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Efficient self-consistent quantum transport simulation in complex geometry devices

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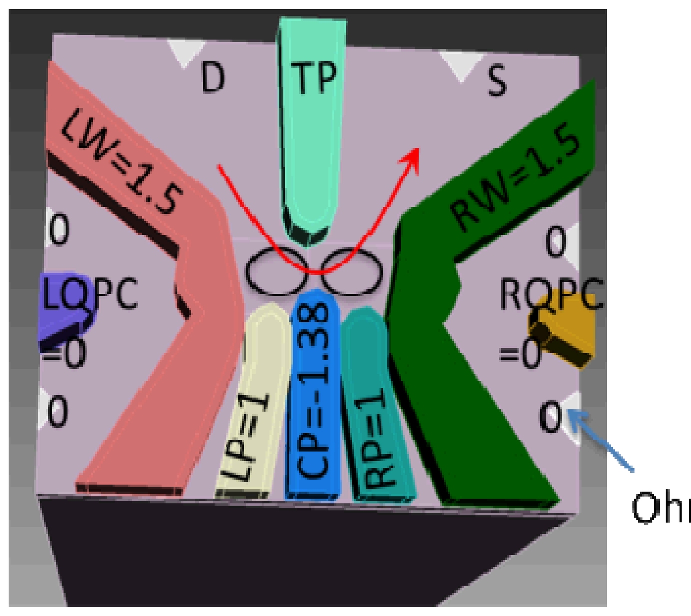
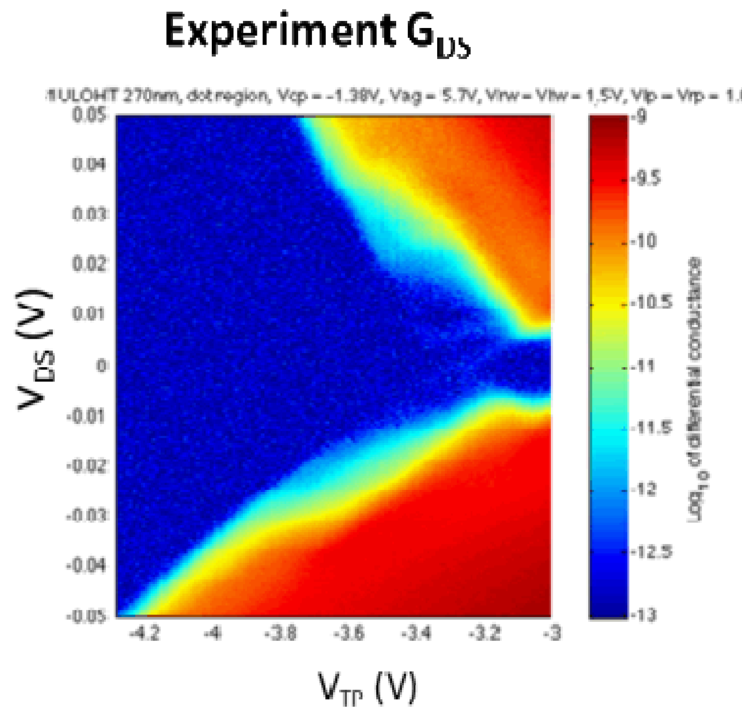
Motivation

