Research Spotlight Forum

6.4.19 Quantum Information Sciences

Simulating Quantum Computers and Using Quantum Computers for Simulation

PRESENTED BY:

Andrew Baczewski, Quantum Computer Science, adbacze@sandia.gov

Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.
SAND2019-6181 PE

SAND2018-14303 O

Quantum Computer Science at Sandia

I work in the Quantum Computer Science group (manager, John Aidun)

- 10 technical staff
- 2 postdocs
- 3 student interns (2 from UNM/CQuIC)

Wide-ranging expertise

- Physical device modeling and experimental support
- Qubit characterization and performance assessment
- Basic quantum algorithms research

I am a computational physicist

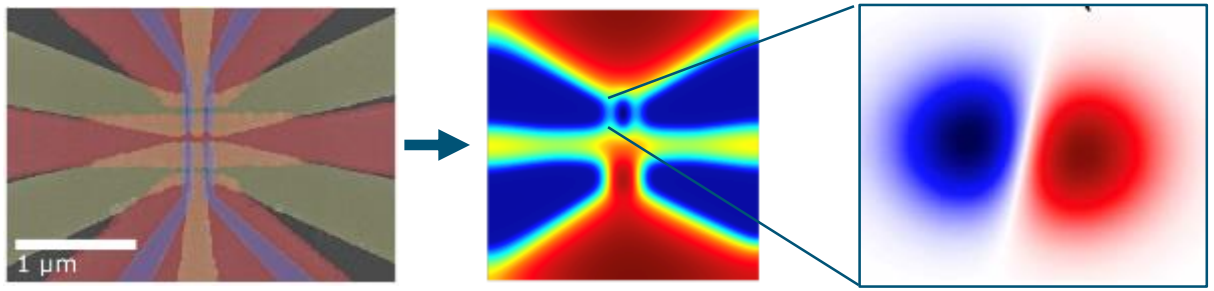
- PhD in physics and EE (Michigan State, 2013)
- Fast methods for integral equations, accurate methods for PDEs, applications in light-matter interaction
- Took the leap into QIS 6 years ago, using electronic structure theory to model semiconductor spin qubits

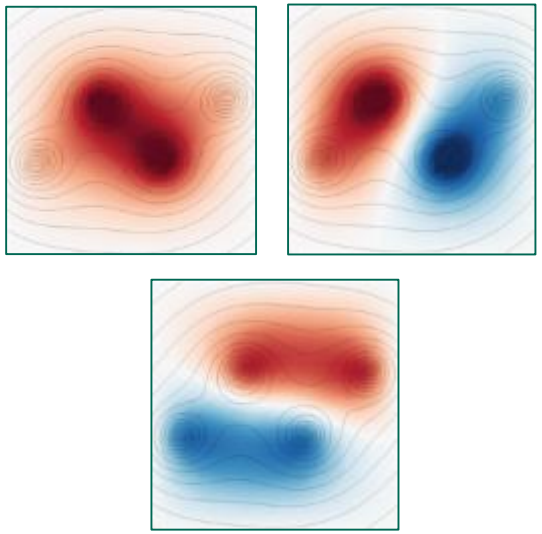
Topic for today: simulating quantum computers and using quantum computers for simulation

Physical Device Simulation

I am the lead developer of a device simulator, Laconic

- Contributors: Mitchell Brickson, Toby Jacobson, Leon Maurer, Vanita Srinivasa, and Wayne Witzel
- Sandia LDRD has funded a lot of this development





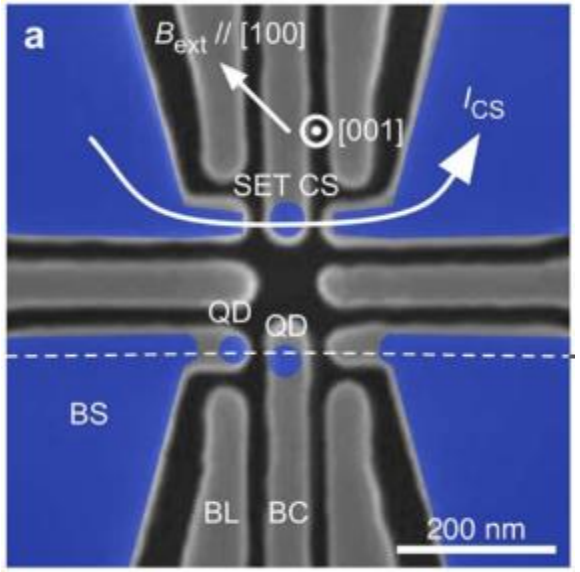
Features:

