Accurate Simulation of 2-Well Quantum Devices

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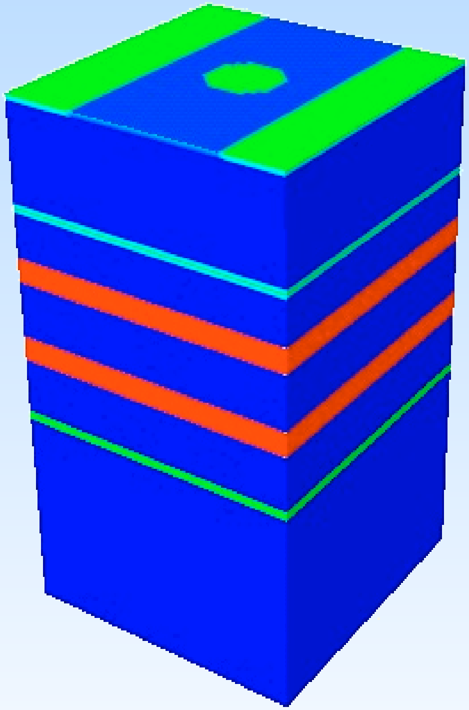
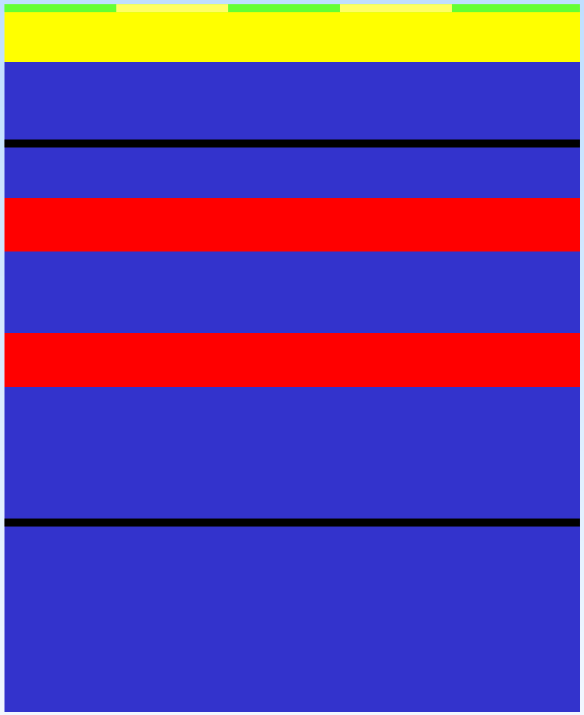
The Target Device

- Creates and confines a quantum dot electrostatically
- Senses dot using a quantum wire.





Side Gate Center Gate Side Gate

AlInAs

InP

δ-doping

InGaAs

InP

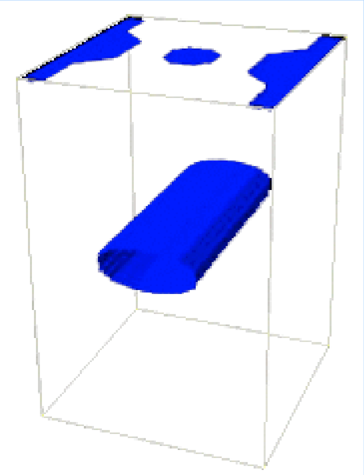
InGaAs

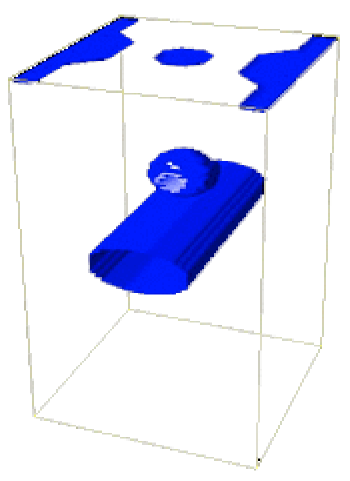
InP

δ-doping

Device
Structure

Device Operation





Side voltage applied

⇩

quantum wire

Multiple states in the lower well.
Confinement in 2 directions.