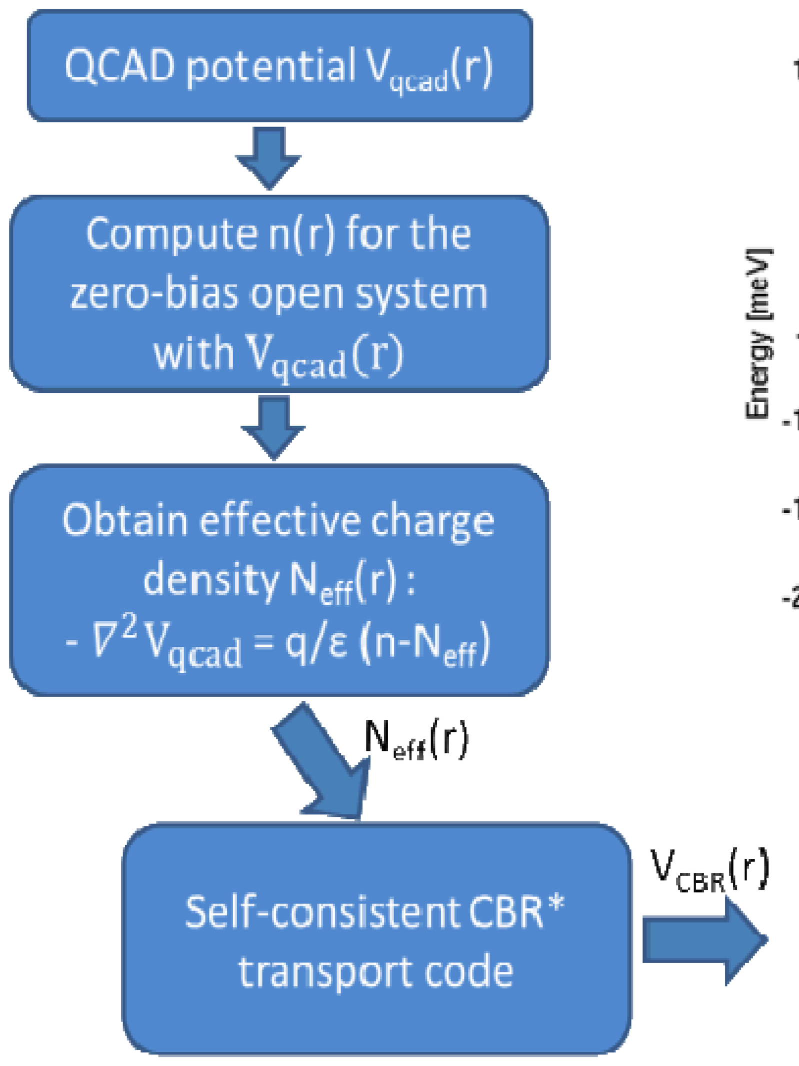
Silicon double quantum dots are designed and fabricated for qubit applications at Sandia National Laboratories.

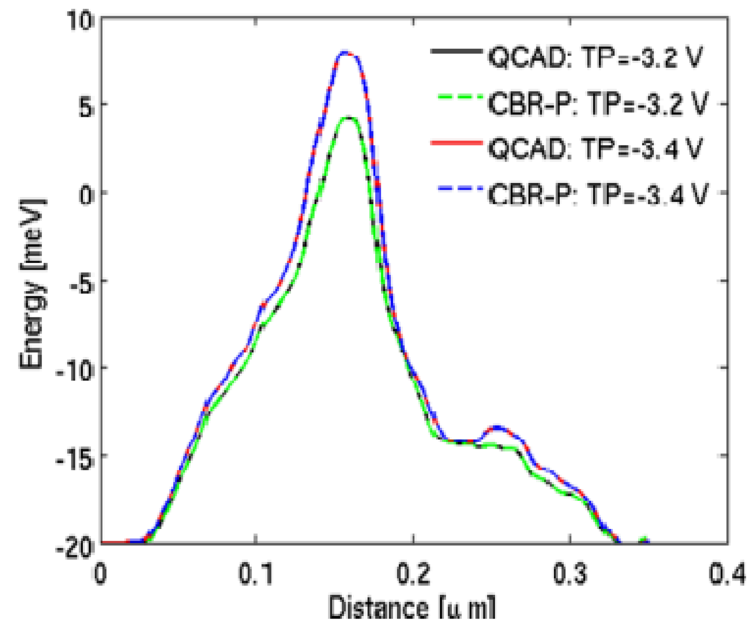




- Characterization of tunnel barriers (e.g., dot and QPC barriers) -> information on barrier shape and disorder defect -> controllability of tunnel barriers
- Typical measurements of dot barrier: fix all the depletion gates and Ohmic contacts, while TP and SD voltages are being varied.
- **To aid the experiment and improve DQD designs, a quantum transport modeling capability is needed.**

How to feed an external potential to a self-consistent transport scheme: effective charge?

