Quantum Testbed Stakeholder Workshop

Hosted by the
Advanced Scientific Computing Research Program

Argonne National Laboratory

Quantum Computing Capabilities and Interests

February 14 – 16, 2016

U.S. DEPARTMENT OF ENERGY | Office of Science

Argonne NATIONAL LABORATORY

Argonne National Laboratory Capabilities and Interests Summary

Primary Expertise & Interest Areas

Superconducting and semiconducting spin qubits, including device fabrication

Quantum microarchitectures and systems level deployment

Quantum sensing

Quantum algorithms

Supercomputing and computational science

Most Differentiating Factor

Across the stack expertise in quantum science and technology

Cleanroom capability with existing qubit and superconducting device technology

The Quantum Factory: comprehensive capabilities for the growth of semiconductor, oxide, nitride and carbide heterostructures

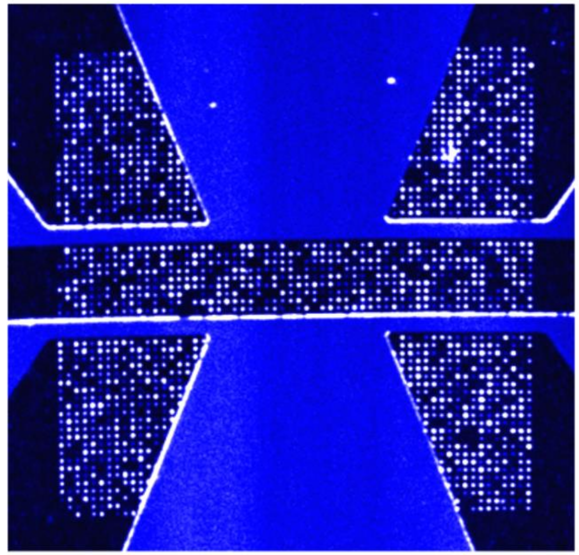
Synergistic leadership-level computing

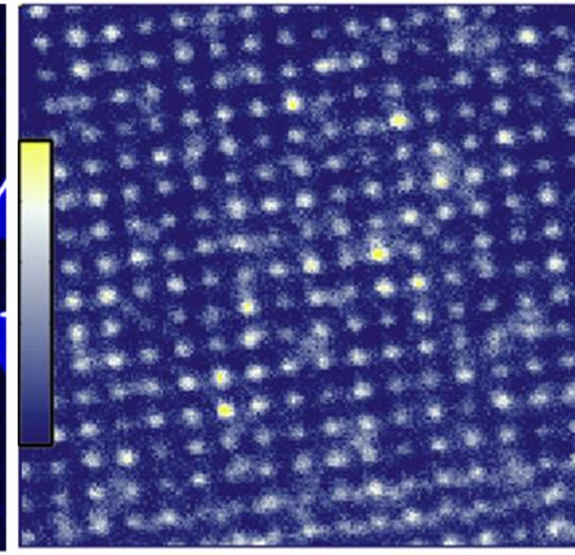
Main Contribution/Role

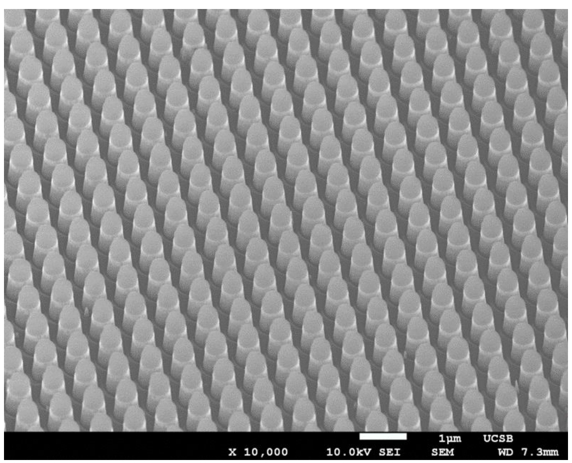
Development and fundamental science behind superconducting, semiconducting and hybrid qubits and coherent interconnects. We have the capability to develop and build quantum chip sets centered around the 30,000 sq. ft. cleanroom space at ANL and U Chicago, and using our experience at the Center for Nanoscale Materials, the user infrastructure to make available these chipsets remotely for users to interrogate. This would include setting up the remotely available test capabilities, abstractions and interfaces to control software, compilers, and programming languages development. Large-scale simulations would also help guide physics and algorithmic exploration.

