COMSOL CONFERENCE
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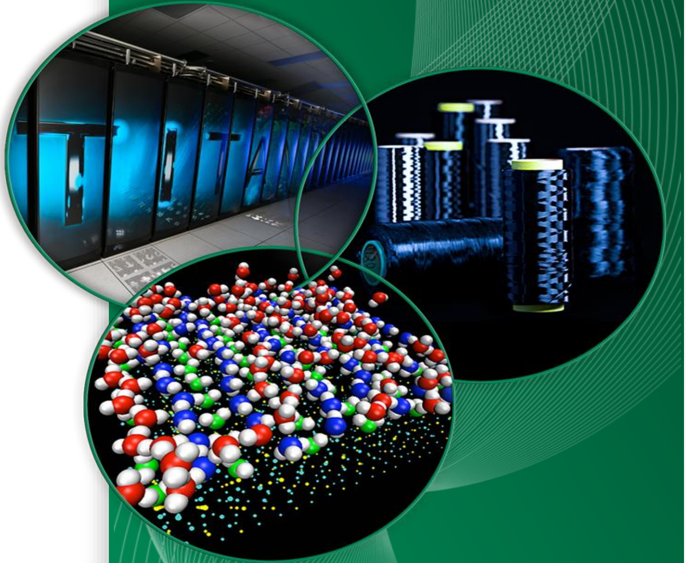
Session : MEMS & Nanotechnology 2



Simulation of Silicon Nanodevices at Cryogenic Temperatures for Quantum Computing

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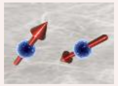
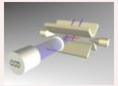
Quantum Computation

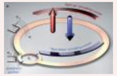
Qubit → Two level system obeying quantum mechanics
Examples