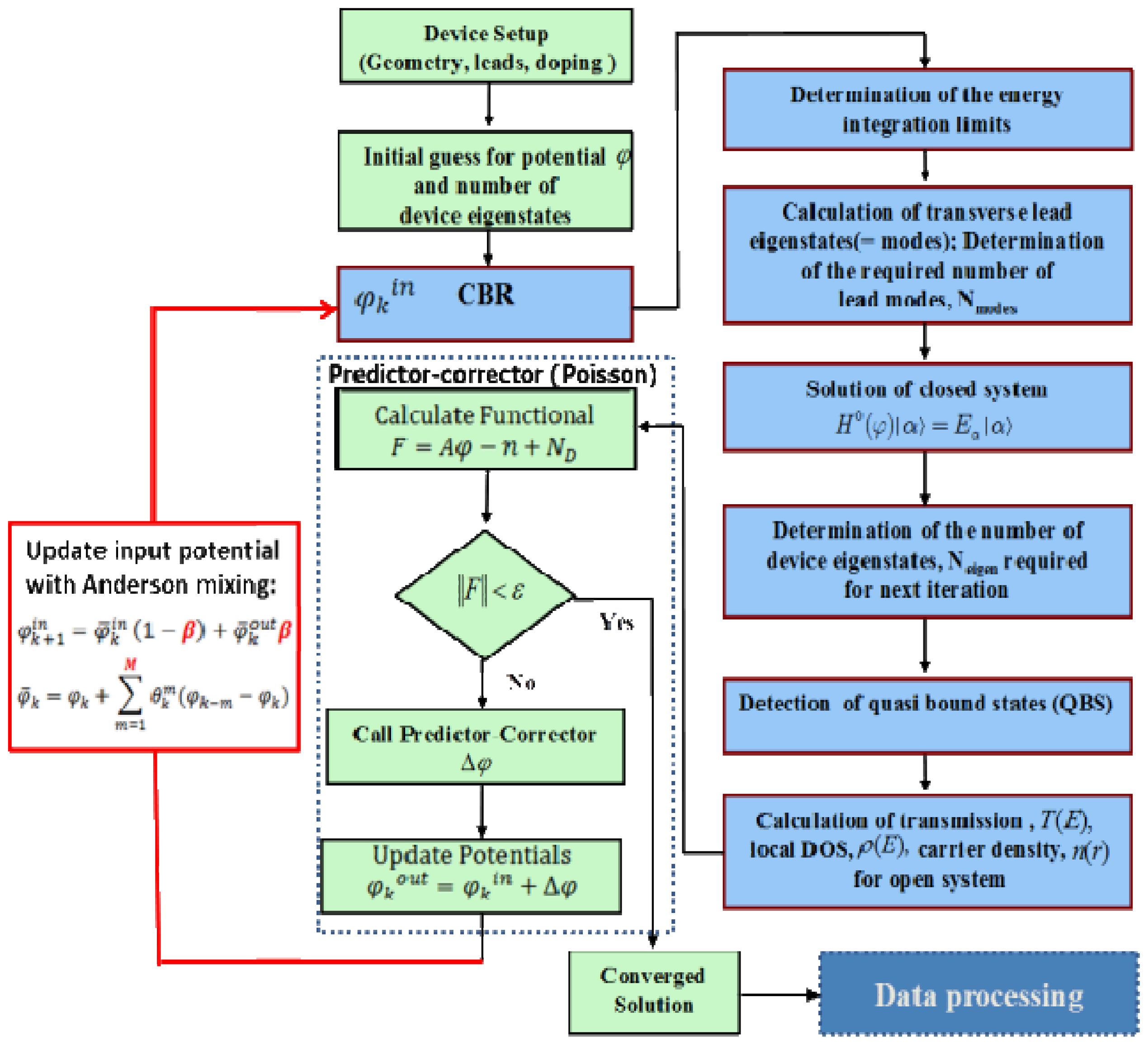




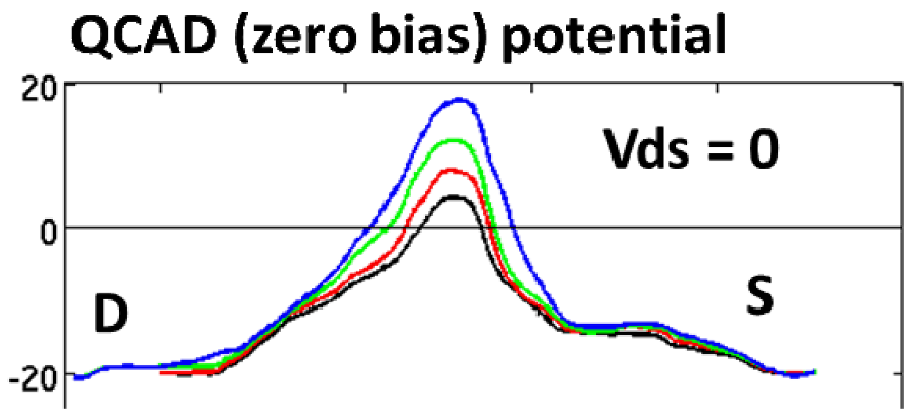
For zero bias, $V_{CBR}(r)$ should be the same as $V_{qcad}(r)$ at convergence

