Poisson-Schrodinger Solvers in QCAD

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October 2 , 2012

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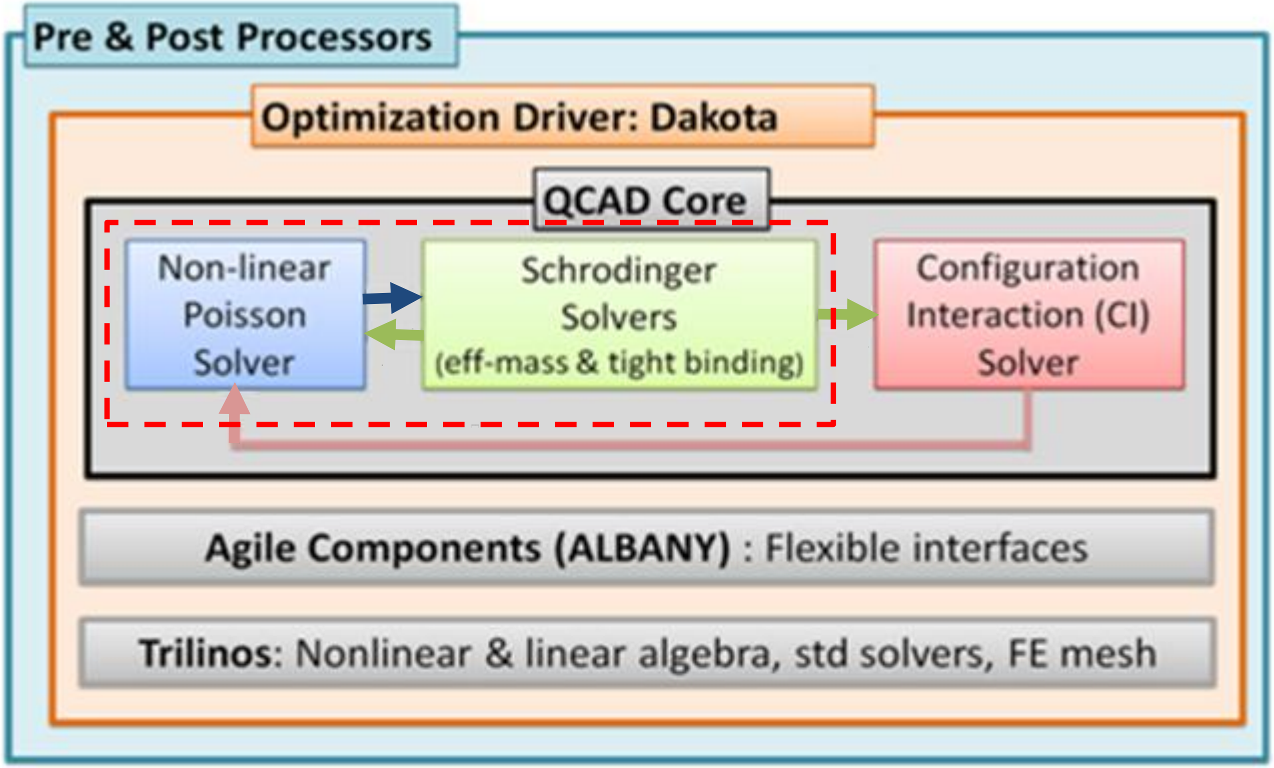
QCAD Framework



QCAD core has **nonlinear Poisson**, **Schrodinger**, and **CI solvers**, which can run **individually** or are **combined self-consistently**.

Erik's talk will cover some aspects of the optimization and the pre & post processors and their powerful applications to complex quantum dots devices.

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Motivation

Rick has given some motivations for the QCAD project in his morning talk. Here I will illustrate on two specific motivations.

