

# Poisson\_CCD: A Dedicated Semiconductor Simulator for Silicon CCDs.

Craig Lage

October 3, 2017

Acknowledgements:

Tony Tyson, Andrew Bradshaw, Kirk Gilmore, Perry Gee

# Outline

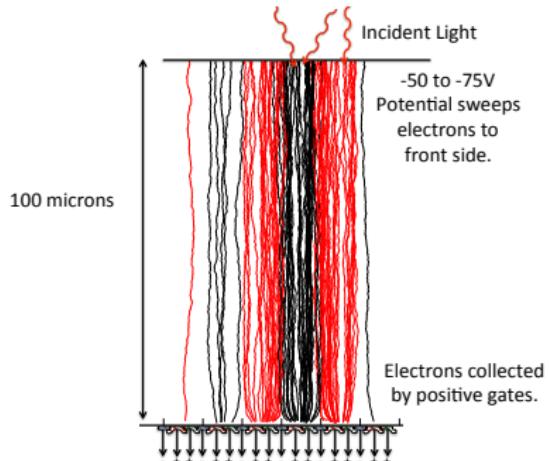
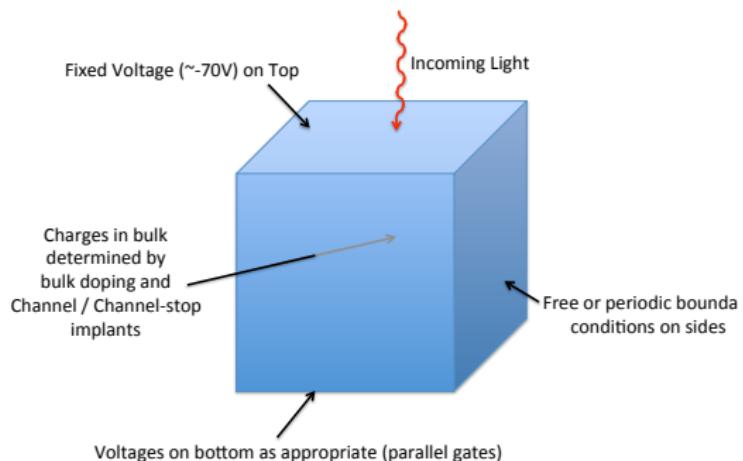
- Why build a CCD simulator?
- Overview of basic output
- Verification and results
  - Need for CCD physical characterization.
  - Brighter-Fatter effect
  - Array edge astrometric shift
  - Saturation
  - Chip edge
  - Tree rings
- Methods
  - Numerics
  - Electron diffusion and tracking
  - Electron density methods
  - “Stretched” Z-axis.

## Why build a physics-based simulation of the sensor?

- Allows one to turn physical effects (such as diffusion) on and off.
- Allows study of small effects without interference from extraneous problems:
  - Noise
  - Crosstalk
  - Optical Distortion, ...
- Allows study of the impact of sensor differences:
  - Doping
  - Thickness
  - Vendor, ...
- Allows study of the impact of environmental effects:
  - Temperature
  - Voltage, ...

