

The QCAD Framework for Quantum Device Modeling

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Problem

Background

- Few-/single-electron quantum dots as qubits

Goals

- Design guidance:** which layouts perform best (allow few e- in each dot and simultaneous control of barriers)? given a dot device, what gate voltages lead to few-electron behavior?
- Device calibration:** seek a systematic method of calibrating device parameters (threshold voltage, capacitance, etc.)

Challenges

- many device layouts & complex geometries
- large parameter space (many gates)
- low temperature
- quantum effects
- defects / disorder

Approach

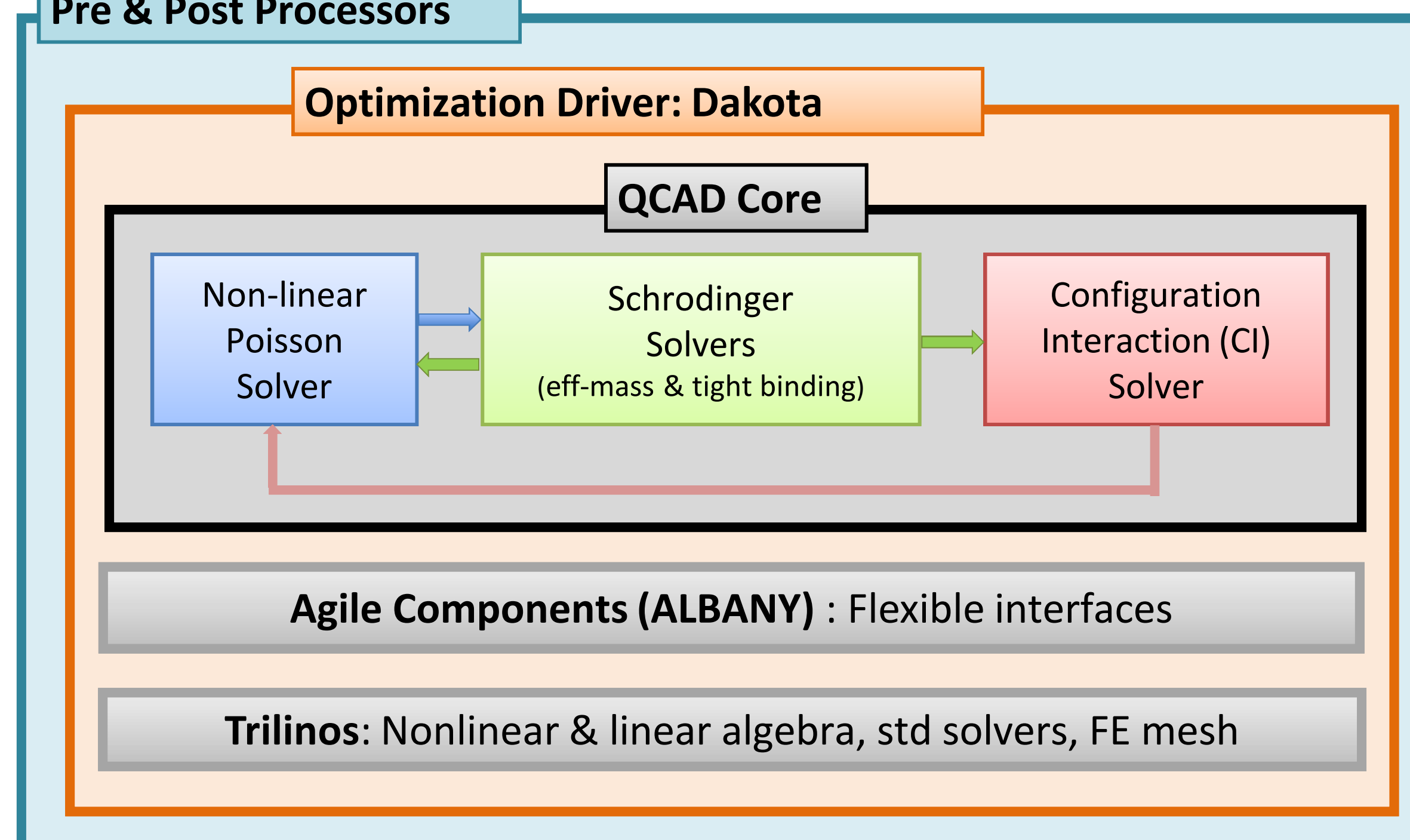
Solution

- Albany agile framework interfaces Trilinos and Dakota, provides rapid FEM framework for developing tools