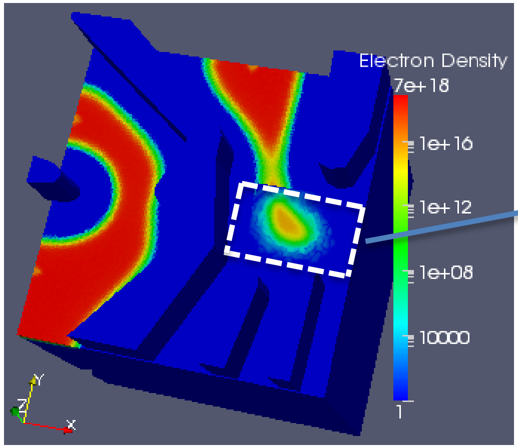
Commercial TCAD cannot solve nonlinear Poisson equation at cryogenic temperatures, where quantum dot qubits operate at.

Commercial TCAD solves

$$-\nabla(\varepsilon_s \nabla \phi) = q(p - n + C) = q\left[n_i \exp\left(\frac{E_i - E_F}{k_B T}\right) - n_i \exp\left(\frac{E_F - E_i}{k_B T}\right) + C\right]$$

$$n_i = \sqrt{N_C N_V} \exp\left(\frac{-E_g}{2k_B T}\right) \rightarrow 0 \text{ as temperature } T \rightarrow 0$$

Commercial TCAD do not have 3D quantum models, which are essential for accurately modeling quantum dot devices.



3D spatial confinement requires a 3D self-consistent Poisson-Schrodinger quantum model for the dot region

QCAD Approach

Nonlinear Poisson Solver – recast the equation [1] using well-defined quantities and carefully address the blowup issue of $\exp(a/k_BT)$ function near 0 K

$$-\nabla(\varepsilon_s \nabla \phi) = q(p - n + C) = q\left[N_V F_{1/2}\left(\frac{E_V - E_F}{k_B T}\right) - N_C F_{1/2}\left(\frac{E_F - E_C}{k_B T}\right) + C \right]$$

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

Fermi-Dirac integral of 1/2 order

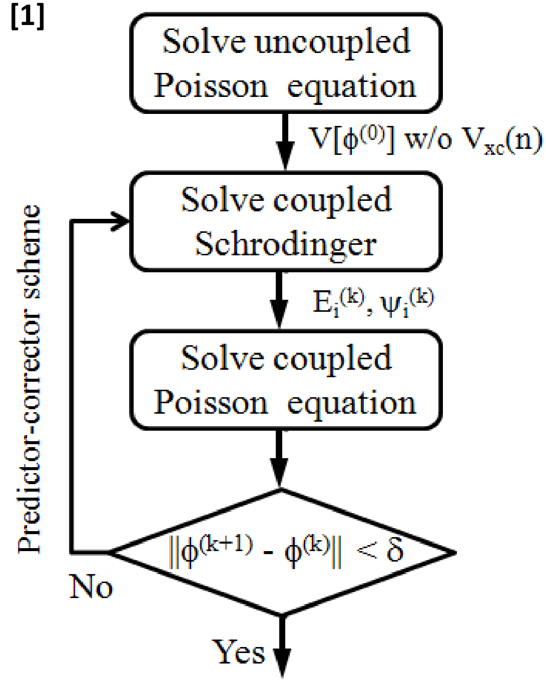
Self-Consistent Poisson-Schrodinger (P-S) Solver [1]

Coupled nonlinear Poisson equation:

$$-\nabla(\varepsilon_s \nabla \phi) = q[p(\phi) - \underline{n(\phi, E_i, \psi_i)} + C(\phi)]$$

Coupled Schrodinger equation:

$$\frac{-\hbar^2}{2} \nabla\left(\frac{1}{m^*} \nabla \psi_i\right) + \underline{V(\phi, n)}\psi_i = E_i \psi_i$$



[1] X. Gao, E. Nielsen, et al., Proceedings of IWCE (submitted).