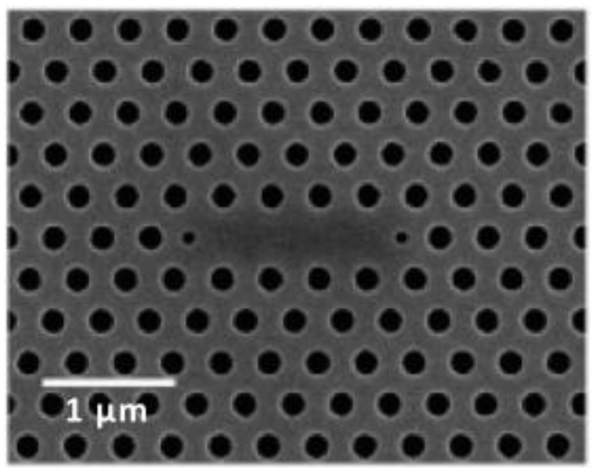
Spin Qubits: Diamond and SiC (Awschalom)

- Implanted spin arrays in diamond and SiC via wafer ion implantation
- Entanglement in a solid-state electron-nuclear spin ensemble at ambient conditions
- Tomography protocol yields fidelities up to 0.88±0.07









- Diamond growth of pillar spin arrays
- 2D photonic crystals with integrated spins
- Quantum control of single electron spin in SiC wafers with 95% contrast
- Superadiabatic control demonstrated for rapid quantum state transfer

Similar work is being pursued for other materials, like AlN, with theory support from the Galli group using the ALCF.

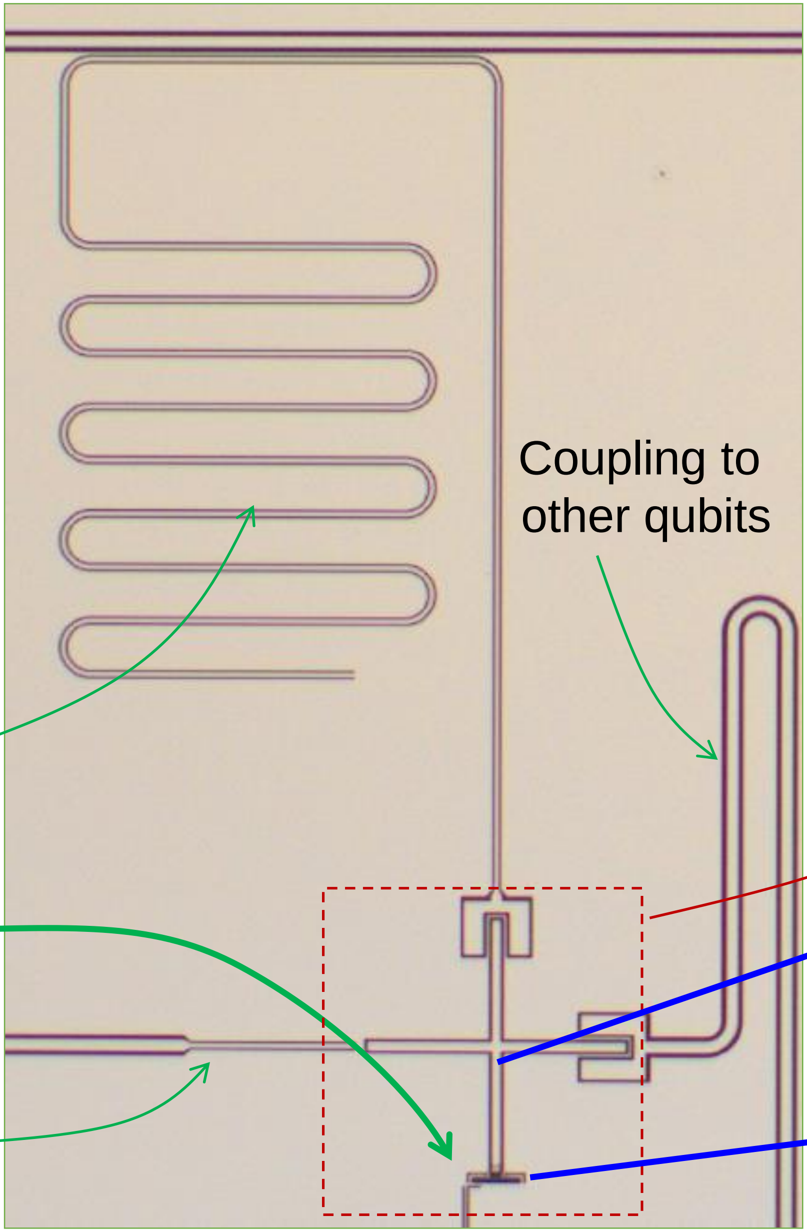
Superconducting Qubits (Cleland, Schuster)

