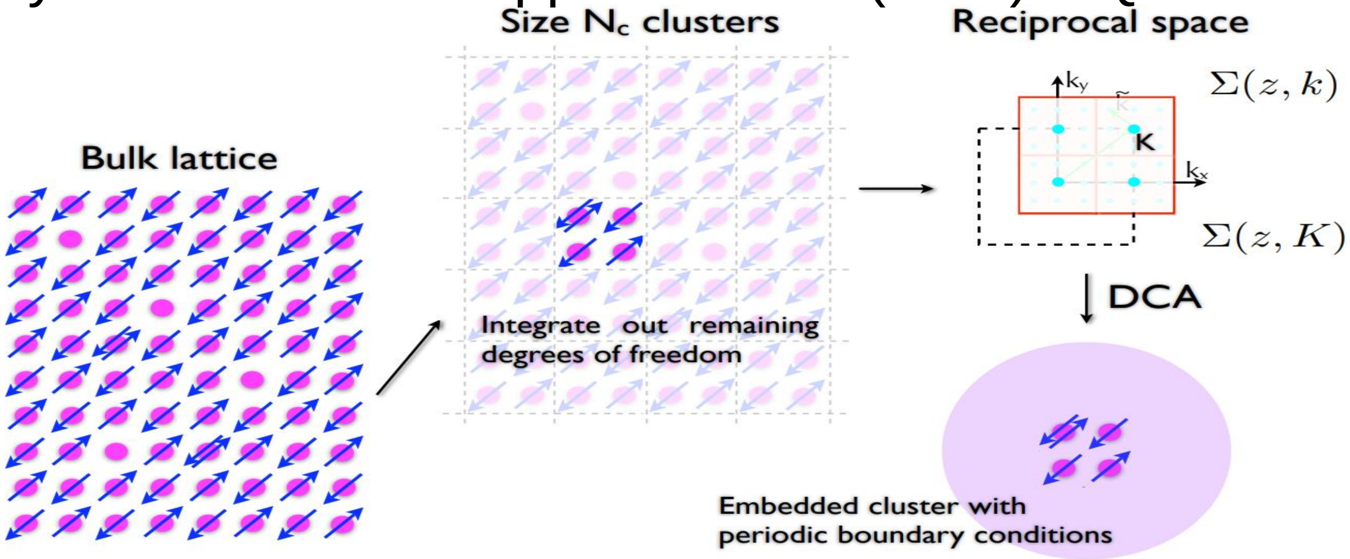
$$T_n = \frac{1}{(n!)^2} \sum_{i_1, i_2, \ldots, i_n} \sum_{a_1, a_2, \ldots, a_n} t_{a_1, a_2, \ldots, a_n}^{i_1, i_2, \ldots, i_n} \hat{a}^{a_1} \hat{a}^{a_2} \ldots \hat{a}^{a_n} \hat{a}_{i_n} \ldots \hat{a}_{i_2} \hat{a}_{i_1}$$

Scientific Applications: Strongly Correlated Electrons

- Strongly correlated electron systems Fermi Hubbard & Hubbard Holstein Models



- Dynamical Cluster Approximation (DCA) + Quantum Monte Carlo



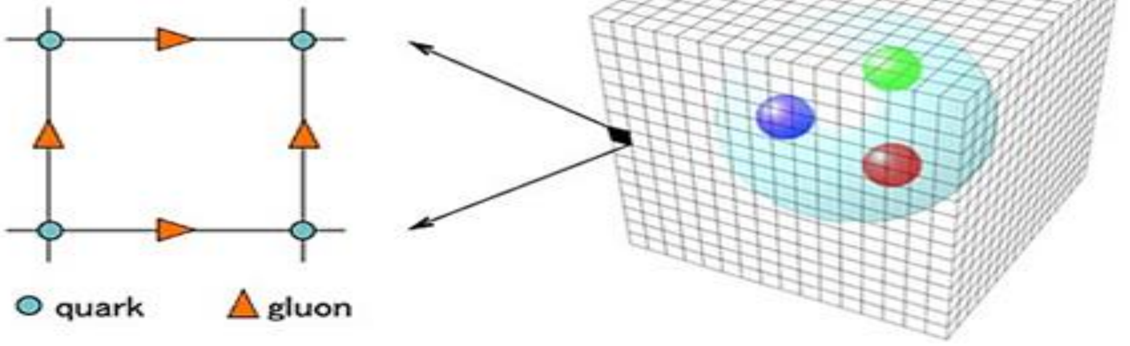
Maier et al., Rev. Mod. Phys. ’05

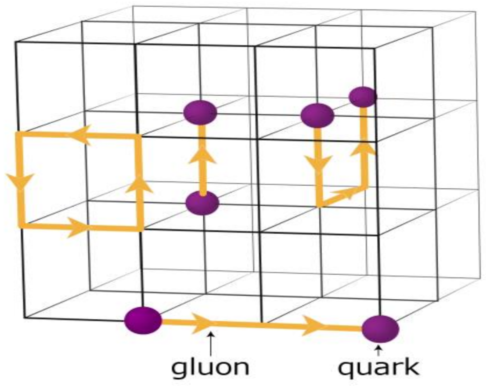
Scientific Application: Nuclear Physics

- Lattice QCD for nuclear physics applications

QCD Lagrangian

$$\mathcal{L} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} + \sum_{q=u,d,s,c,b,t} \bar{q}\left[i\gamma^{\mu}(\partial_{\mu} - igA_{\mu}) - m_q\right] q$$





- Nuclear structure via coupled cluster approach

The CC wavefunction takes on a different form:

$$\Psi_{CC} = e^{\hat{T}}\Phi_0$$

Coupled Cluster Wavefunction
Φ_0 is the HF solution

$$e^{\hat{T}} = \hat{1} + \hat{T} + \frac{1}{2}\hat{T}^2 + \frac{1}{6}\hat{T}^3 + \cdots = \sum_{k=0}^{\infty}\frac{1}{k!}\hat{T}^k$$

Exponential operator generates excited Slater determinants

$$\hat{T} = \hat{T}_1 + \hat{T}_2 + \hat{T}_3 + \cdots + \hat{T}_N$$

Cluster Operator

N is the number of electrons

G. Hagen et al, Rep. Prog. Phys. 77, 096302 (2014)

Uncertainty Quantification

- Quantifying simulation uncertainty
- Analyzing error propagations
- Measuring quantum advantage quantitatively

Software Toolchain

- Developing a software toolchain that enables utilization of the proposed QA as a part of the existing HPC simulation codes.

Thank you!
Questions?