Side and dot voltage applied

⇩

quantum wire + quantum dot

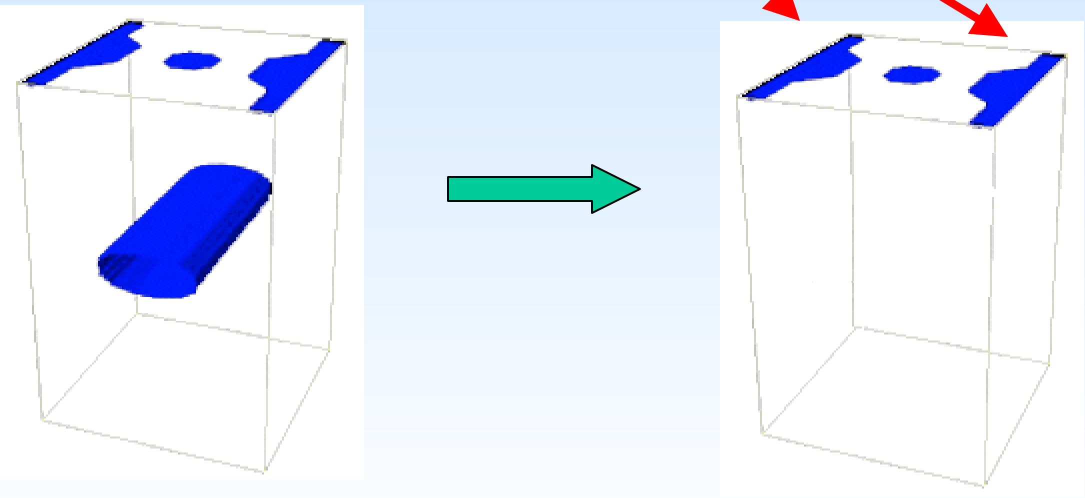
Single state in the upper well.
Confinement in 3 directions

Multiple states in the lower well.
Confinement in 2 directions

Operational Behavior Discrepancy

The predicted side gate bias required to pinch off the lower well quantum wire is too high.

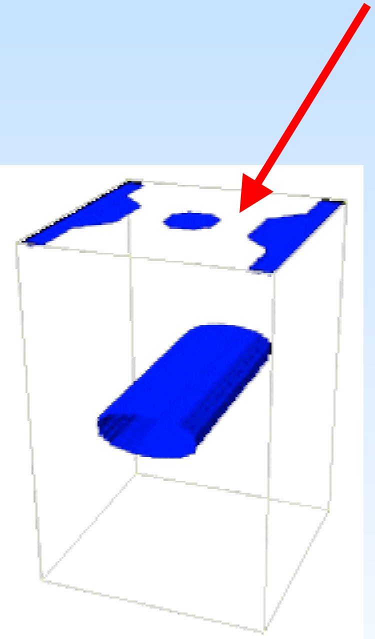
Pinchoff V_{side}=
~10 V (simulation)
~1 V (experiment)



Discrepancy Resolution

Use a fixed charge boundary condition rather than a fixed potential boundary condition on the ungated surface.