# Overview of Basic Output

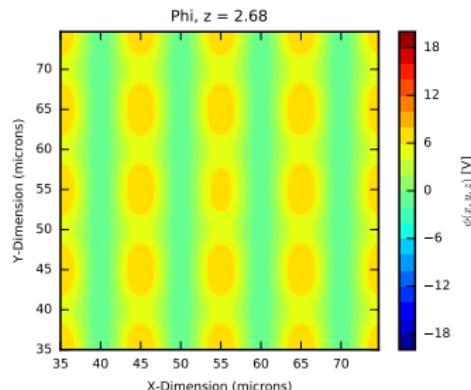
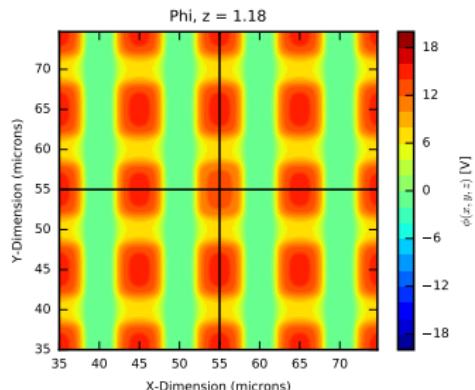
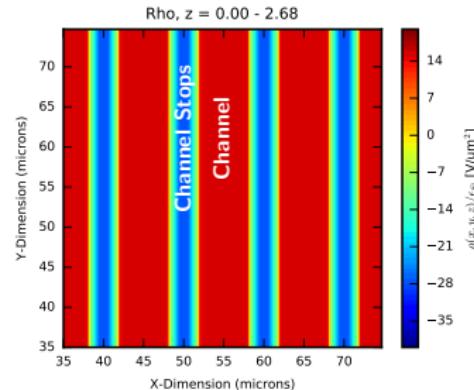
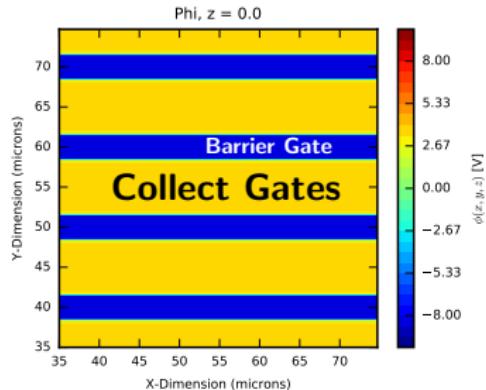
# Typical Simulation 100 $\mu$ m Cube.



- Poisson's equation solved using multi-grid methods.
- 100 $\mu$ m Cube. - 10 X 10 pixels in X and Y.
- 32 grid cells per pixel - cell size = 0.31  $\mu$ .

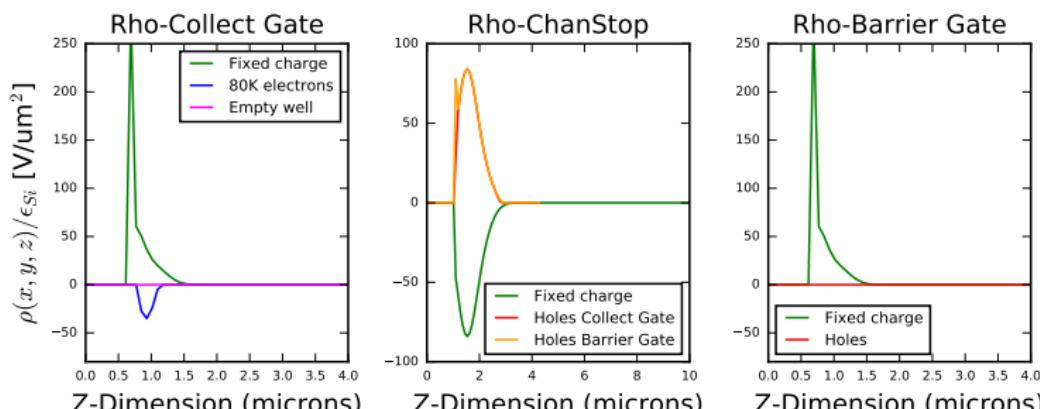
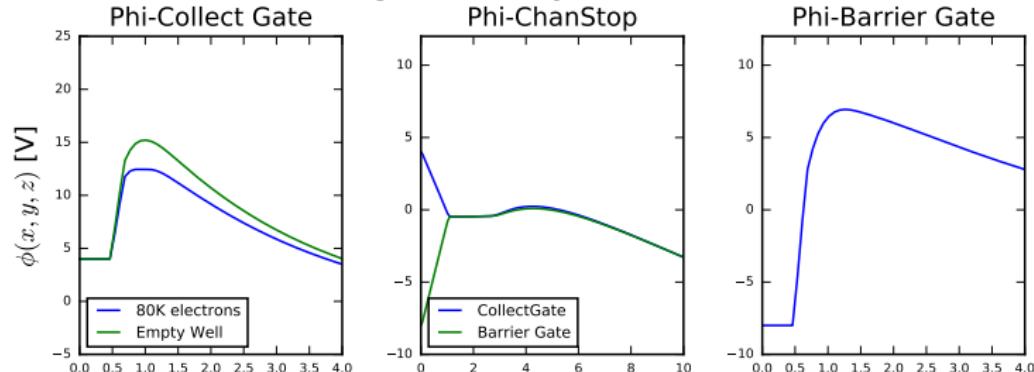
# Pixel Array Summary Plot

