

# The Quantum Computer Aided Design (QCAD) Framework for Quantum Device Modeling

## Sandia National Laboratories

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## Problem

Trial-and-error approach to developing few-electron quantum dots for qubits is untenable; a systematic tool would accelerate development

**Goals:** A simulation tool that supports:

- **Design:**
  - which layouts perform best (allow a few e<sup>-</sup> in each dot and simultaneous control of barriers)?
  - given a dot device, what gate voltages lead to few-electron behavior?
- **Calibration:**
  - we seek a systematic method of calibrating device parameters (threshold voltage, and capacitance)

### Challenges for Schrodinger-Poisson Solvers

- many device layouts and complex geometries
- large parameter space (many gates)
- low temperature Fermi-Dirac statistics
- quantum effects
- defects/disorder

## Approach

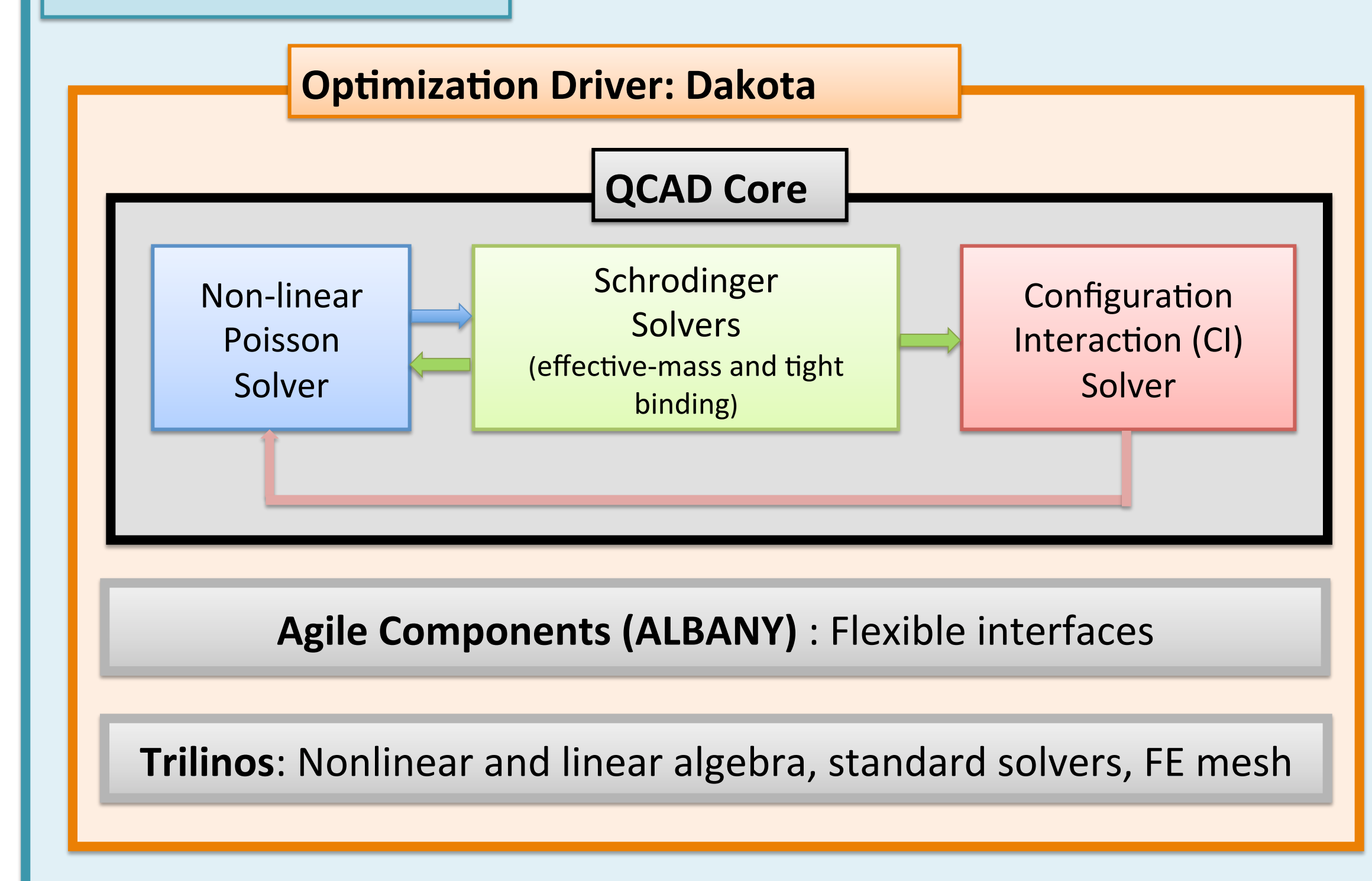
### Solution

- Albany interfaces Trilinos and Dakota, and provides a framework for the rapid development of solvers for finite element method (FEM) problems