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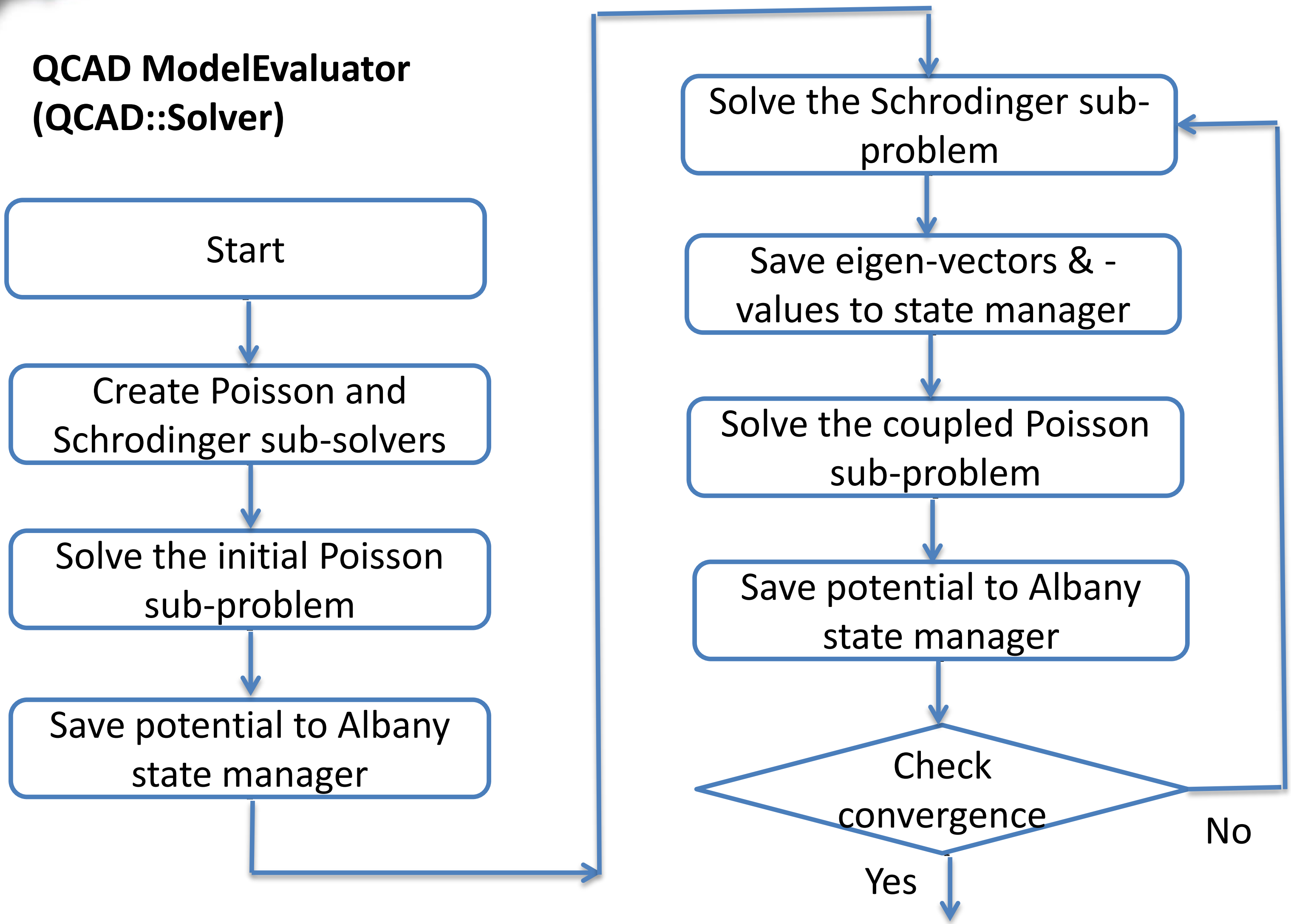
QCAD P-S Implementation

QCAD ModelEvaluator (QCAD::Solver)