Spins in Silicon

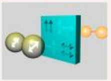


Electronic states of ions

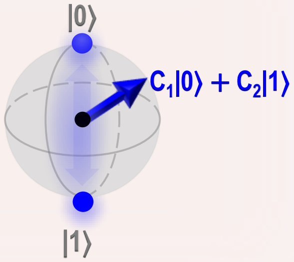




Flux in Superconductors

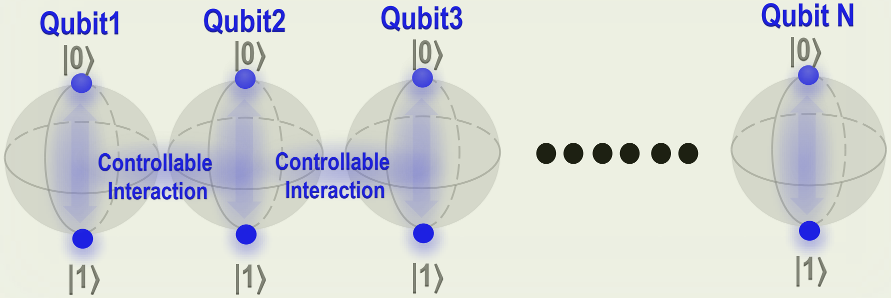


Photon Polarization



Encodes information of 2 complex numbers - C_1 & C_2

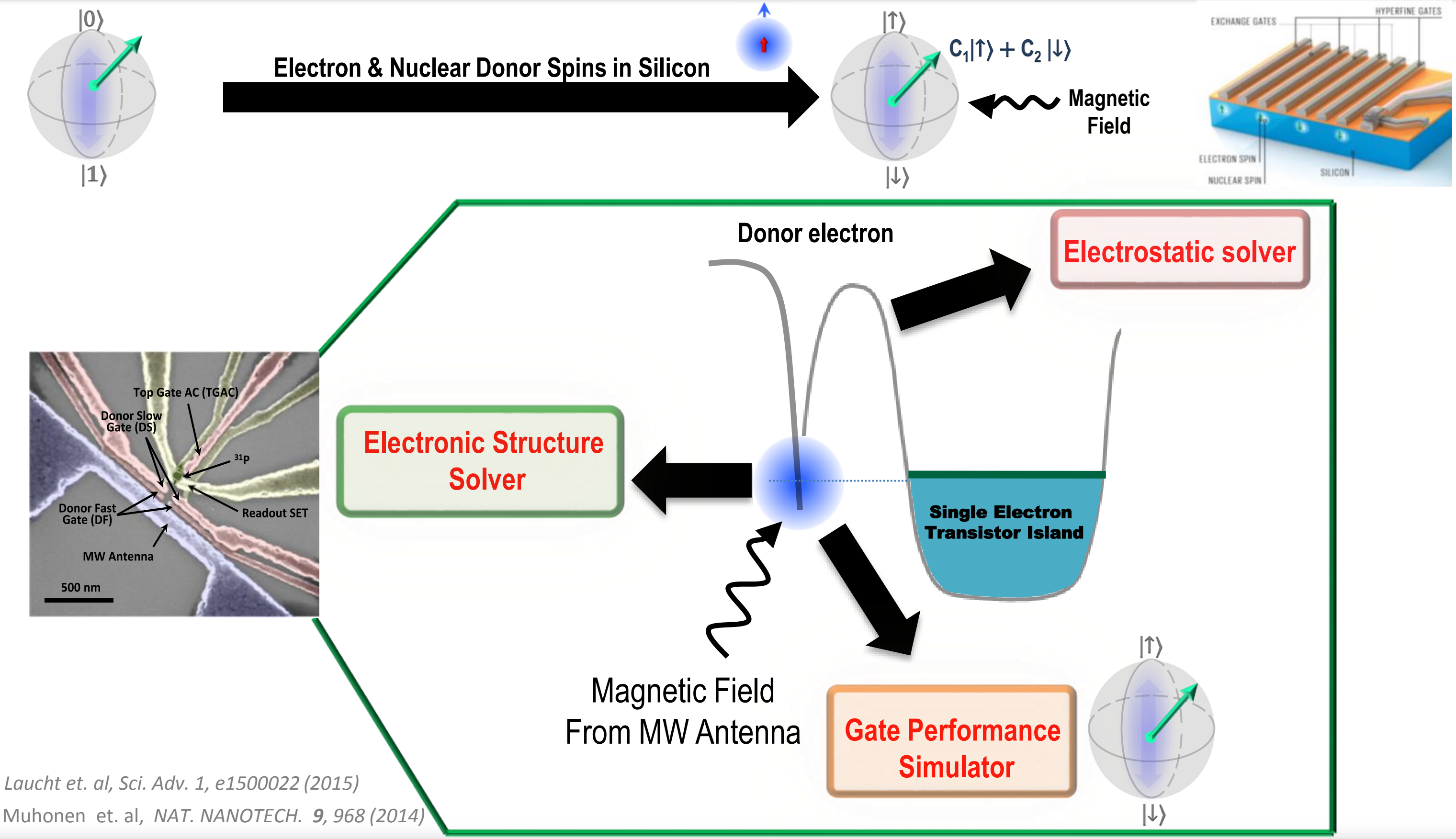
Quantum Computer → An array of several interacting qubits



Encodes information of 2^N numbers

Quantum mechanical laws allow qubits to represent & process exponentially more information than bits !
Information on 300 qubits → Number of particles in the entire universe !

Silicon Quantum Computation – Modeling Parameters



Laucht et. al, Sci. Adv. 1, e1500022 (2015)