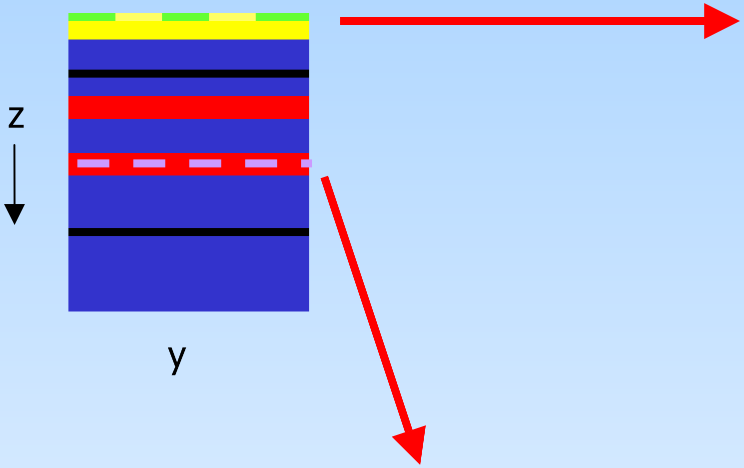
Specify $\kappa_1 \frac{\partial \phi_1}{\partial \vec{n}} - \kappa_2 \frac{\partial \phi_2}{\partial \vec{n}} = \sigma_{\text{surface charge}}$

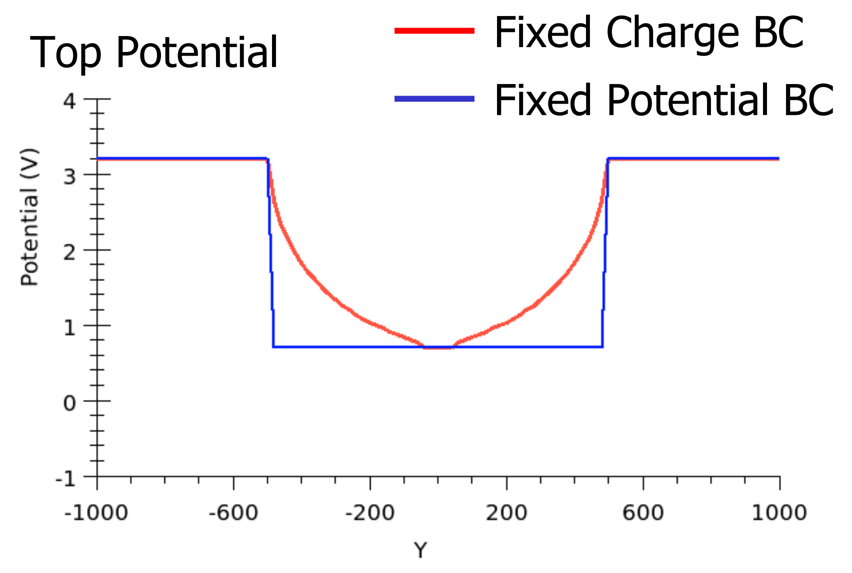


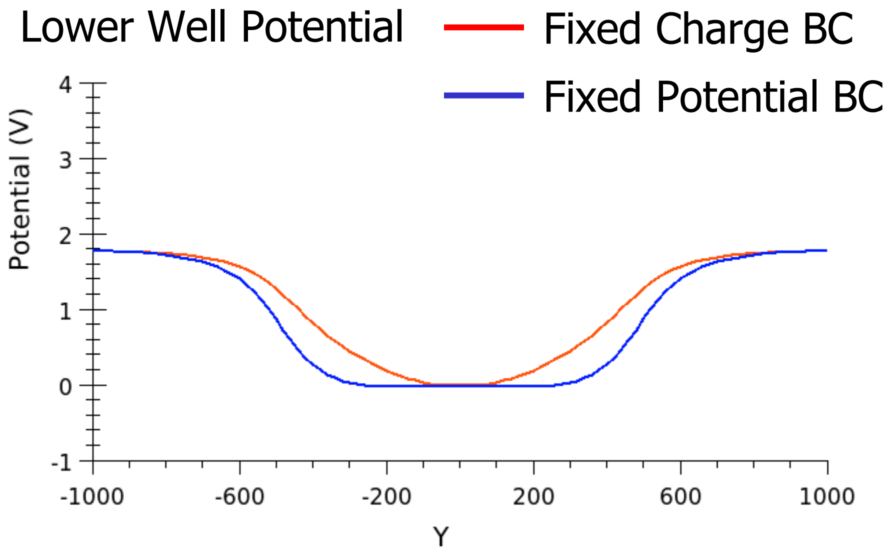
ϕ_1 = potential inside device

ϕ_2 = potential outside device

Boundary Condition Comparison (2D)