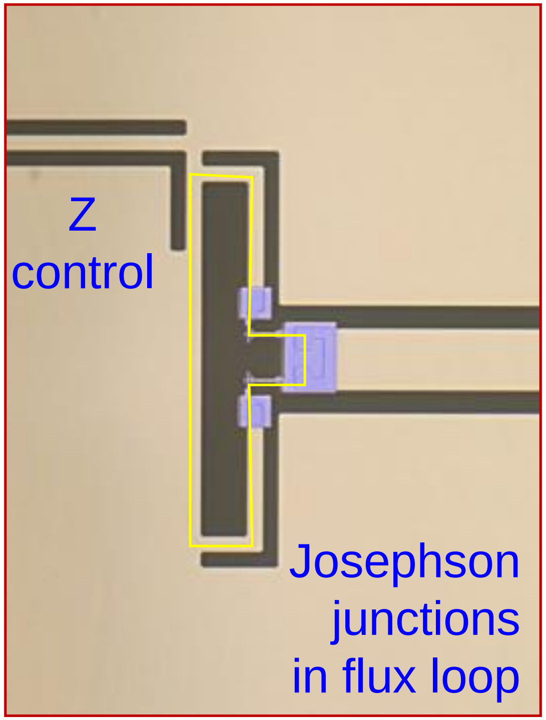
- Xmon, gmon and transmon: Proven design & fabrication
- Multi-layer scalable fabrication

Measurement:
- Dispersive readout

Z rotations:
- Flux tuning varies *L*
- Changes qubit ω

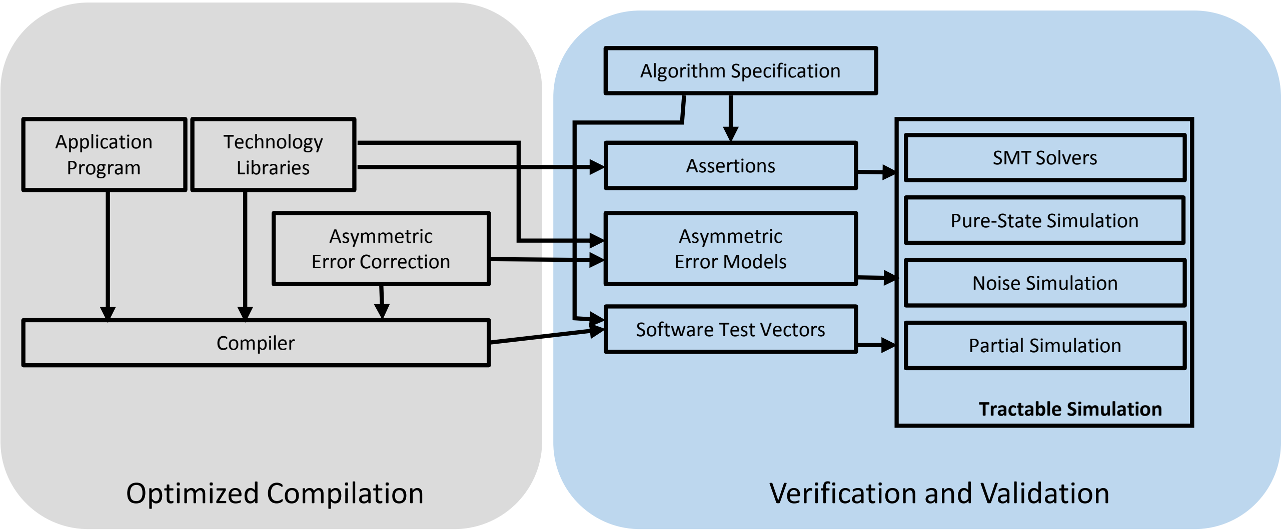
X and Y rotations:
- Microwaves at ω





Quantum Computer Science Capabilities (Chong)