Features

- Automatic differentiation
- Evaluation order determined by graphs
- Distributed parallel computing
- Sandia-developed and freely distributable

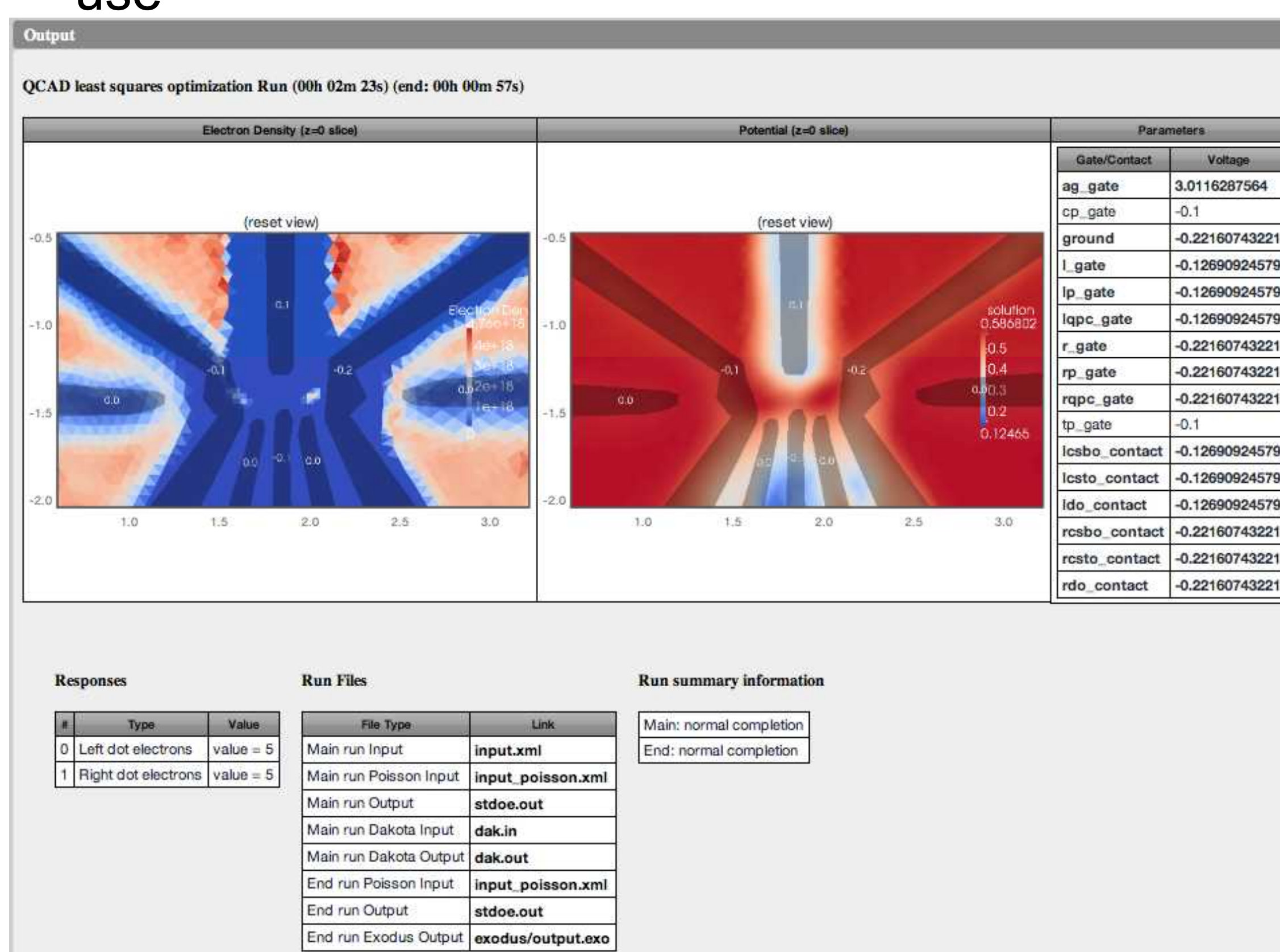
Pre & Post Processors



Results

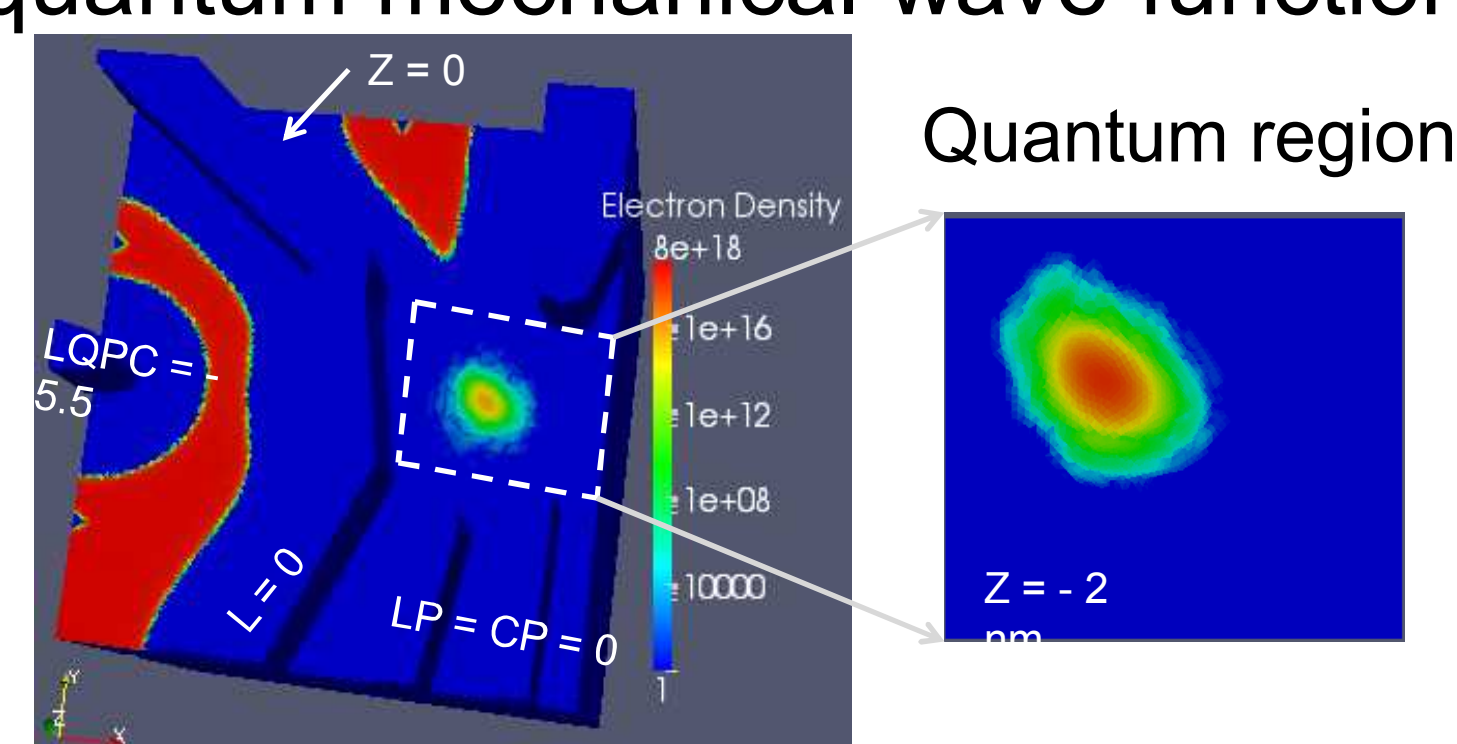
Rapid Feedback for Experimental Designs

- Number of electrons in various regions, capacitances, electron density in tunnel regions, etc.
- iQCAD web app allows QCAD to be used by experimentalists, fast enough for nearly-interactive use



Schrodinger-Poisson simulation of dots

- Coupled S-P solution allows determination of quantum mechanical wave function & potential.



Significance

- QCAD software tool developed enables **design comparison and guidance** for semiconductor quantum dot devices.
- High throughput of simulations through scripting, automated meshing and web portal allows **fast feedback** to experiment team.
- Self-consistent quantum models in QCAD allows for **analysis of quantum effects** on device behavior.