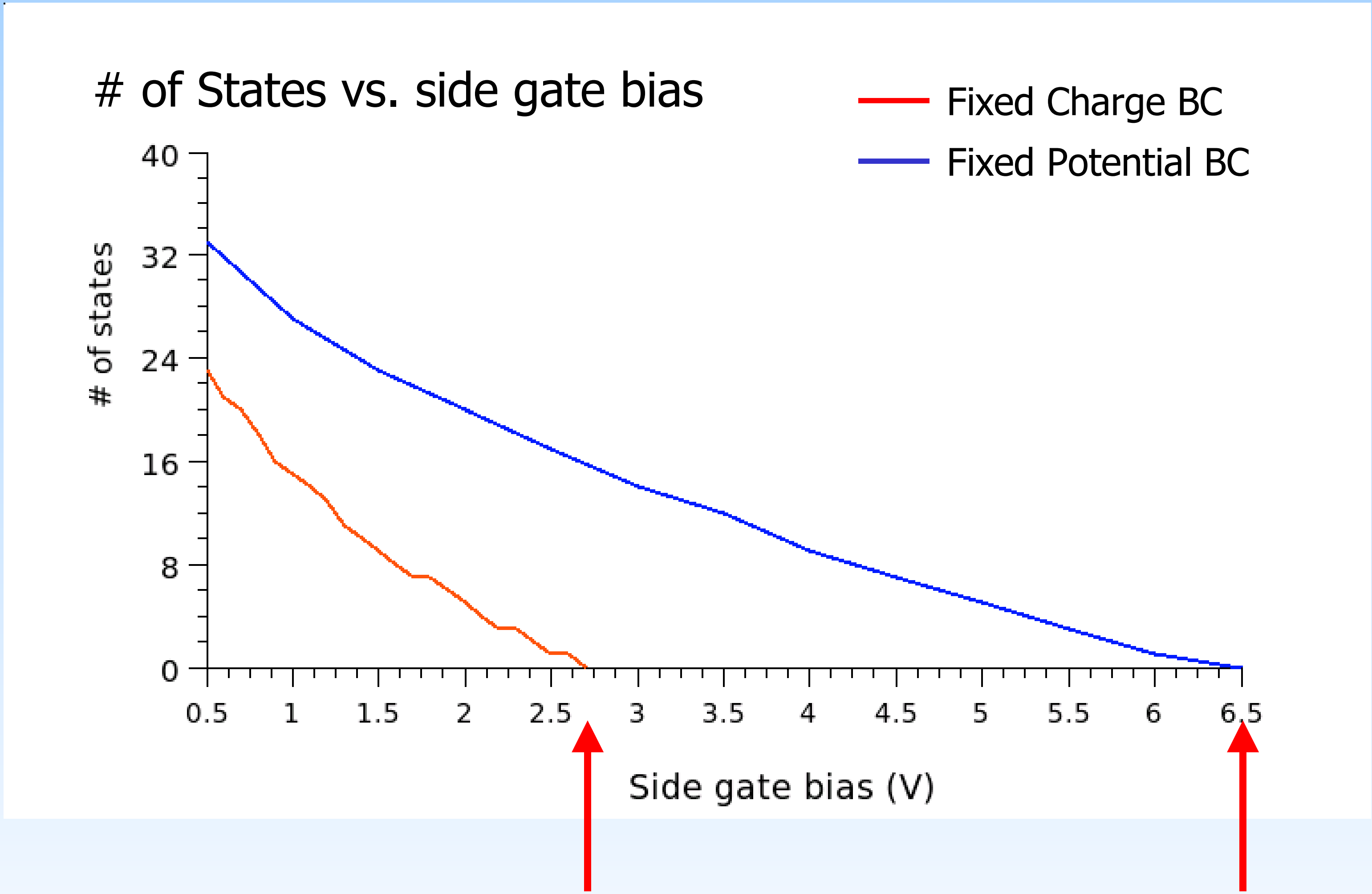



Top Potential


Lower Well Potential

Using fixed charge boundary conditions at the ungated surface “narrows” the potential between the side gates.