CCD Charge Collection. Grid = 320\*320\*320.



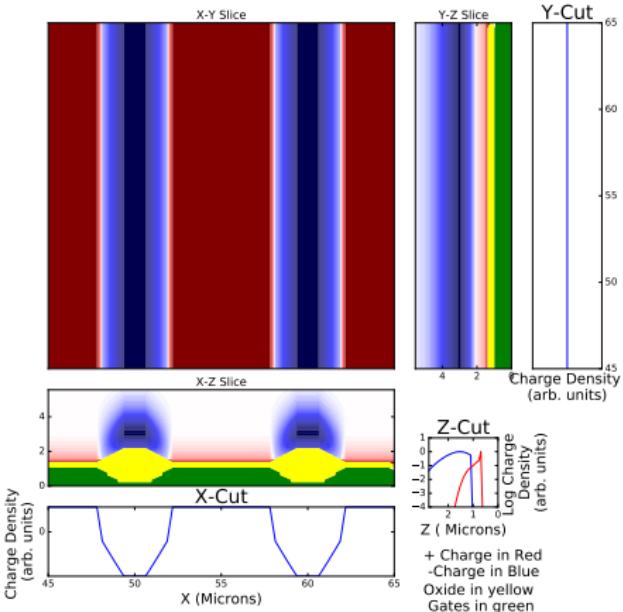
# Pixel Array 1D Slices

1D Potential and Charge Density Slices. Grid = 320\*320\*320.

