SAND2011-5266 C
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QCAD – Computer Aided Design for Quantum Dots

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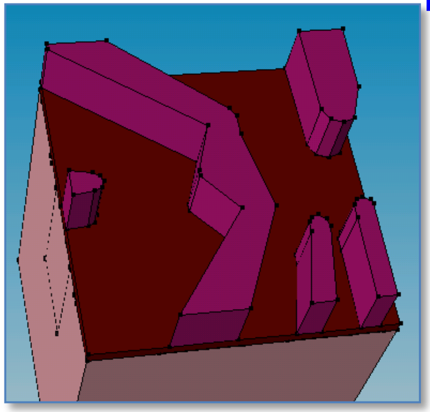
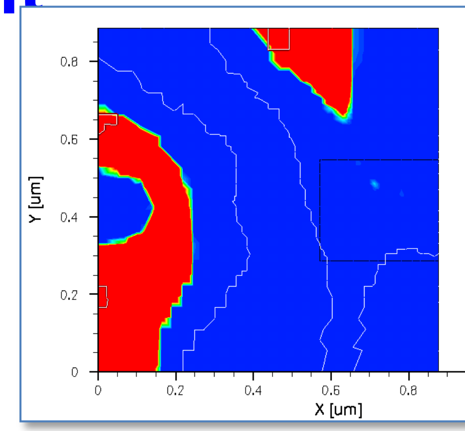
TCAD Calculations Drive Quantum Dot Development





- We have used TCAD calculations in QIST and Weisshorn projects to
  - Simulate the dot shape resulting from gate architectures
  - Predict voltages leading to few-electron regimes
  - Make estimates of lengths and characteristics of tunneling regions
  - Provide input and validation to capacitance calculations

- However, TCAD:
  - Is commercial, expensive, limiting the number of calculations we can run at any given time.
  - Targets many electron devices at room temperature; we're concerned with few electron devices at near 0° K.
  - Is difficult to modify to insert new physics, including quantum effects, atomic-scale roughness and valley splitting, etc.

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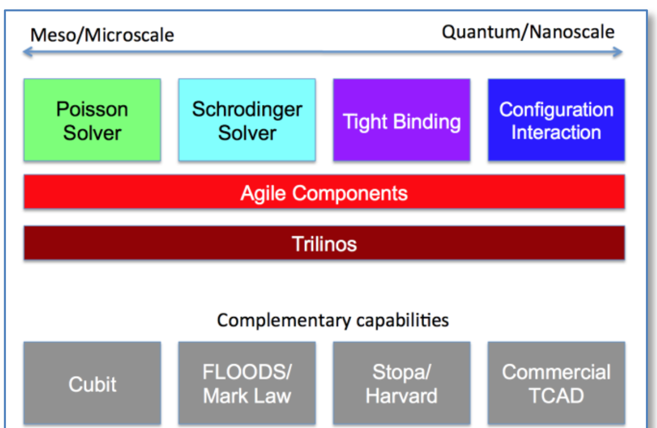
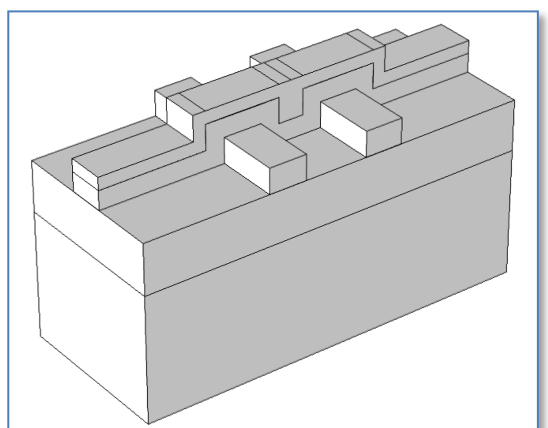
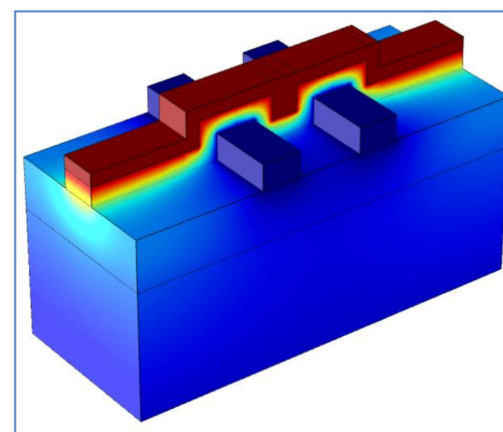
QCAD Approach