Boundary Condition Comparison (2D)

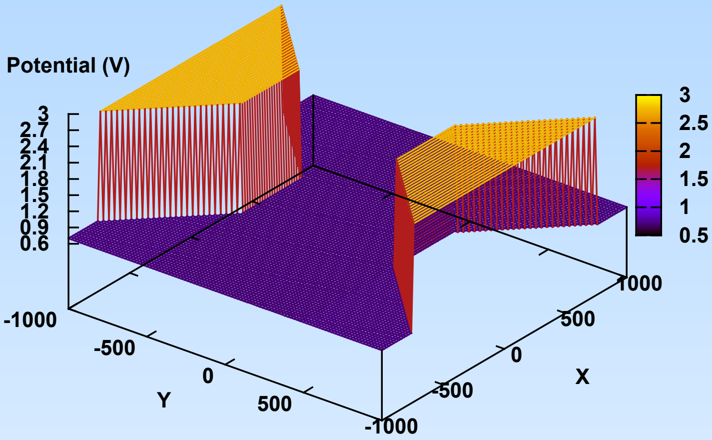


Using a fixed charge boundary condition at the ungated surface lowers the pinchoff voltage.

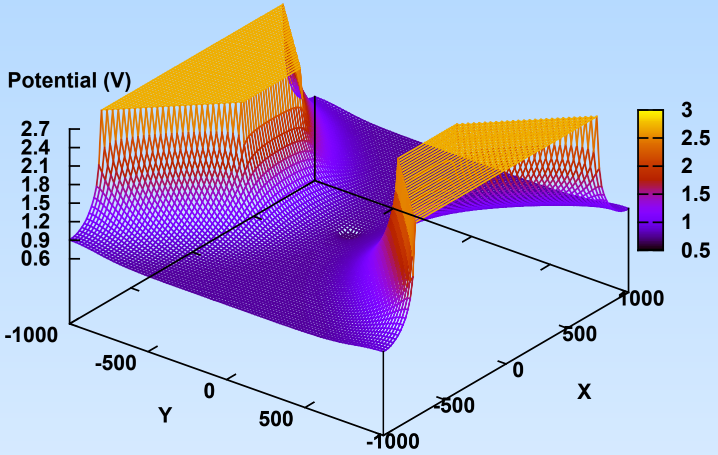
Boundary Condition Comparison (3D)