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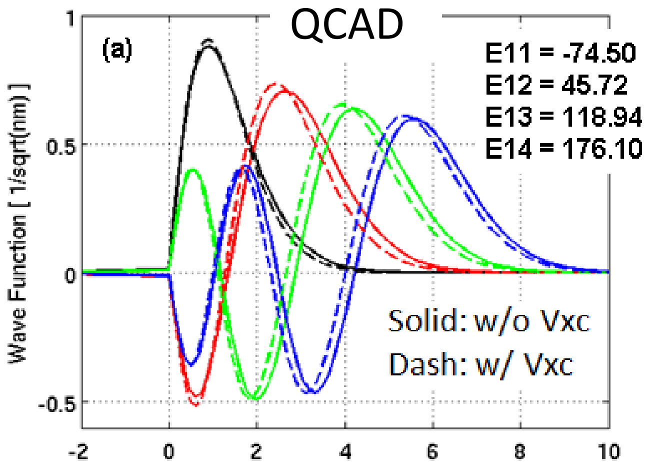
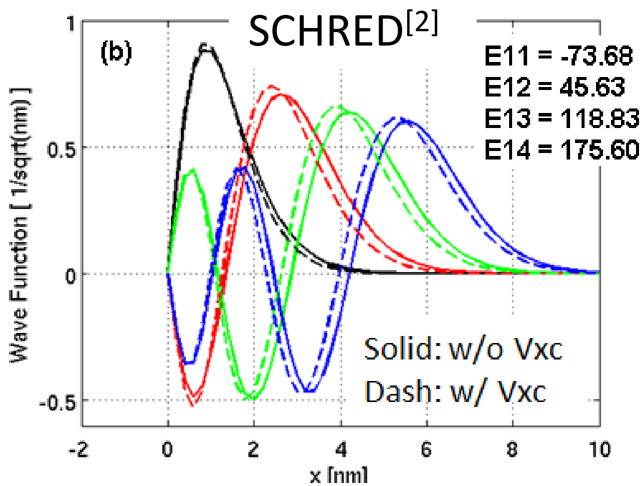
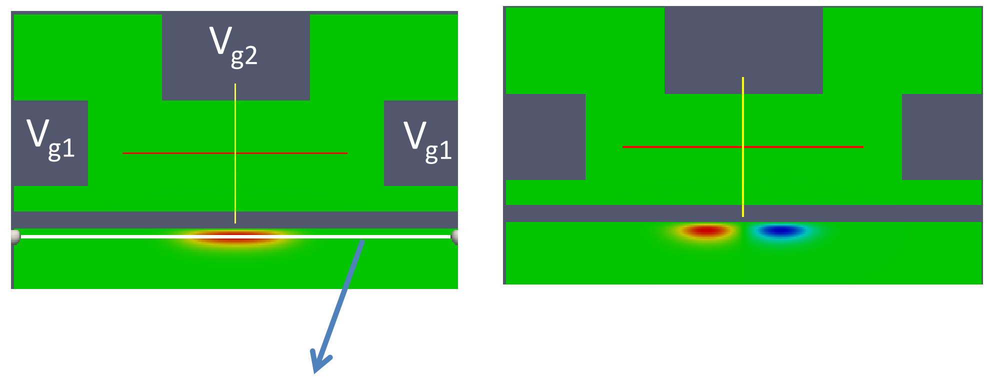
Model Validation

1D MOS capacitor (T = 50 K)





2D Application: gate-induced quantum wire (T = 10 K)



