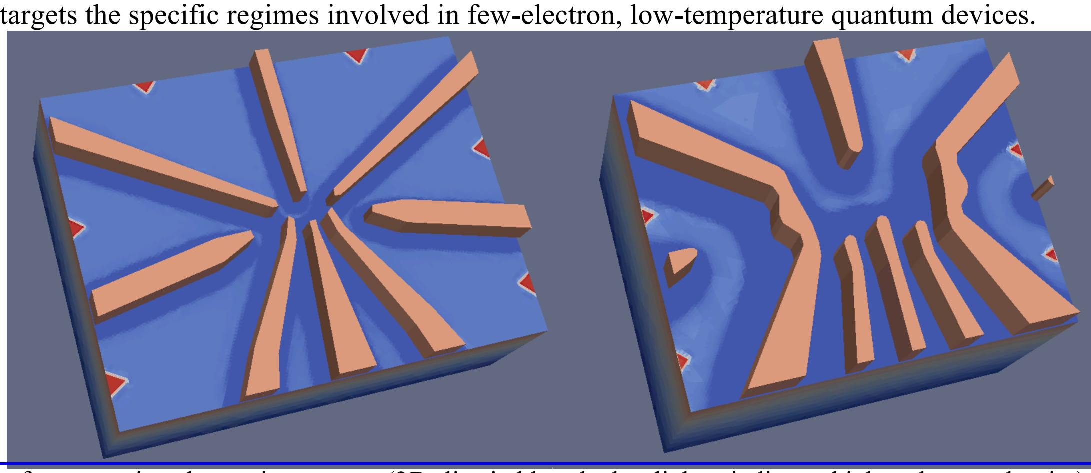
Quantum Dot Computer Aided Design

Challenge

As semiconductor processing chips become further miniaturized for the next-generation of computing and other smart electronic devices, it is likely that they will approach or reach the limits of nanoscale miniaturization, that is the atomic scale—the sizes of single atoms or molecules. This means that, in addition to the macro- and mesoscopic properties already under consideration, scientists and engineers must now also consider quantum mechanical effects described by the Schrodinger equation (the fundamental equation of physics for describing quantum mechanical behavior). These effects become relevant at that atomic scale, and are present, but normally masked by the electromagnetic properties that result from the large population of atoms/molecules of which a device is composed (described by the Poisson equation). Some properties arising from quantum effects—such as entanglement—may be useful as positive capabilities, while others will likely be problematic. It is therefore important to be able to model these phenomena to guide nanoengineering initiatives. In addition to semiconductor devices, current initiatives to design quantum bits (qubits) for quantum computers will also benefit from such modeling capabilities. This project is developing a suite of computational tools, including Schrodinger-Poisson and other capabilities, in order to address current and future issues critical to simulating such quantum-scale electronics.

Research

The Quantum Computer Aided Design (QCAD) LDRD project is developing computational simulation tools to design quantum dots for use as qubits in quantum devices, leveraging a number of existing Sandia software tools, including the Trilinos solver library and the Albany/agile tool chain, the Dakota optimization toolbox, and the Cubit mesher. Existing device simulation tools focus on room-temperature, many-electron devices; by contrast the QCAD project targets the specific regimes involved in few-electron, low-temperature quantum devices.



Simulation of comparative electronic structure (2D slice in blue shades, lighter indicates higher electron density) induced by a set of electronic gates in two different configurations, designed to function in electron confinement for qubits.

QCAD uses Sandia's high-performance computing resources to explore multiple candidate structures in multiple configurations in parallel. The project has developed a semiclassical capability, and is developing a corresponding quantum capability, as well as maturing the optimization tools to enable better discovery of promising quantum dot structures. The resulting capability is already finding application to direct-funded projects in quantum computing.

Impact

The outcome of this project should be a significant increase in the knowledge of the requirements for high-fidelity simulation of quantum-scaled devices, including new algorithms for converging electronic structure calculations at low temperatures, as well as more general convergence calculations for coupled multiphysical regions. As a corollary, further development of several software packages will occur, including the Agile Components in Trilinos, and the Charon device simulation package. In addition to strengthening Sandia's position as a leader in the engineering of devices for use in nanoelectronics circuits—by enabling predictive simulation of such 3D electronic devices—this simulation capability will move researchers a step closer to the actualization of qubits, and therefore, of quantum computers.

Point of Contact: Robert Muller rmuller@sandia.gov

Funding: LDRD