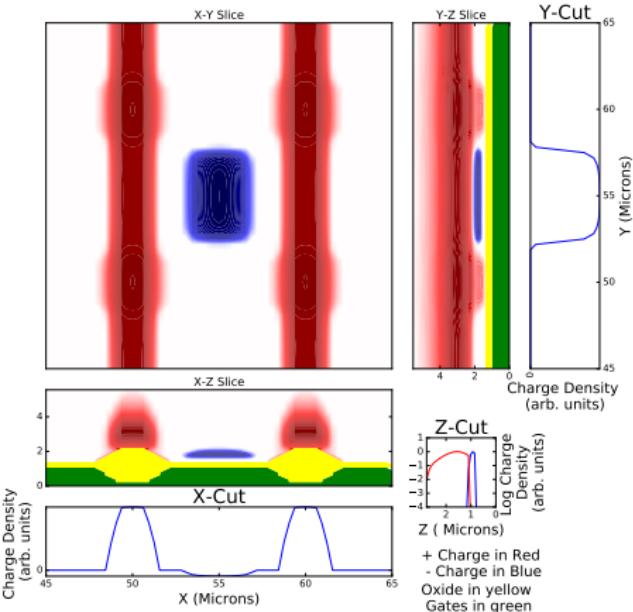


# Fixed and Mobile Carriers

Fixed Charge Distribution



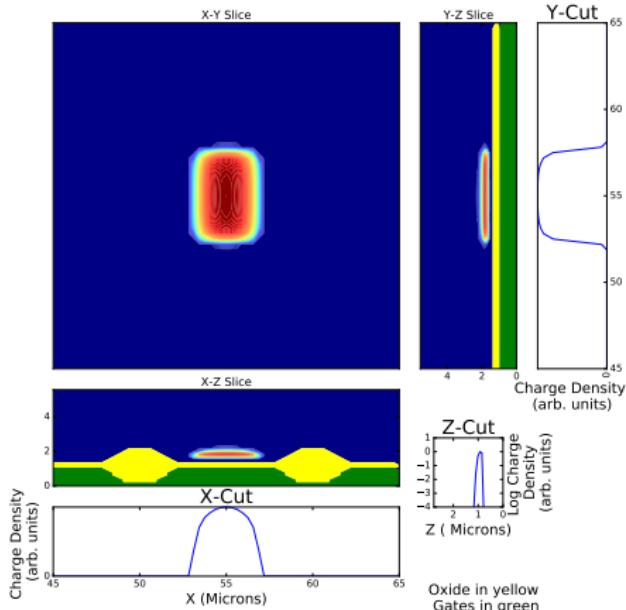
Mobile Charge Distribution



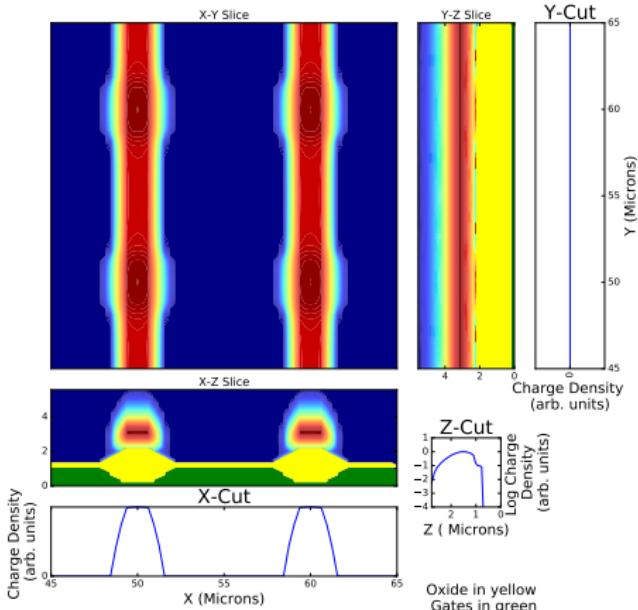
Z-axis has a 2X scale multiplier

# Electrons and Holes

Electron Charge Distribution



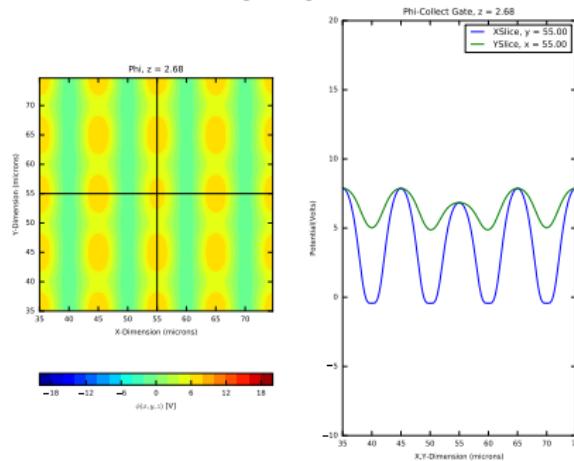
Hole Charge Distribution



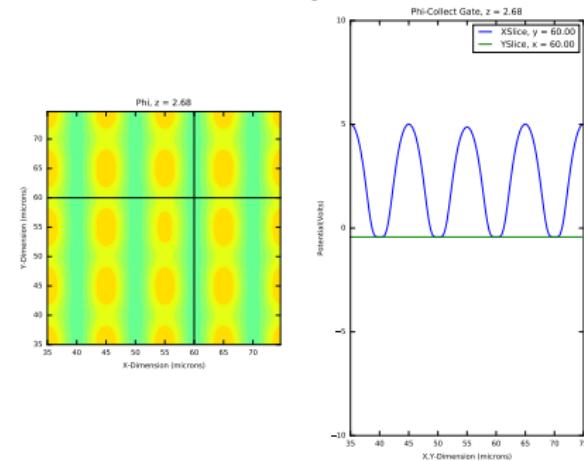
Z-axis has a 2X scale multiplier

# Other 1D Slices

1D Potentials in Storage Region. Grid = 320\*320\*320.