Muhonen et. al, *NAT. NANOTECH.* ***9****, 968 (2014)*

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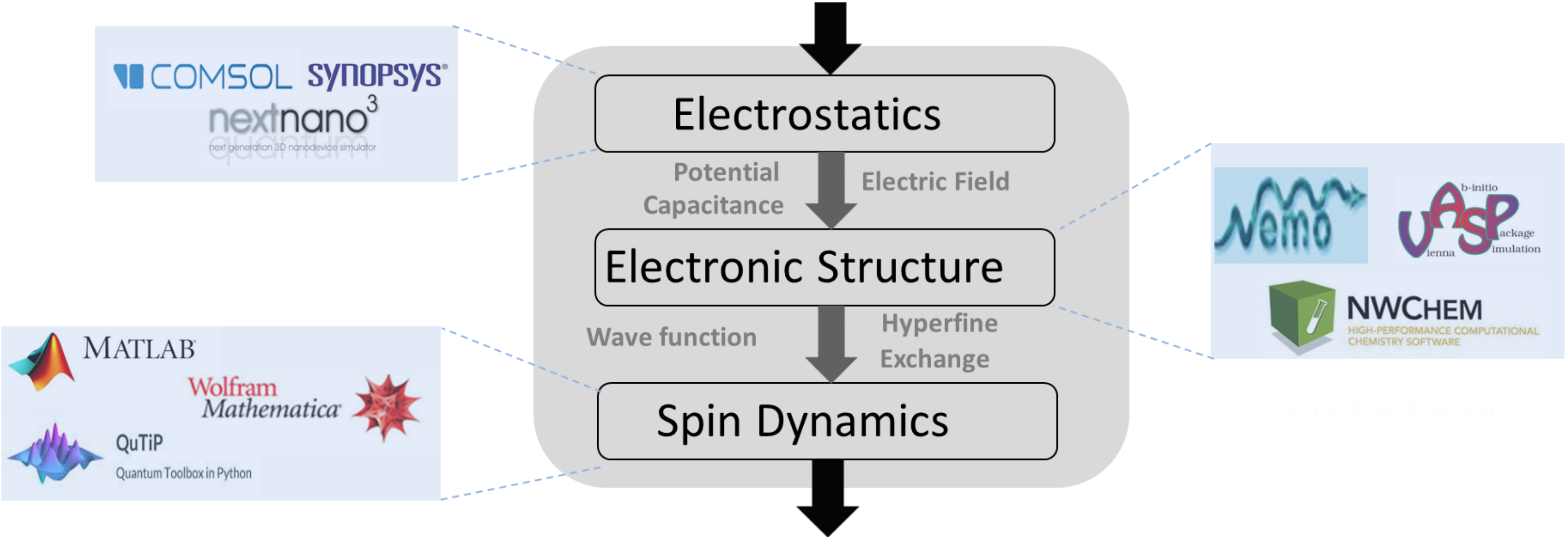
Computational Workflow for Designing Silicon Donor Qubits

Input : Device Geometry, Gate Voltages, Magnetic Fields, Material Model



Output : Spin States, Coherence/Relaxation times, Quantum Gate Fidelity

T. S. Humble et. al, Nanotechnology, 27, 42 (2016)

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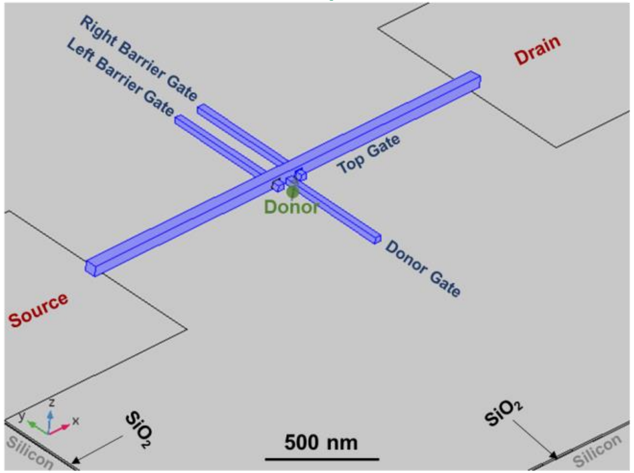
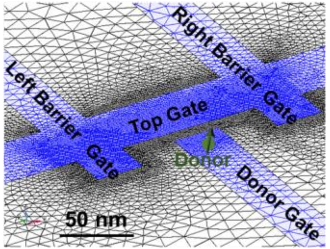
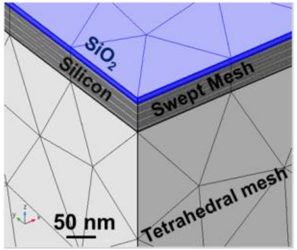
Test Device Model & Equations