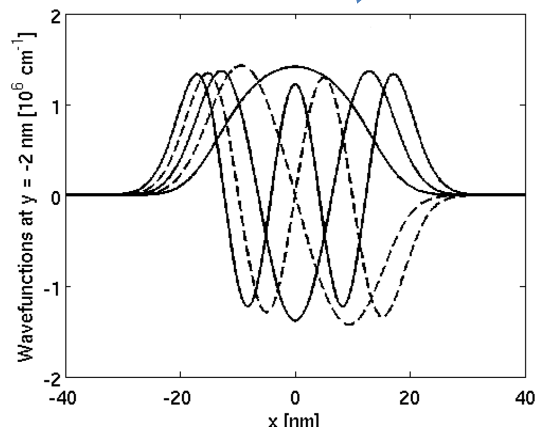
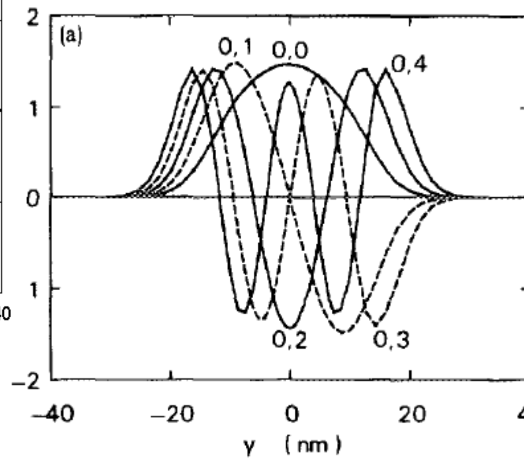
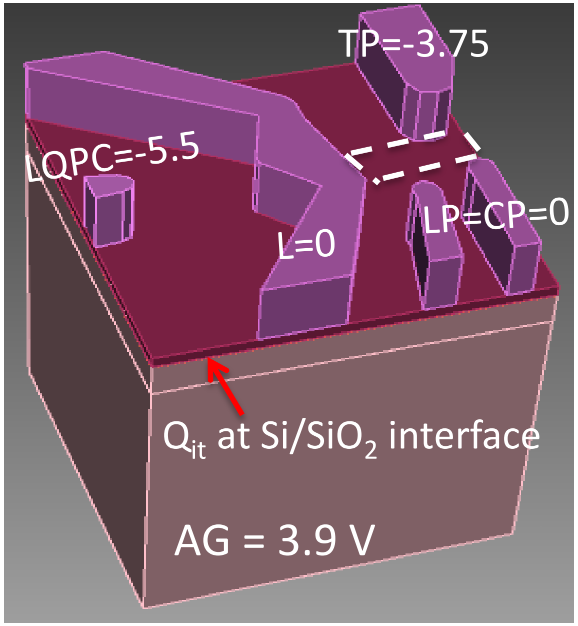


Fig. 4(a) in Ref.[3]