- Develop a set of tools that allow semiclassical and Schrodinger-Poisson simulations in an extensible framework. Focus on regimes relevant to quantum dots (low T, few e).
  - Albany: Agile development framework in Trilinos
- Interface with a variety of existing capabilities.







Equations

In the semiconductor region of a MOS capacitor, the Poisson equation reads:

$$-\nabla(\varepsilon_s \nabla\phi) = q(p - n + N_D^+ - N_A^-) \qquad (-\nabla(\varepsilon_s \nabla\phi) = 0 \quad \text{in the oxide region})$$

For Maxwell-Boltzman statistics,

$$n = N_C \exp\left(\frac{E_F - E_C}{k_B T}\right) \qquad p = N_V \exp\left(\frac{E_V - E_F}{k_B T}\right)$$

For Fermi-Dirac statistics,

$$n = N_C F_{1/2}\left(\frac{E_F - E_C}{k_B T}\right) \qquad p = N_V F_{1/2}\left(\frac{E_V - E_F}{k_B T}\right)$$

Conduction band effective density of states

$$N_C = 2\left(\frac{m_{dn}^* k_B T}{2\pi\hbar^2}\right)^{3/2} = 2.5094\times 10^{19}\left(\frac{m_{dn}^*}{m_0}\right)^{3/2}\left(\frac{T}{300K}\right)^{3/2} \text{ cm}^{-3}$$

Valence band effective density of states

$$N_V = 2\left(\frac{m_{dp}^* k_B T}{2\pi\hbar^2}\right)^{3/2} = 2.5094\times 10^{19}\left(\frac{m_{dp}^*}{m_0}\right)^{3/2}\left(\frac{T}{300K}\right)^{3/2} \text{ cm}^{-3}$$

m_{dn}^* / m_{dp}^* = Electron/hole density-of-states effective mass including valley degeneracy

Fermi-Dirac integral of order 1/2

$$F_{1/2}(x) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\sqrt{\varepsilon}\, d\varepsilon}{1 + \exp(\varepsilon - x)}$$