Device to readout the spin of donor electron







Poisson &
Current Continuity :
$n\,,\,p,\,V$

$$\nabla\cdot(\epsilon\nabla V) = -q\,(p - n + N_{D+} - N_{A-})$$

$$\frac{\partial n}{\partial t} = \frac{1}{q}(\nabla\cdot \mathrm{J_n}) - U_n$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q}(\nabla\cdot \mathrm{J_p}) - U_p$$

Dependent Variables :
$E_c,\,E_v,\,E_{fn},\,E_{fp}\,,\,n_i$

$$n = N_C\,F_{1/2}\left(\frac{E_{F_n}-E_c}{k_BT}\right) \qquad N_{D+} = \frac{N_D}{1+g_D\exp\left(\frac{E_{F_n}-E_D}{k_BT}\right)}$$

$$p = N_V\,F_{1/2}\left(\frac{E_v-E_{F_p}}{k_BT}\right) \qquad N_{A-} = \frac{N_A}{1+g_A\exp\left(\frac{E_A-E_{F_p}}{k_BT}\right)}$$

$$E_c = -\chi - qV \qquad E_v = -\chi - E_g - qV$$

$$n_i = \sqrt{N_cN_v}\exp\left(-E_g/2k_BT\right)$$

Ohmic Boundary Condition

$$n_{eq} - p_{eq} + N_a^- - N_d^+ = 0$$

$$n_{eq} = \frac{1}{2}\left(N_d^+ - N_a^-\right) + \frac{1}{2}\sqrt{\left(N_d^+ - N_a^-\right)^2 + 4\gamma_n\gamma_p n_i^2}$$

$$p_{eq} = -\frac{1}{2}\left(N_d^+ - N_a^-\right) + \frac{1}{2}\sqrt{\left(N_d^+ - N_a^-\right)^2 + 4\gamma_n\gamma_p n_i^2}$$

$$V_{eq} = V_0 - \chi - \frac{E_g}{2q} + \frac{k_BT}{q}\left(\log\left(\frac{n_{eq}}{\gamma_n n_i}\right) + \frac{1}{2}\log\left(\frac{N_v}{N_c}\right)\right)$$