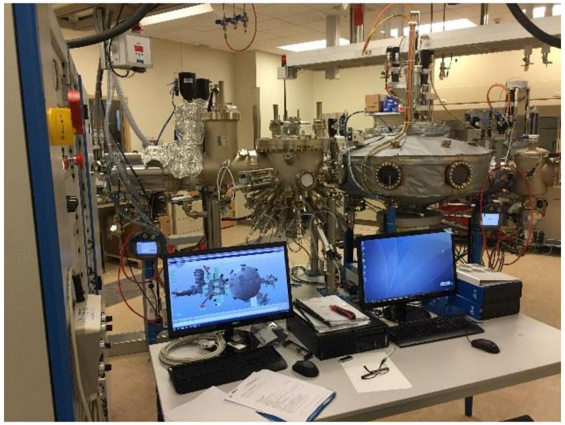
- Extensive software toolchain
  - Scalable, open source, compatible with MSR, Intel and Delft efforts
- Extensive architecture work
  - Technology and error correction comparisons, adaptation to physical characteristics
- Strong ties to experimental effort
  - Physical models and error control, quantum transduction to scale machines
- Formal methods & simulation for correctness
  - Argonne supercomputing resources



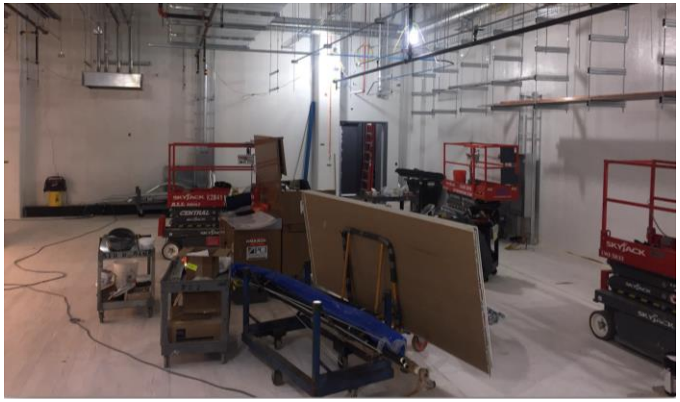
Synthesis, Fabrication and Characterization Capabilities

- UC Pritzker Nanofabrication Facility
  - General purpose nanofabrication facility
  - Fully equipped for qubit fabrication
  - Fully staffed and open user facility

- ANL-IME Quantum Factory (6000+ sq. ft)
  - Quantum materials discovery platform
  - 9M$+ invested by ANL-UC & DOE
  - Nitrides, carbides, oxides, & oxy-chal-cogenide qubit heterostructures
  - MBE, MOCVD, CVD, sputtering, plasma

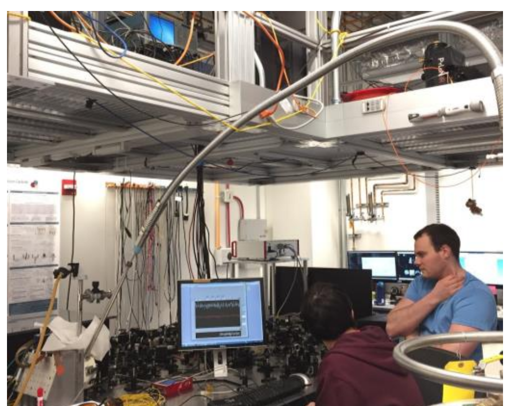


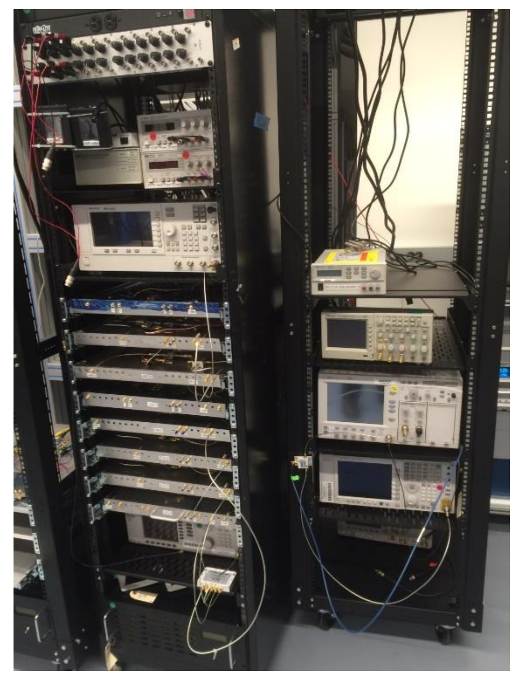
- ANL-CNM Cleanroom
  - 12,000 sq. ft. professionally staffed & fully equipped nanofab facility
  - Undergoing $9M+ expansion by 6000 sq. ft.
  - Fully developed superconducting qubit & superconductor technology process flows