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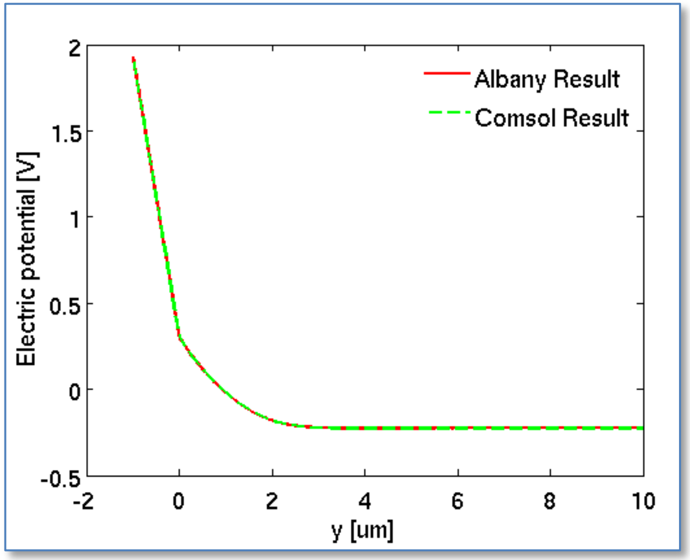
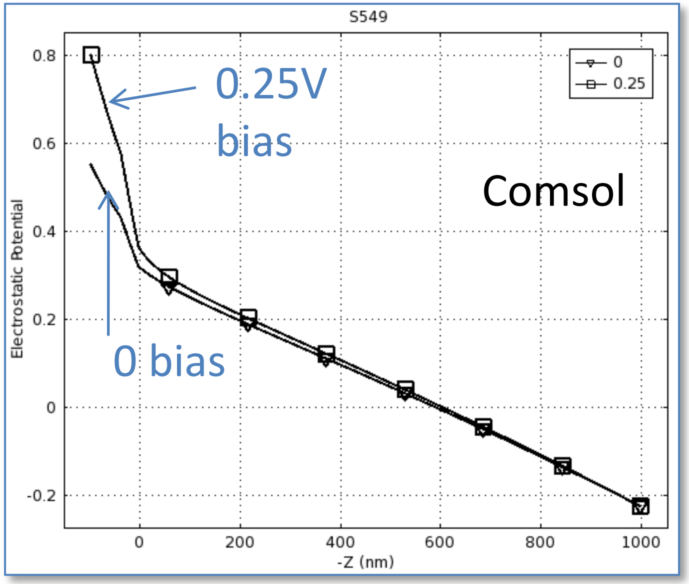
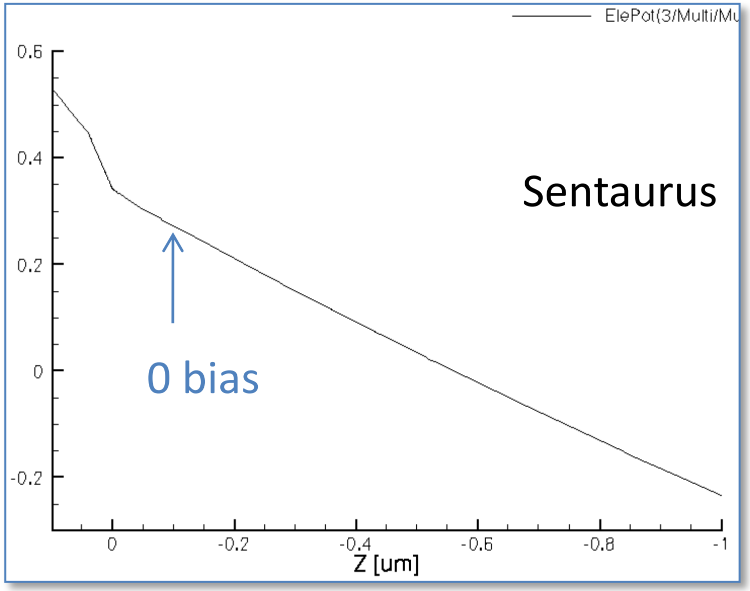
QCAD Comparison to Sentaurus

- Simple test cases help verify results of Comsol and Albany capabilities.