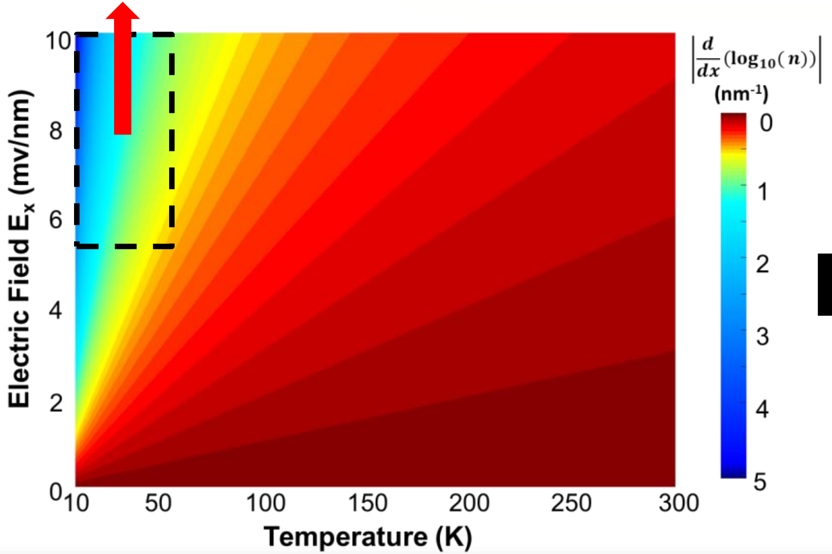
Challenges at Low Temperature

Exponential dependence of densities with temperature

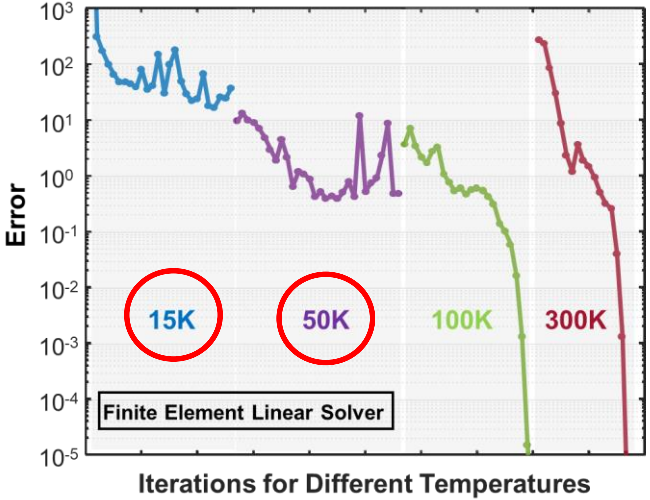
$$n = N_C\, F_{1/2}\left(\frac{E_{F_n} - E_c}{k_B T}\right) \qquad N_{D^+} = \frac{N_D}{1 + g_D \exp\left(\frac{E_{F_n} - E_D}{k_B T}\right)} \qquad E_c = -\chi - qV \qquad E_v = -\chi - E_g - qV$$

$$p = N_V\, F_{1/2}\left(\frac{E_v - E_{F_p}}{k_B T}\right) \qquad N_{A^-} = \frac{N_A}{1 + g_A \exp\left(\frac{E_A - E_{F_p}}{k_B T}\right)} \qquad n_i = \sqrt{N_c N_v} \exp\left(-E_g / 2 k_B T\right)$$

Huge spatial gradients in electron density



Convergence Plots



Guidelines for Low Temperature Convergence

1. Approximate hole densities $p = n_i^2/n$

Reduce Number of degrees of freedom to be solved for

2. Use Finite Element Log Discretization

Solve for the Log of electron density which has smaller spatial gradients than electron density

3. Modify equations appropriately

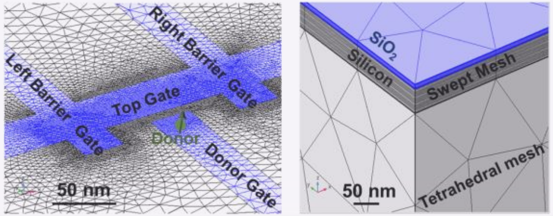
Minimize divide-by-zero-errors

e.g. $n_i = \sqrt{N_c N_v}\exp\left(-E_g/2k_BT\right)$

$$V_{eq} = V_0 - \chi - \frac{E_g}{2q} + \frac{k_BT}{q}\left(\log\left(\frac{n_{eq}}{\gamma_n n_i}\right) + \frac{1}{2}\log\left(\frac{N_v}{N_c}\right)\right) \rightarrow V_{eq} = V_0 - \chi + \frac{k_BT}{q}\left(\log\left(\frac{n_{eq}}{\gamma_n N_c}\right)\right)$$