Capabilities in Engineering & Supporting Technology

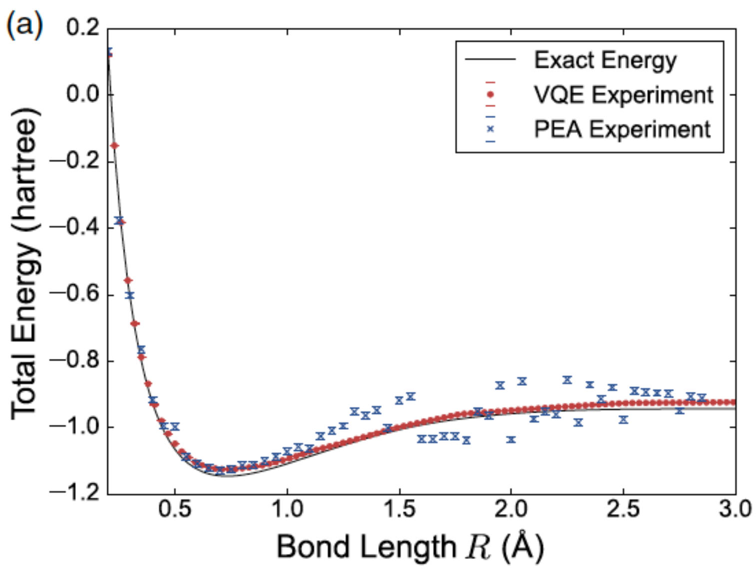
- AWG microwave electronics with complex pulse shaping
- Single photon detection, femtosecond operation from 3K to 300K
- Dry cryostats wired for continuous multi-qubit operation below 10 mK
- Custom FPGA microwave electronics for complex multi-qubit operations
- Leadership computing for exploration and validation of arrays of qubits



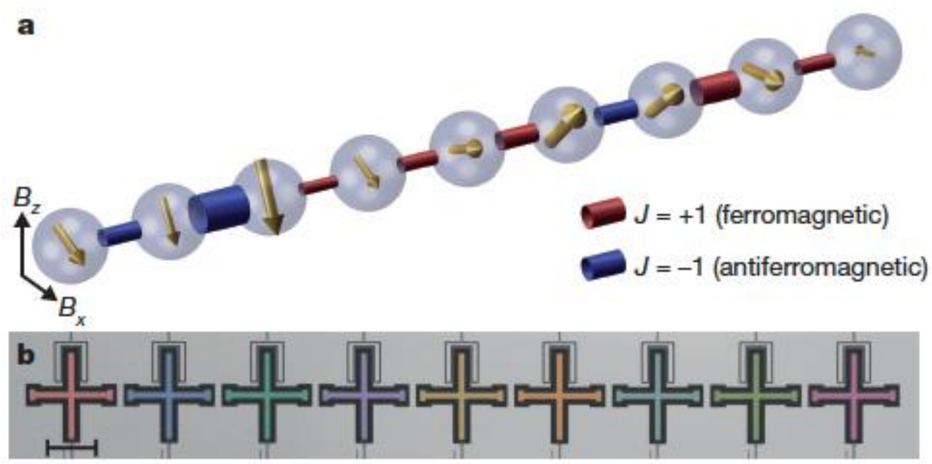


Applications to Domain Science

- Materials discovery utilizing machine learning, including quantum variants
- Quantum chemistry & energy landscapes from quantum/classical hybrids
- Hybrid quantum/classical approaches to correlated electrons
- Simulation of small molecules relevant for future technologies (Li_xO_x, etc.)
- Solution of quantum spin systems on frustrated magnetic lattices
- Quantum control and quantum metrology