### Features

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

### Pre & Post Processors



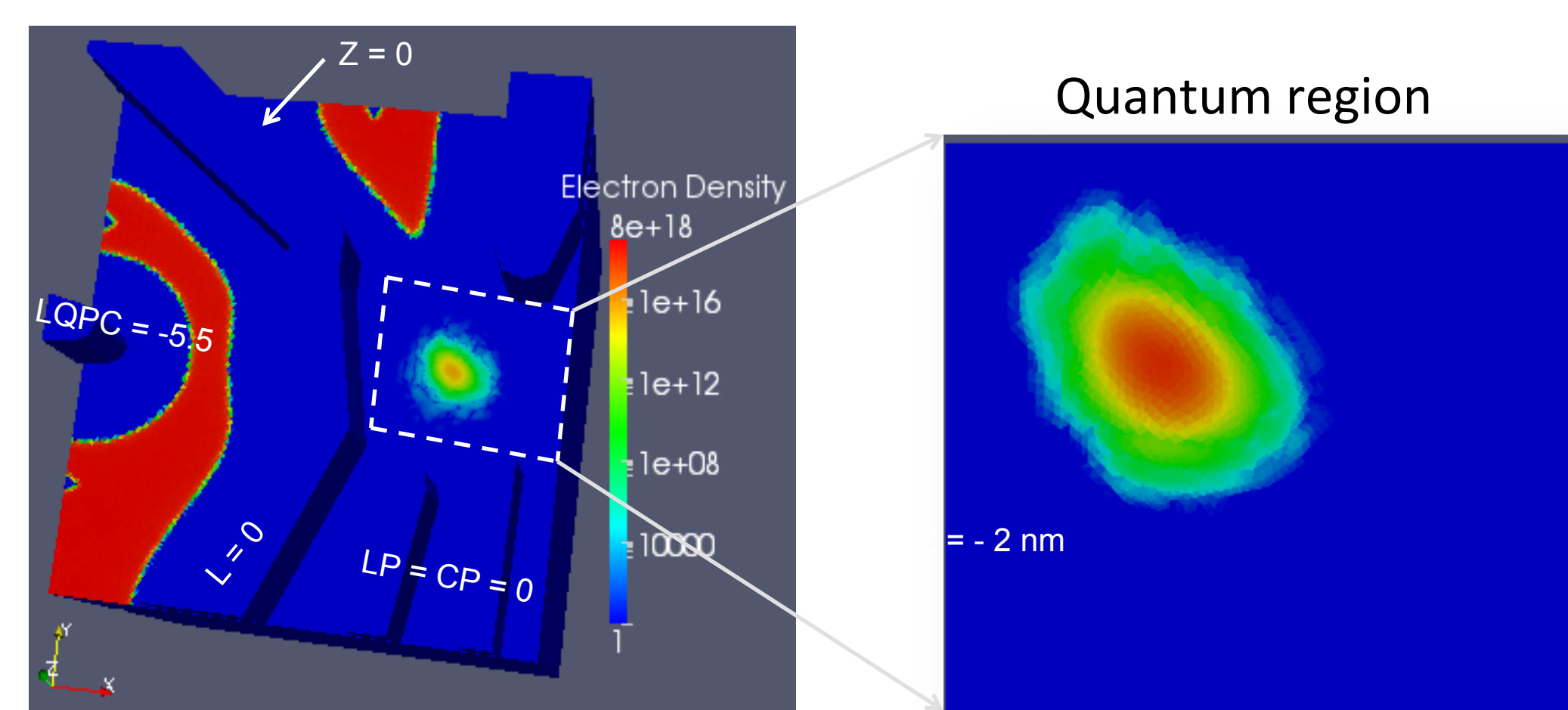
## Results

### Rapid Feedback for Experimental Designs

- QCAD reports the number of electrons in various regions, capacitances, and electron density in tunnel regions