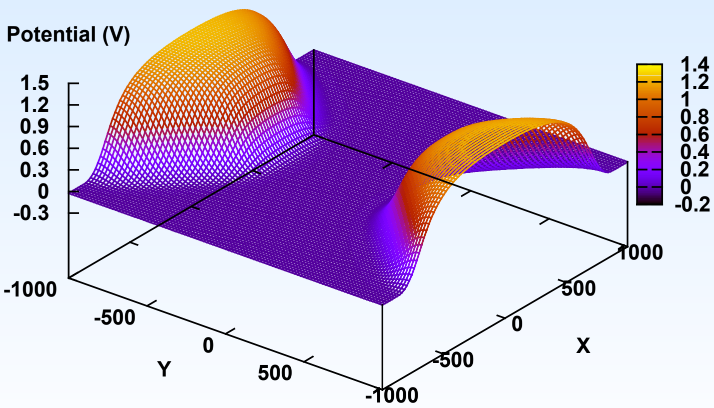
Fixed potential boundary conditions

Fixed charge boundary conditions

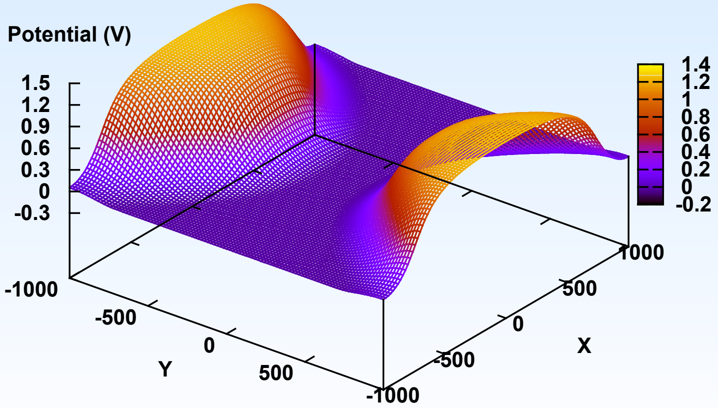


top potential (transverse slice)