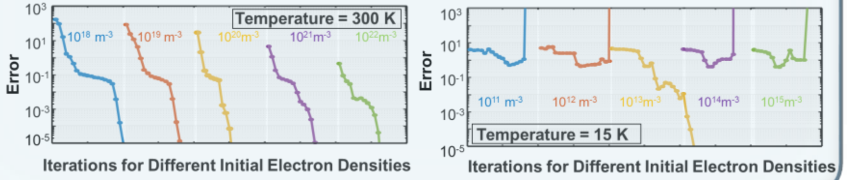
4. Choose Appropriate Meshing

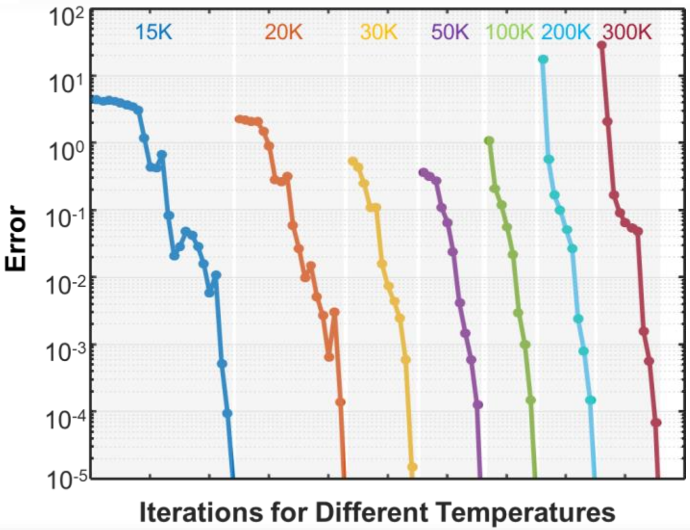
High densities near gates & swept mesh across domains



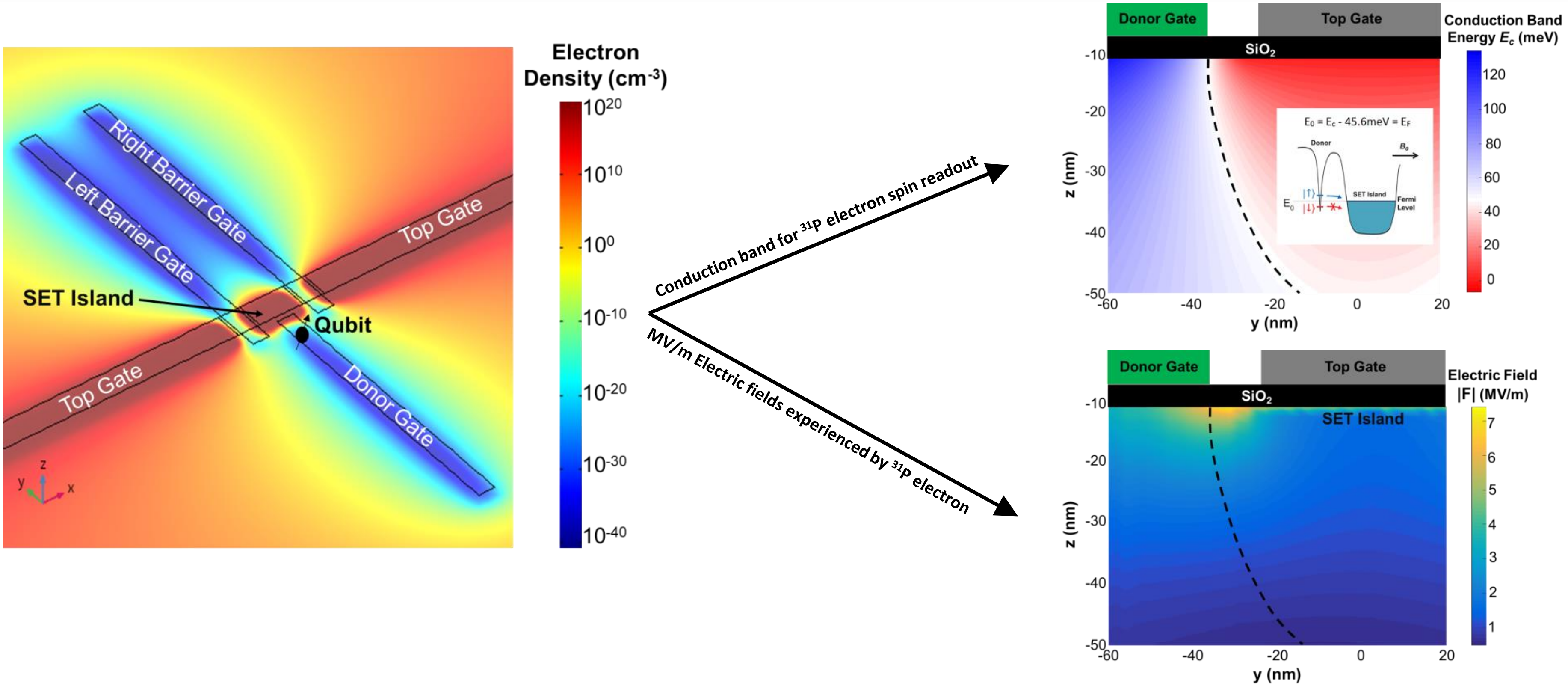
5. Use proper initial guesses for electron density