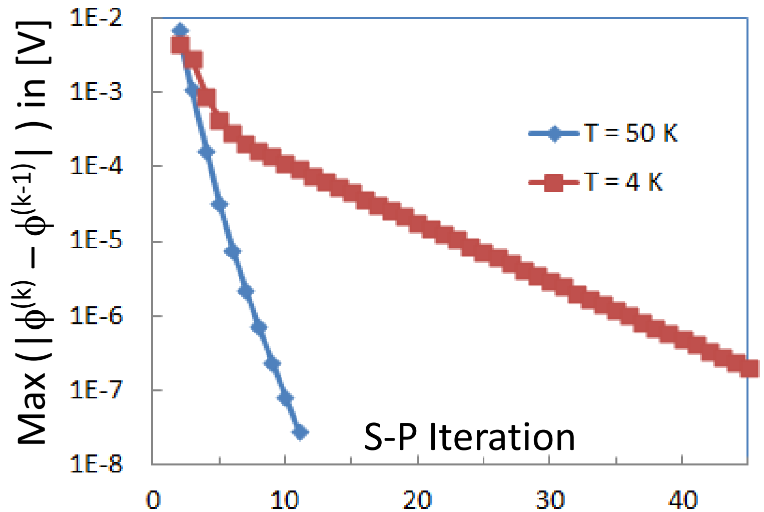


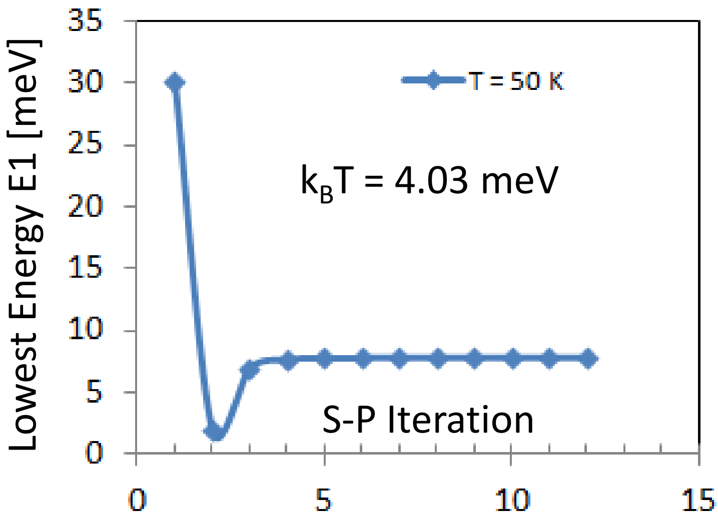
[2] https://nanohub.org/tools/schred . [3] S. Laux and F. Stern, Appl. Phys. Lett. **49**, 91 (1986).

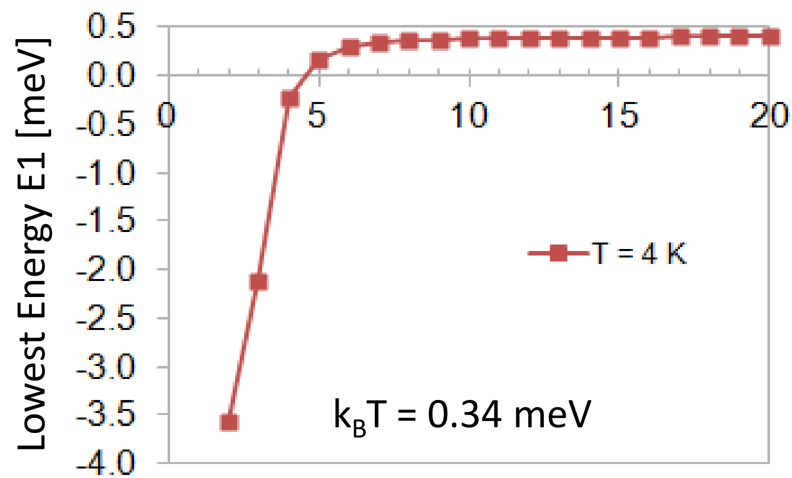
3D Quantum Dot - Convergence



Monotonic 3D S-P convergence is observed.