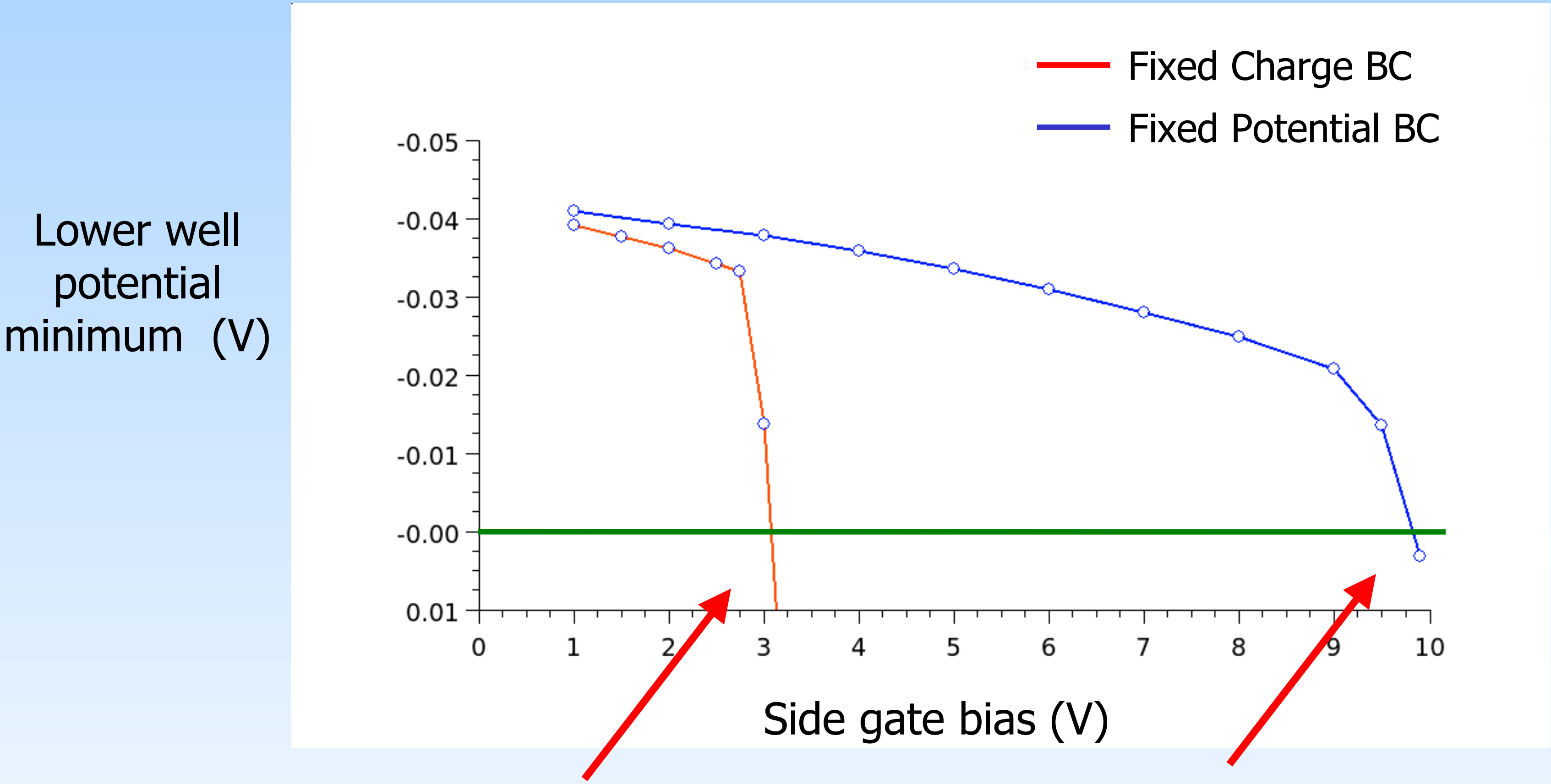


lower well potential (transverse slice)



Boundary Condition Comparison (3D)

Lower well pinchoff comparison*



Using a fixed charge boundary condition at the ungated surface lowers the pinchoff voltage.

** Calculations done using "local" density of states calculation*

Consequences

- The simulation results with fixed charge boundary conditions more accurately reflect experimental results (See E. Croke and M. Gyure poster)

- The use of fixed charge boundary conditions leads to a problem for the potential that is no longer separable.

Handling the Numerical Consequences

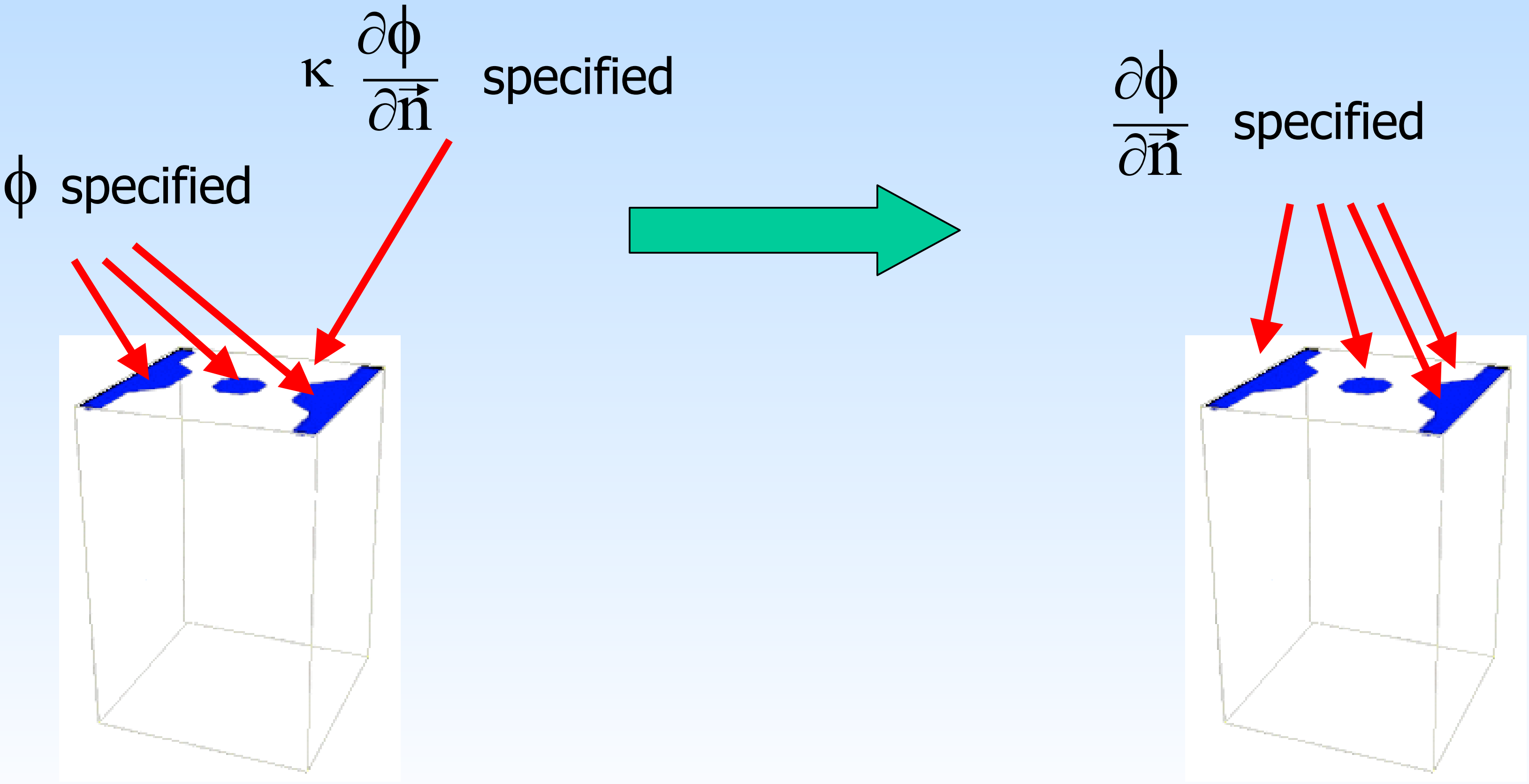
Problem: How to solve a non-separable elliptic PDE using a solver* that explicitly depends upon separability?