Set appropriate scaling factors in the Jacobian Matrix





Device Electrostatics at 15 K

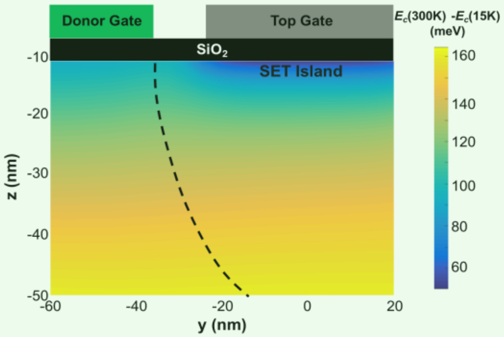


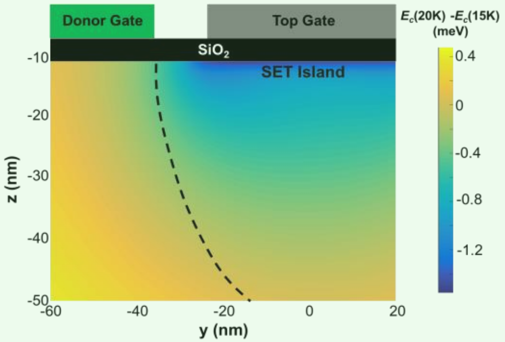
Device electrostatics (n, E_c and F) from COMSOL can (a) simulate locations for spin-readout and (b) electric fields experienced by ^{31}P electron qubits, and is consistent with our understanding and other semiconductor packages.