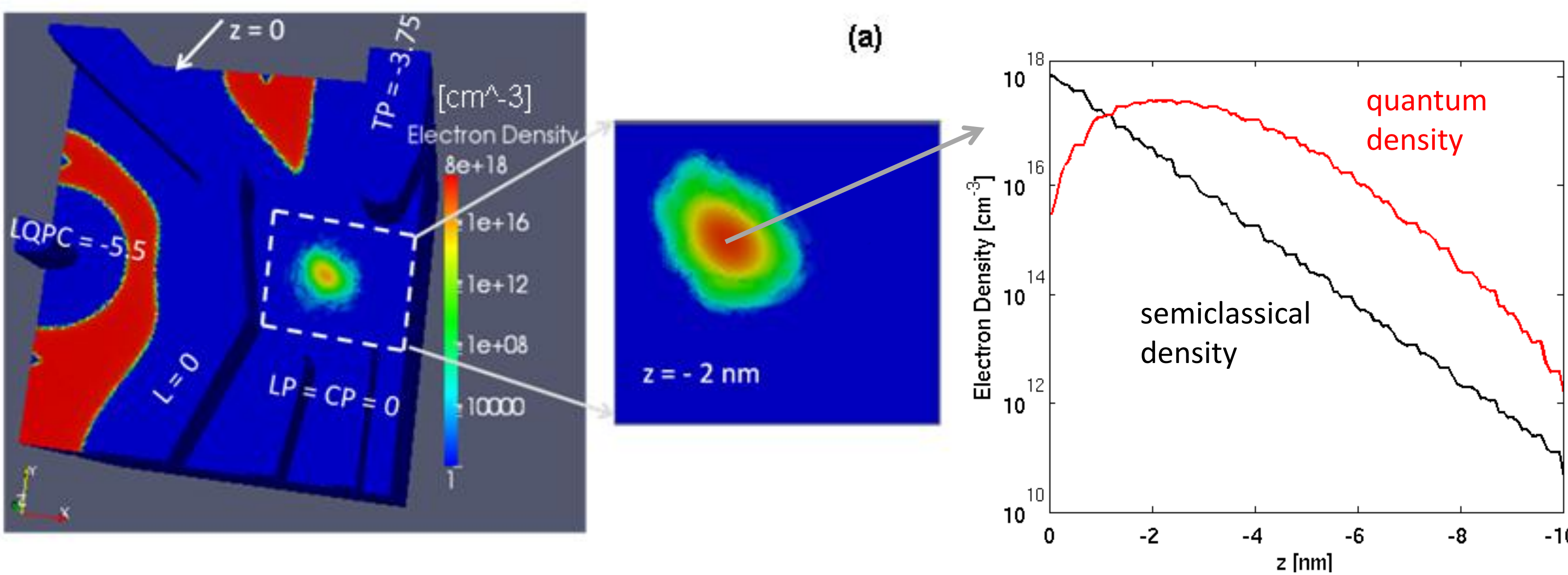




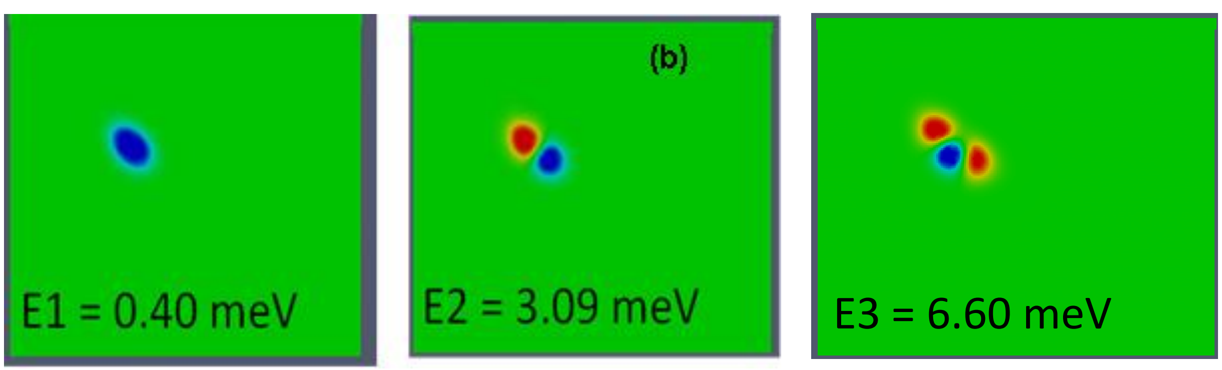


3D Quantum Dot – Electron Density

Quantum confinement pushes electrons away from the interface



Lowest three wave functions in the z = -2 nm plane



T = 4 K

Q_{it} = -4.43x10^{11} cm^{-2}

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Collaborative Teamwork

- The exciting opportunity of working with experts from different areas.
- Irina's work on preconditioners leads to the use of ML preconditioner with Zoltan repartitioning, which gives 2-5x speedup of linear solves in parallel.
- Discussions with Andy and Heidi lead to 2x speedup in QCAD S-P solver by modifying LOCA/Eigensolver interface code to avoid matrix recalculation. 2x is insignificant for small problems, but important for big problems, e.g., 30 hrs -> 15 hrs. Further possible speed improvement is under investigation.