Solution: Transform the non-separable boundary conditions into separable boundary conditions.

* C.R. Anderson and T. Cecil, "A Fourier-Wachspress Method for Solving Helmholtz's Equation in Three Dimensional Layered Domains" to appear J. of Comp. Physics.

Handling the Numerical Consequences

Transform mixed boundary conditions to equivalent Neumann boundary conditions.



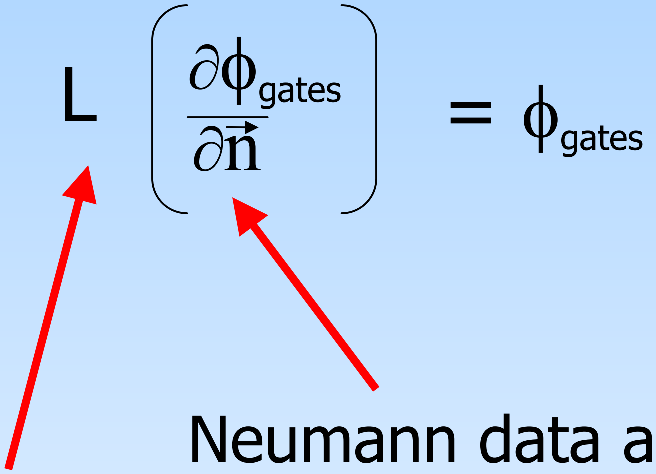
$\kappa \frac{\partial \phi}{\partial \vec{n}}$ specified

ϕ specified

$\frac{\partial \phi}{\partial \vec{n}}$ specified

Transforming boundary conditions ...

Equations to be solved:



$$L \left(\frac{\partial \phi_{\text{gates}}}{\partial \vec{n}} \right) = \phi_{\text{gates}}$$

Neumann data at gates

Neumann - Dirichlet operator: evaluated using FFT's

↑

The critical aspect for efficiency

The transformation equations are solved iteratively using pre-conditioned conjugate gradients (4-5 iterations).

Conclusions

- The simulation results with fixed charge boundary conditions on the ungated surface more accurately reflect experimental results.

- The non-separable nature of the new boundary conditions does not impact the use of FFT’s to evaluate the Neumann-Dirichlet operator.

- The Neumann-Dirichlet operator can be efficiently inverted to obtain equivalent separable boundary conditions.

- The non-separable potential calculation takes only 2x the time of the separable problem!