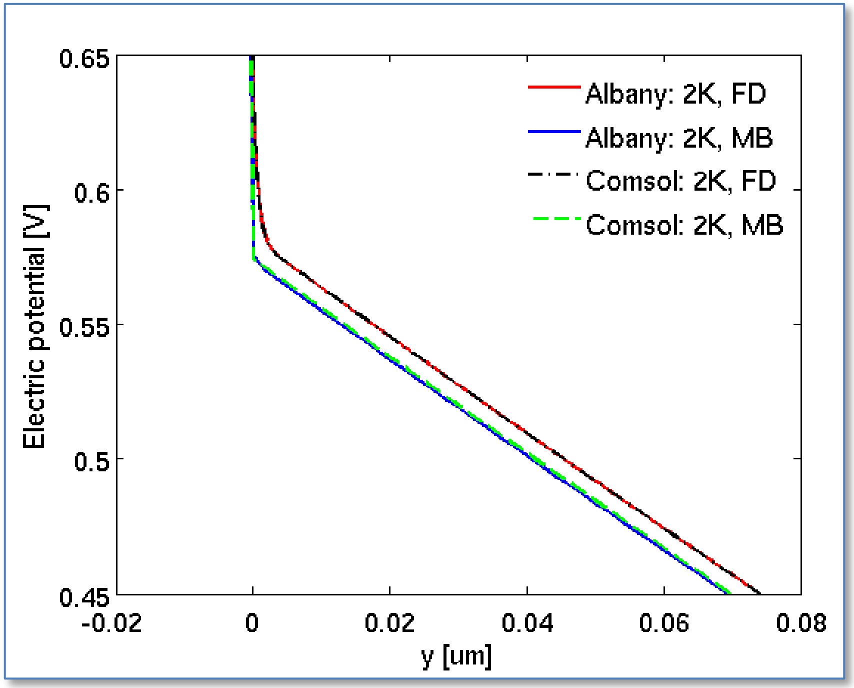
RY simulated quantum dot structures





Nonlinear Low Temperature Poisson Simulation

- Sentaurus Fermi Dirac simulation have serious robustness issues at T < 50° K.
  - Use the wrong expansion for low temperature requiring extended precision for proper convergence
- We implemented proper low T expressions in QCAD and see no robustness issues whatsoever.
  - We have similarly implemented a variety of other nonlinear Poisson solvers.
- Agile tool chain (Albany, Sacado, Phalynx, NOX, STK) allow new physics to be implemented flexibly and robustly. This is very promising moving forward.



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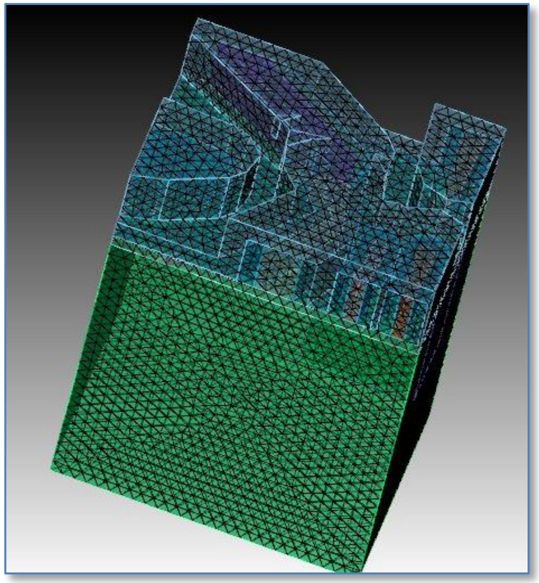
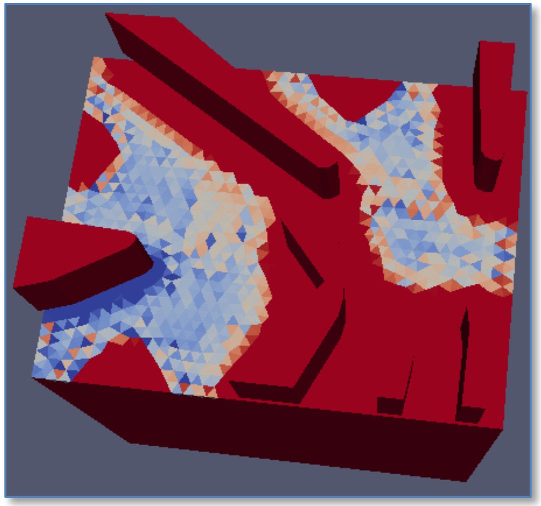
QCAD Import of TCAD Structures

- We are able to import existing TCAD geometry files and remesh, allowing use of the Sentaurus process emulation capability and reuse of existing structures.
- Top figure shows Cubit tetmesh for sample 581, bottom shows semiclassical charge density at 0.2° K.
- Currently running 2M element meshes in parallel Red Sky simulations.