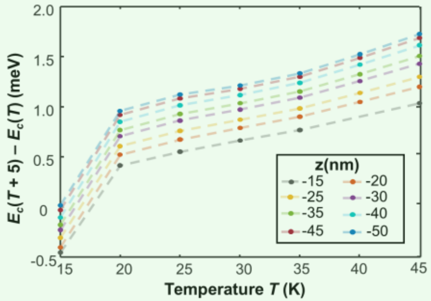
Comparison with Higher Temperatures

300 K – 15 K | 20 K – 15 K | Gradients over 5K

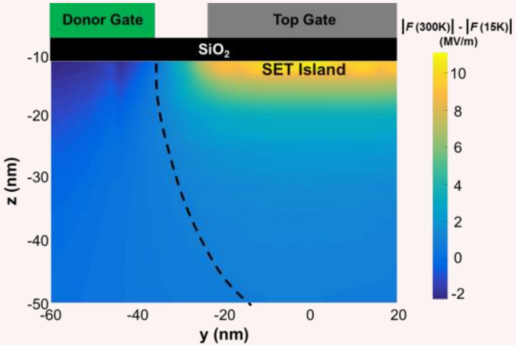
Conduction Band Energy

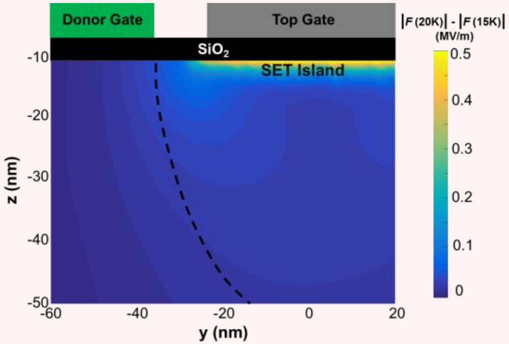


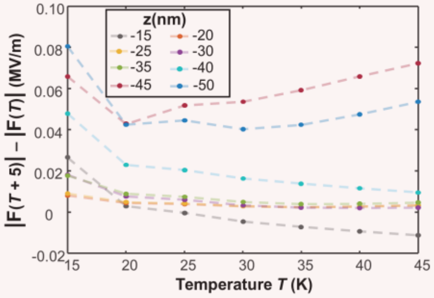




Electric Field





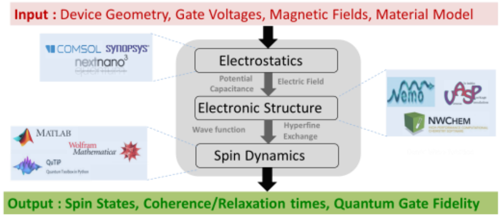


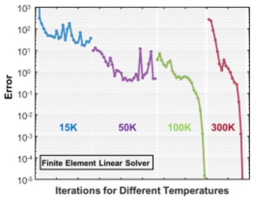
Over 5 K, typical accuracies of conduction band energy is ~ 1 meV and electric field ~ 0.1 MV/m

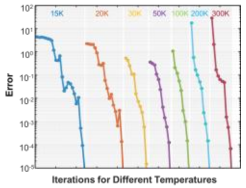
Summary

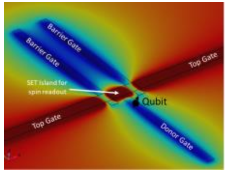
- **Electrostatic calculations are an integral part of a computational workflow needed to design silicon donor qubits for quantum computing.**
- **Simulating electrostatics at low temperature poses convergence issues as several parameters such as carrier densities scale exponentially at low temperature.**
- **We have provided a guideline of simulating electrostatics at low temperatures and have achieved convergence down to 15 K for a test nanostructure.**
- **The electrostatics at 15 K with COMSOL yield expected results for the position of charge reservoirs, donors, conduction band and electric fields.**
- **We then compared the results at 15 K to higher temperatures to quantify the accuracy of device electrostatics with temperature.**

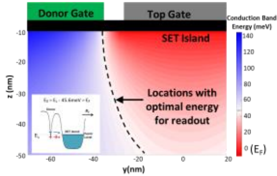
F.A. Mohiyaddin et. al, COMSOL Conference 2017 (2017)

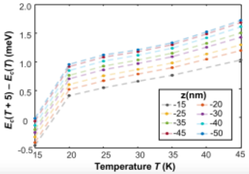


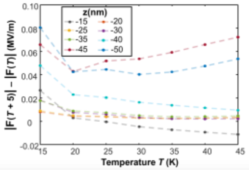












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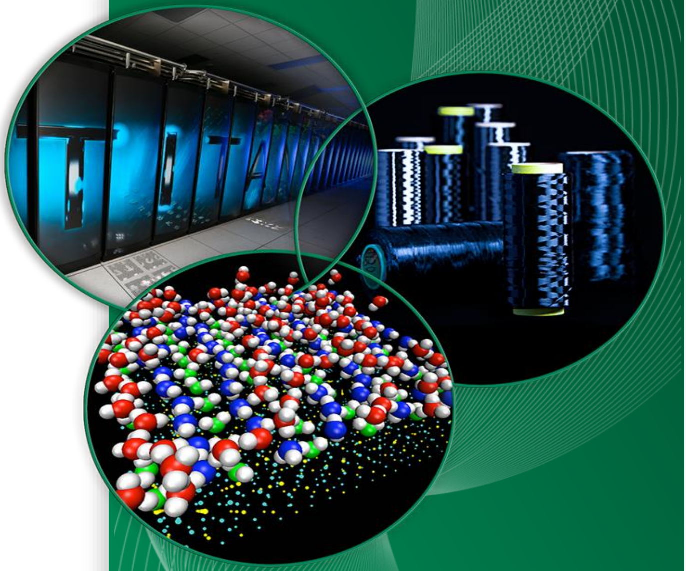

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5 October 2017

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