1D Potentials in Isolation Regions. Grid = 320\*320\*320.

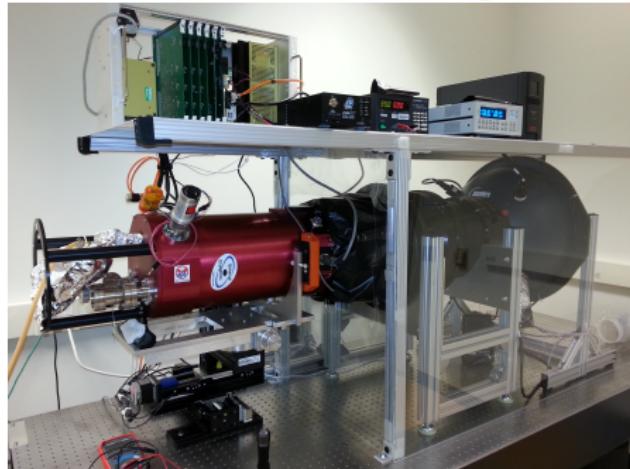


- Left hand plot shows confining potential in X and Y. This shows clearly why blooming happens along the column (in the Y direction), where the potential barrier is much smaller than along the row (in the X direction).

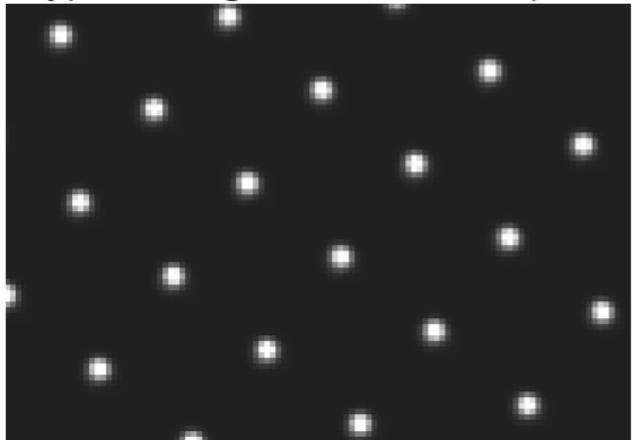
# Verification and Comparison to Measurement