- Implements a discontinuous Galerkin discretization, stitches in semi-analytic solutions where possible
- Dynamical simulation capability (Jacobson, Srinivasa, Witzel)
- Configuration Interaction solver (Maurer and Jacobson)
- Spin-orbit physics and magnetic fields (Brickson)
- New methods for open systems (Brickson)

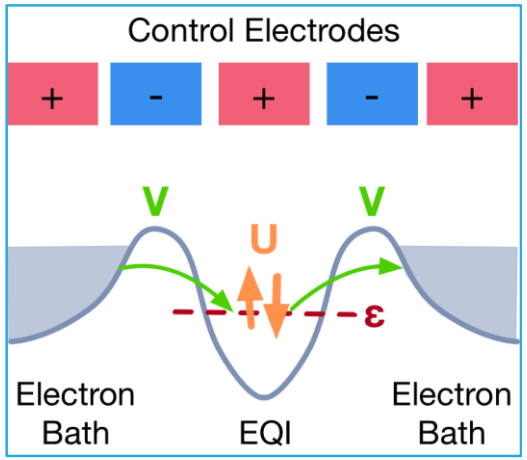
Analog Simulation of Strongly Correlated Materials

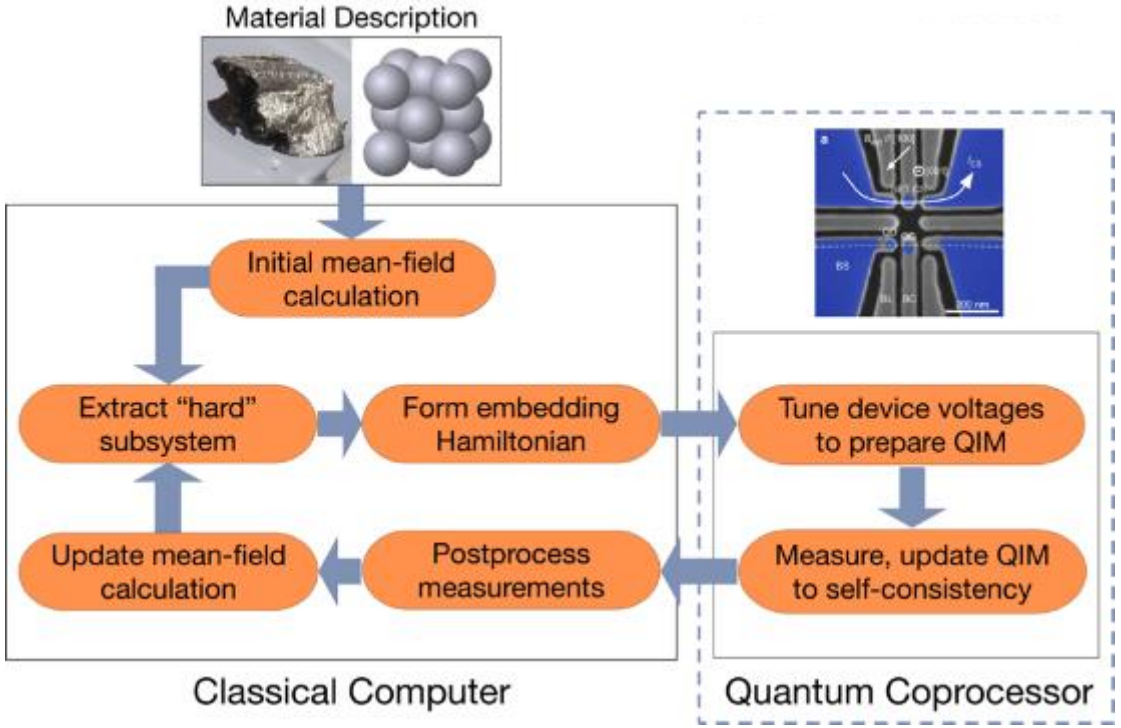
We are using Laconic to develop a new hybrid approach for analog simulation of strongly correlated materials