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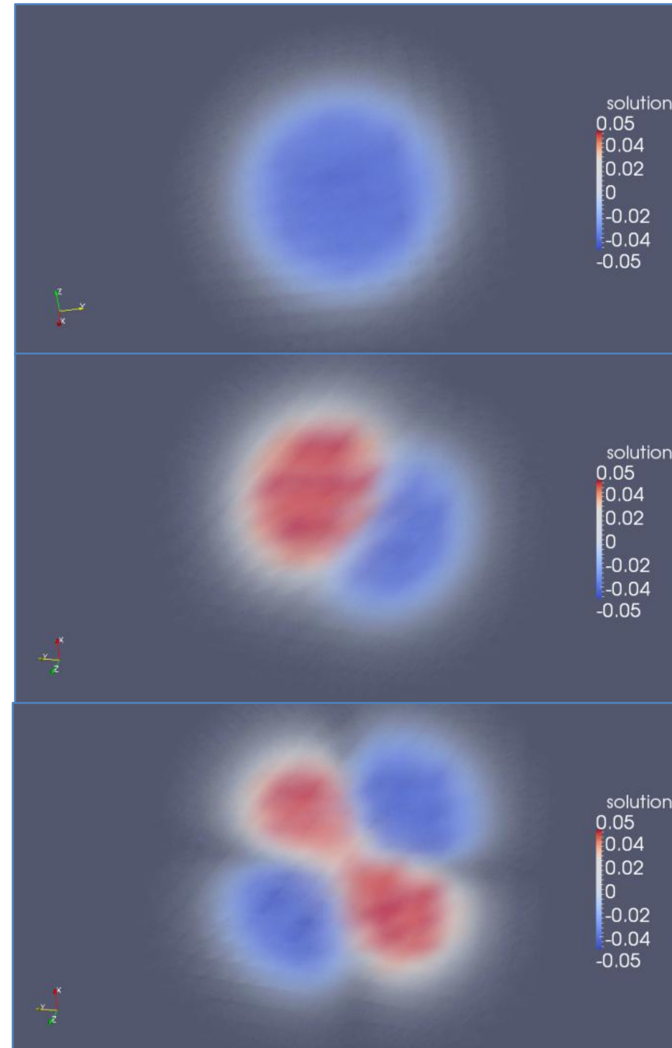
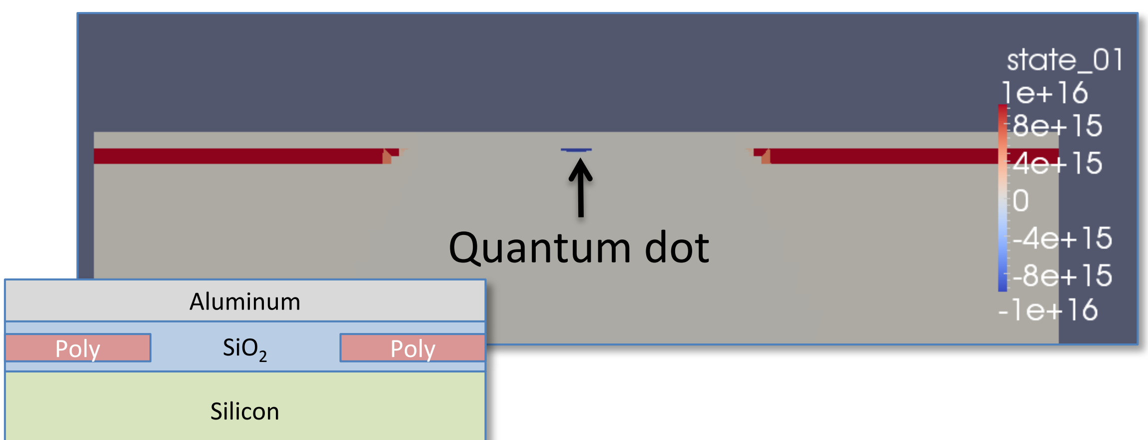
Schrodinger-Poisson Status

- We have implemented a quantum solver a Schrodinger code to solve for quantum behavior in simple parabolic wells. This was a FY12 milestone
- Extended this to iterative Schrodinger-Poisson solutions of simplified quantum dot structures in 2D.





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