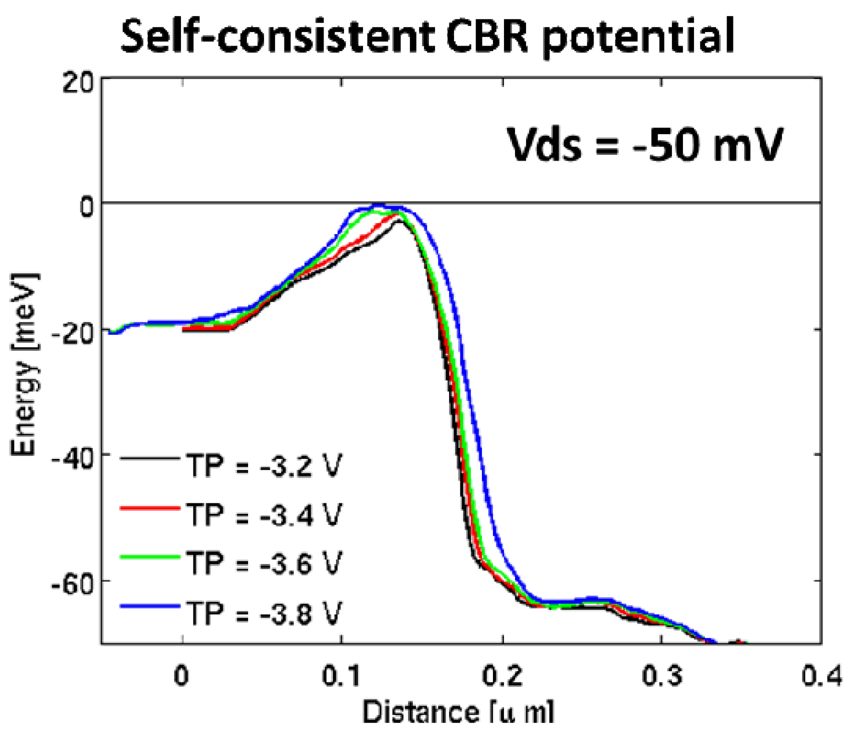
*D. Mamaluy *et. al.*, Phys. Rev. B 71, 245321 (2005); T-ED 54, 784 (2007)