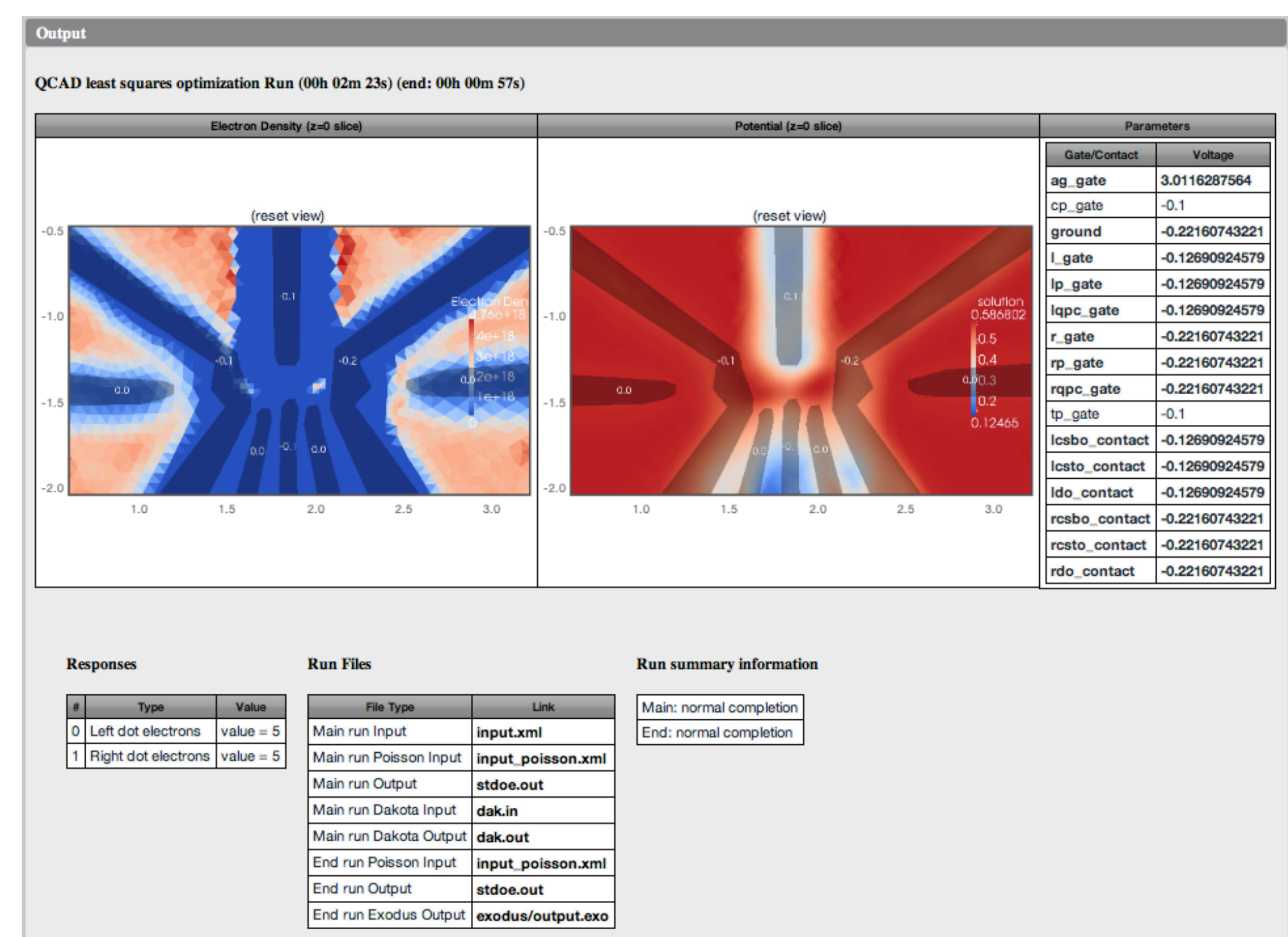
### Schrodinger-Poisson simulation of dots

- Coupled Schrodinger-Poisson solution allows determination of quantum mechanical wave function and potential



### iQCAD Interface

- Extensively used by experimentalists through the iQCAD web application
- Fast enough for interactive use



## Significance

- QCAD software tool 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 allow **analysis of quantum effects** on device behavior