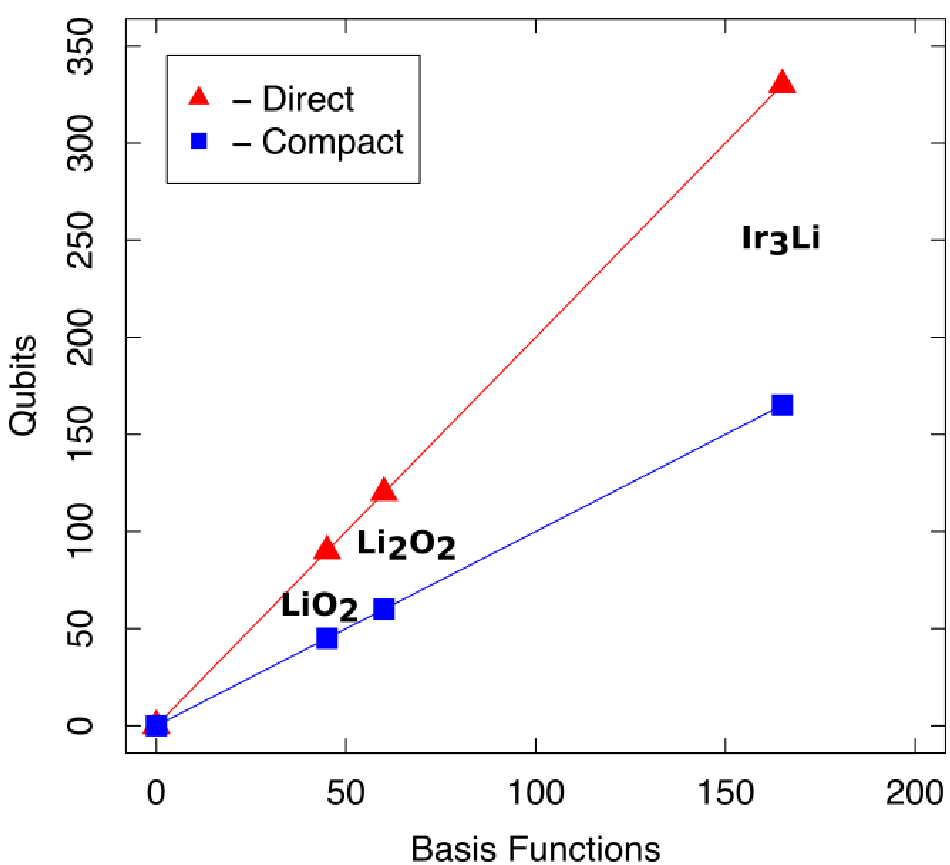
Xmon calculation of H_2 energy curve
O'Malley *et al*, PRX 6, 031007 (2016)



Xmon calculation of quantum spin chain
Barends *et al*, Nature 534, 222 (2016)

Case Study: Battery Research

Developing new generations of batteries is technologically important and scientifically challenging. Quantum computing will enable the most accurate quantum chemistry method, full configuration interaction (FCI), which scales exponentially with the size of the system, but polynomially for quantum computing. A recursive phase estimation algorithm (compact) is proposed to significantly reduce the number of qubits [1]. An example is Li_xO_x for a Li-Air battery system [2].



The number of qubits required to store the wave function is shown as a function of the number of basis functions. The estimate is for the FCI method using a DZP basis set.

[1] Simulated quantum computation of molecular energies, Aspuru-Guzik *et al*, Science 309, 1704 (2005)

[2] A lithium–oxygen battery based on lithium superoxide, Lu *et al*, Nature 529, 377 (2016)

Investments in Quantum Computing Technology

- ANL LDRD Investments (FY14-17)
  - IME Quantum Engineering Staff - Awschalom, Galli, Guha, Cleland
  - M3 Strategic LDRD on “Oxides for novel computational approaches”
- ANL Infrastructure Investments (FY14-17)
  - MEM module to the Energy Sciences Bldg. (Awschalom and Guha Labs)
  - CNM cleanroom expansion

MEM Module

CNM Cleanroom Expansion

Facility Management Experience

- Center for Nanoscale Materials (BES User Facility)
  - Extensive experience with worldwide users and user facilities
  - Fully staffed clean room with extensive user support
  - Quantum sensing, a key strategic thrust for the CNM

- Argonne Leadership Computing Facility (ASCR User Facility)
  - Extensive experience with worldwide users, algorithm development, and support of diverse hardware architecture
  - Developed methodology for high-level and technical support, user training, and management of complex operational constraints
  - Has the potential to field a dedicated quantum-computing testbed with a long-term goal of integrating QC into large-scale machines

External Partnerships

- Partnerships with industry, universities, or other entities outside the lab that are relevant to quantum computing
  - Extensive partnership with UC, with multiple joint appointments with ANL (Awschalom, Cleland, Guha, Galli)
  - Coupling to other UC quantum computing efforts (Chong, Schuster)
  - UC/ANL Computation Institute
  - Industry connections – Intel (software tools, qHipster)
  - Guha managed & expanded IBM's quantum program 2010-2015 prior to joining ANL-UC

- Experience working with industry, including IP protection and technology transition
  - ANL Technology and Commercialization Division
  - UC Chicago Innovation Exchange