All-electrical universal control of a double quantum dot qubit in silicon MOS



Charge sensor is the challenging part for modeling





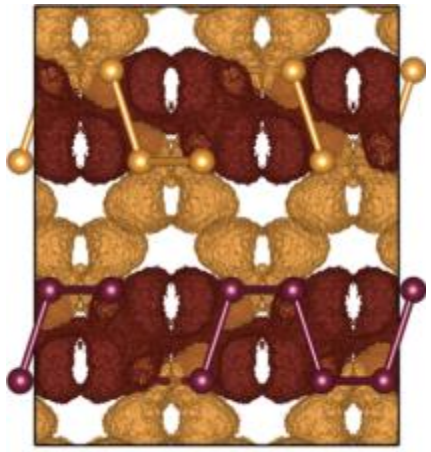
Approach circumvents qubit-to-fermion mapping, utilizes the very large bath Hilbert space that we typically take for granted

Funding from Sandia LDRD

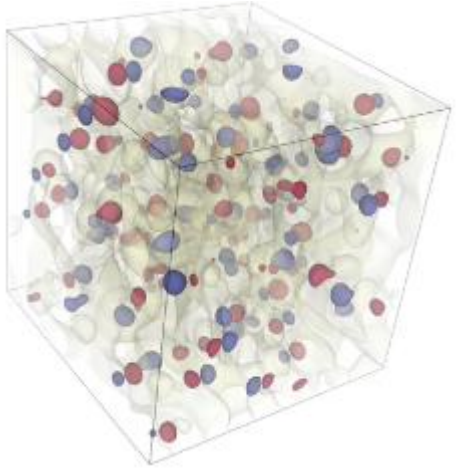
Quantum Simulation for Electronic Structure Problems

Significant fraction of DOE/NNSA supercomputers used for quantum simulation

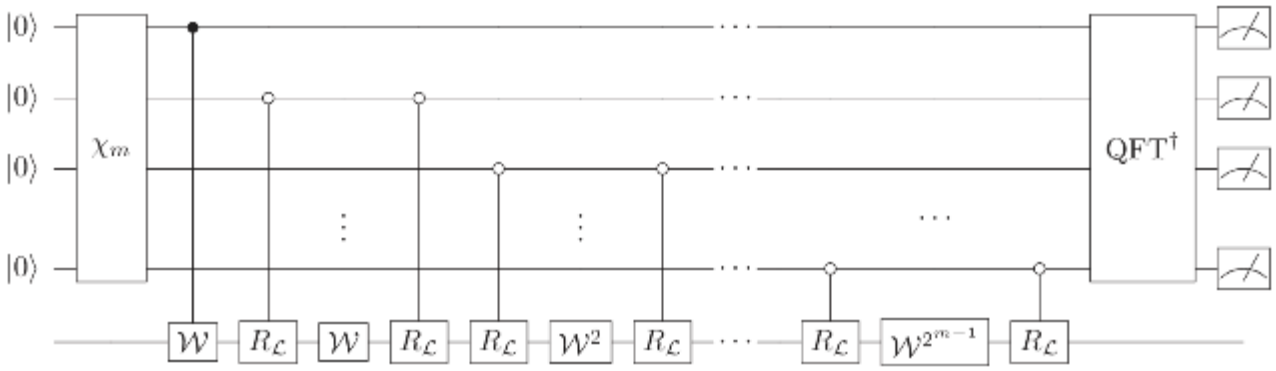
Quantum computers achieve an <u>exponential</u> advantage in <u>systematically improvable</u> quantum simulation



Quantum Monte Carlo (Shulenburger, et al., Nano Letters 2015)



Time-dependent DFT (Baczewski, et al., PRL 2015)



Phase estimation circuit based on qubitization framework (Babbush, et al., PRX 2018)

DOE/NNSA projects developing:

- Algorithms for machine learning, optimization, and simulation (ASCR, QAT – PI, Parekh)
- Near-term quantum software stack (ASCR, QCAT – PI, Sarovar)
- Realistic estimates of what is needed to do impactful quantum simulation (ASC, GBQC – PI, Baczewski)

Research Needs

Ample opportunity for collaboration

Physical device simulation

- Applications/target systems for our simulation tools
- New and improved discretizations, better solvers, better methods
- Techniques for simulating stationary and dynamical properties of interacting open quantum systems
- Control expertise for analog simulation project

Quantum simulation

- New approaches to analog or digital simulation
- Novel applications and use cases, e.g., hard problems, new things to compute
- Classical methods for simulation, hybrid quantum-classical methods, NISQ opportunities…

I'm happy to facilitate connections with other members of the Quantum Computer Science group, too