CBR method with Anderson acceleration

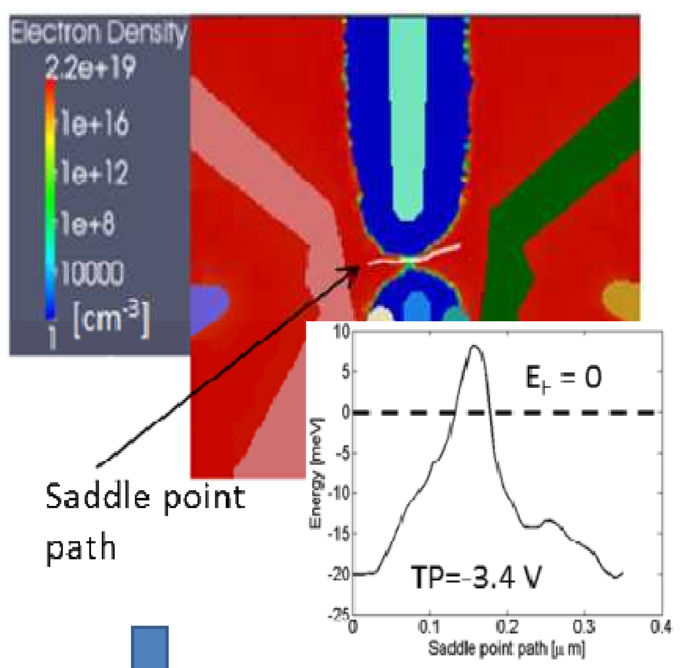


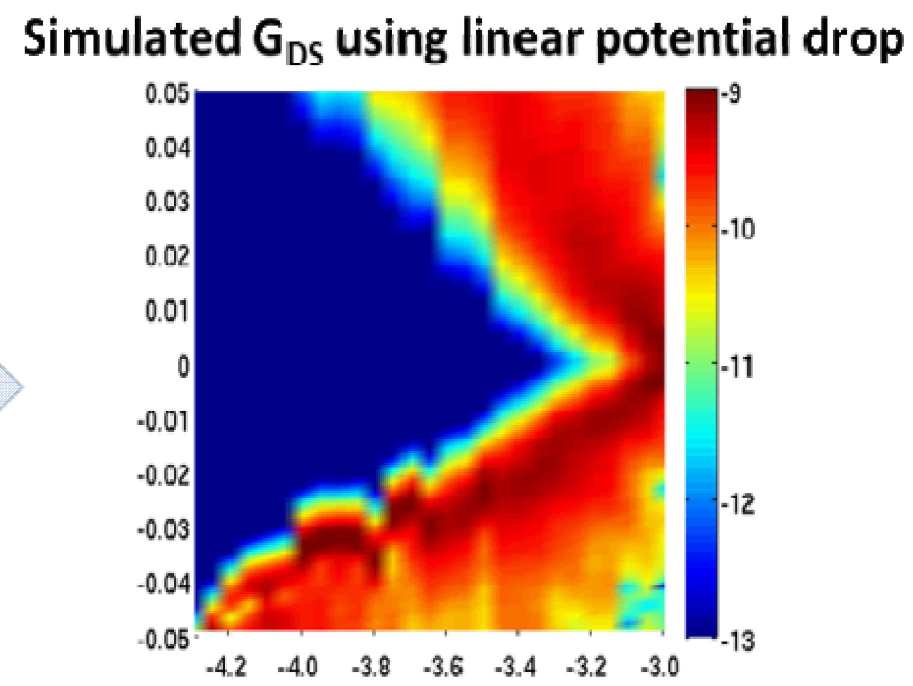
Applying bias:

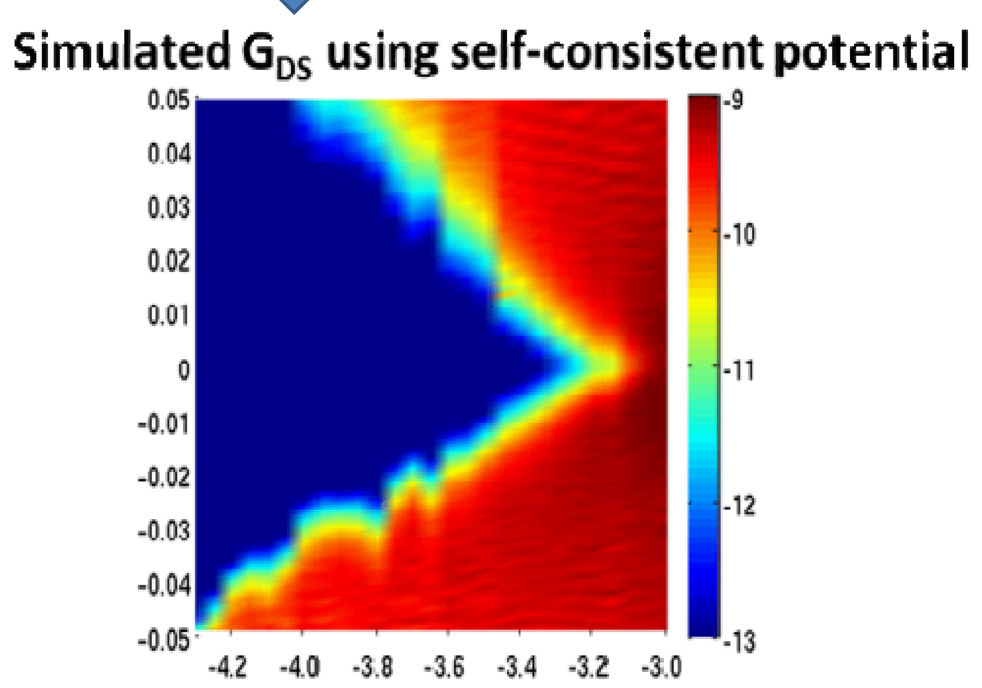




Comparison with Experiment

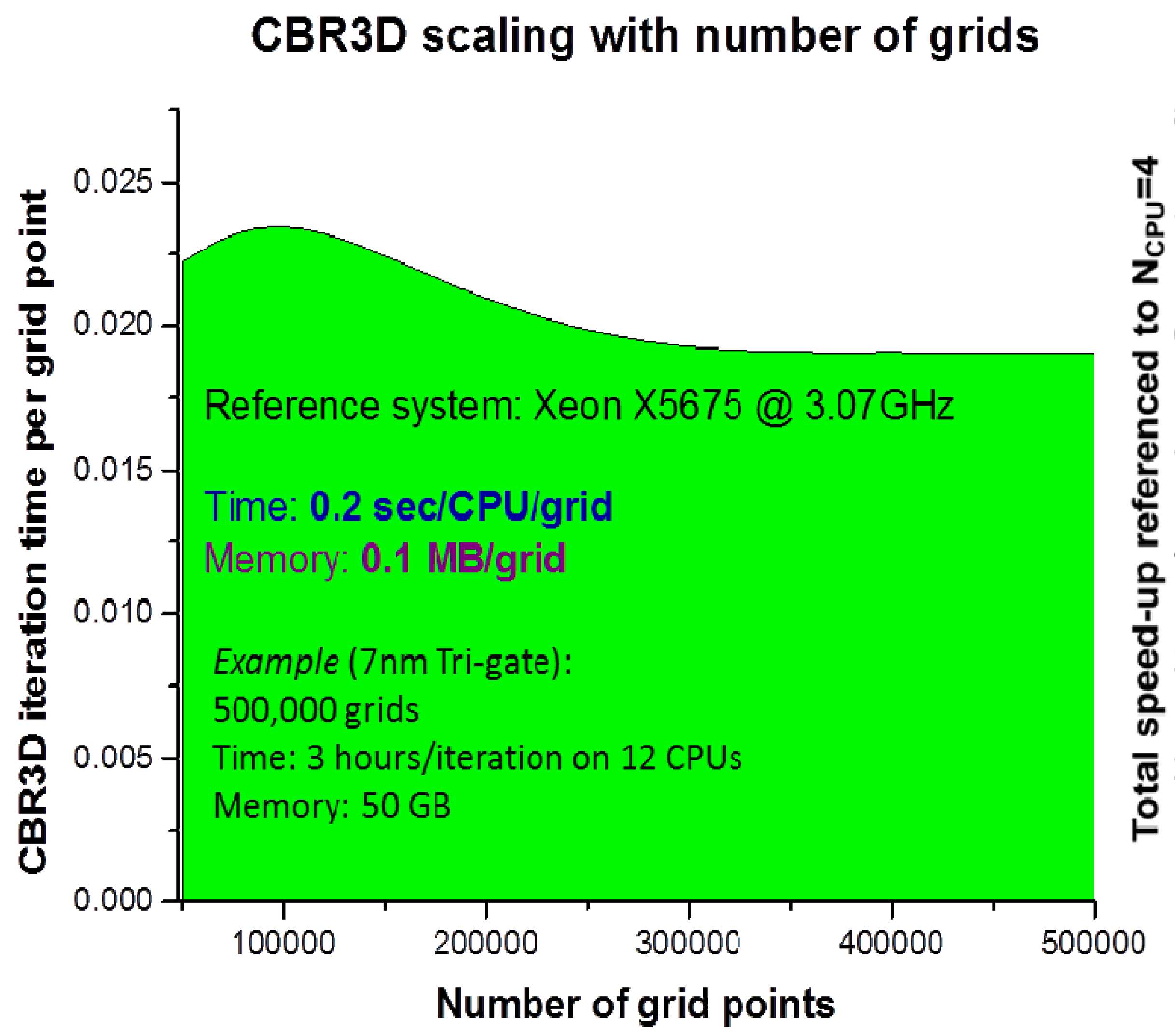


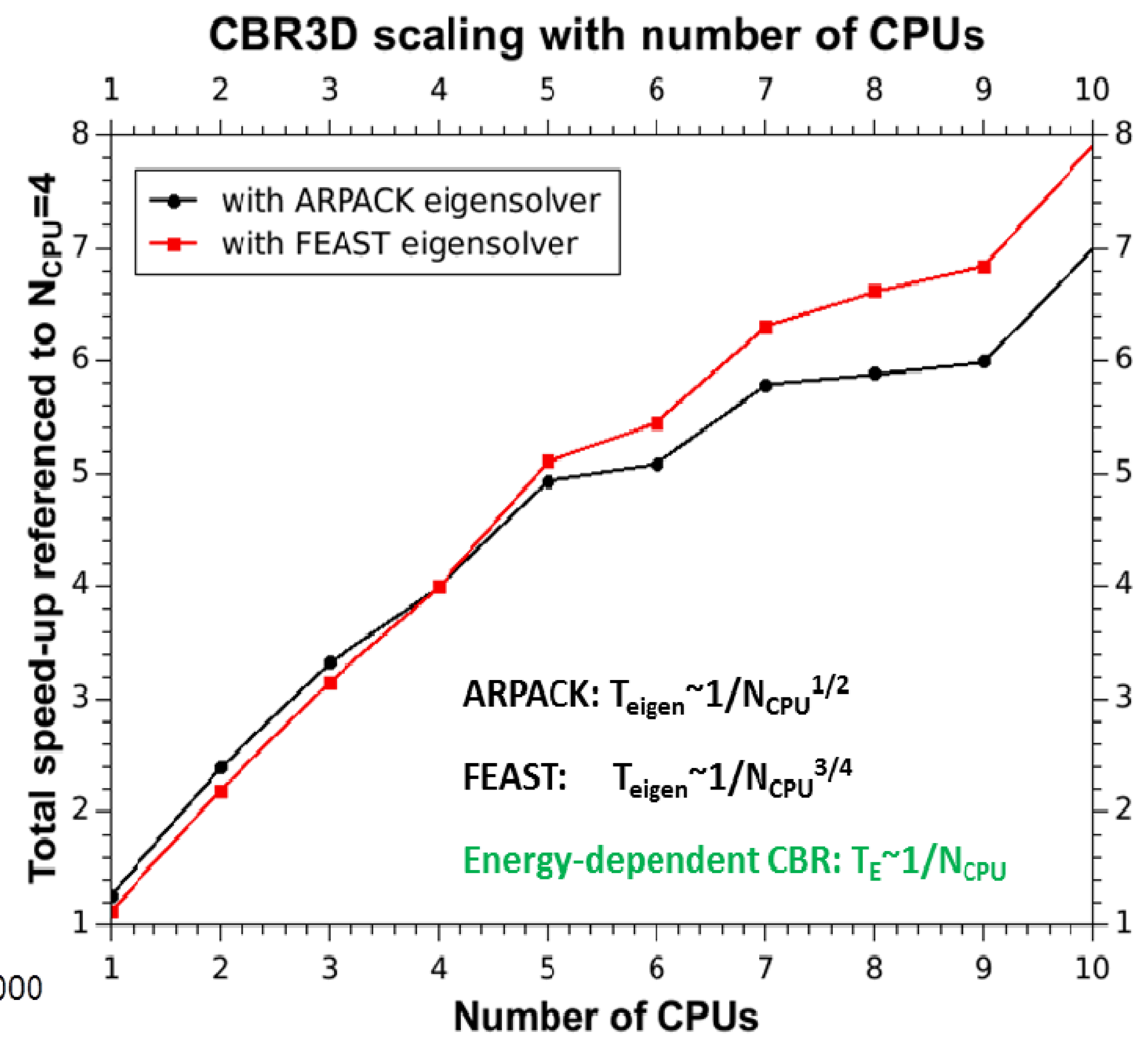




- Self-consistent 1D CBR-Poisson simulation produces differential conductance in better qualitative agreement with the experiment
- The discrepancy in the exp. threshold voltage (high res. island) is due to higher dimensional effects
- More accurate simulation requires the full 3D self-consistent CBR-Poisson

Self-consistent CBR3D scaling*





*D. Mamaluy, Xujiao Gao, "Large scale quantum transport simulations using the CBR method", to be published

Conclusion: in the complex geometry devices for which electrostatic potentials are known from TCAD tools, very fast, yet sufficiently accurate, quantum transport simulations can be performed using the charge self-consistent CBR method and the described effective charge extraction technique. Simulated drain-source conductance using the self-consistent simulator across a tunnel barrier in a silicon DQD device show much better qualitative agreement with experimental data than the non-selfconsistent model assuming a linear potential drop.

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