# LSST Optical Simulator and Typical Spot Images

UC Davis 1:1 Re-Imager



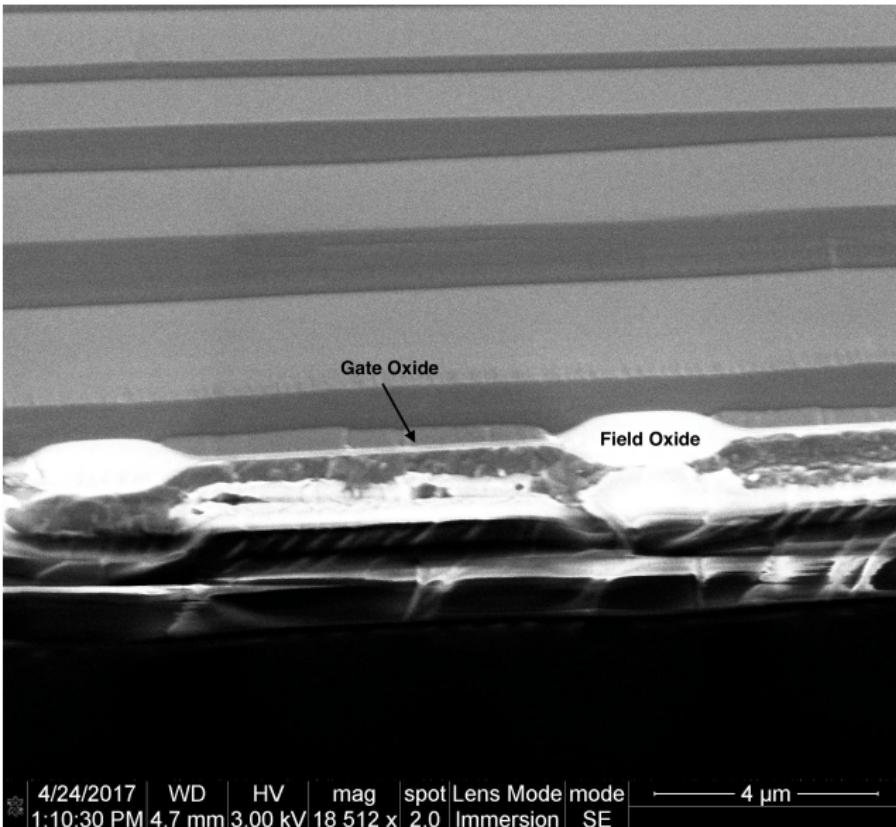
Typical Image of 30 micron Spots:



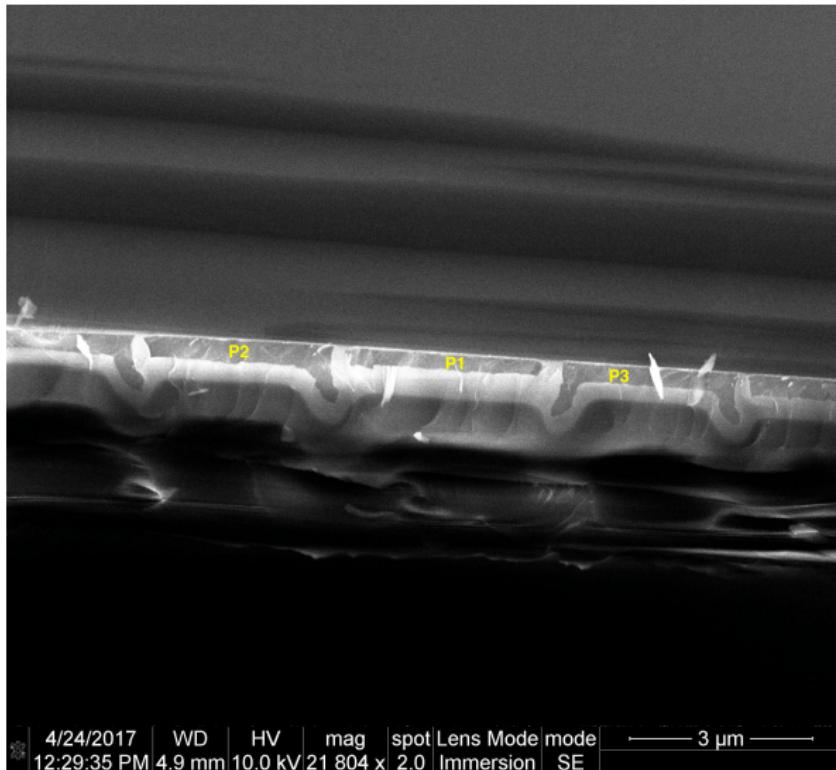
## Need for Physical Characterization

- Trying to infer the physical characteristics of the CCD from the optical measurements simply wasn't working. There are two many degrees of freedom.
- We obtained a “dead” STA3800C device for physical analysis. STA3800C Lot 180928, Wafer 24, Die 4.
- Before performing SIMS analysis, electrical measurements were made on the output device.
- SIMS Analysis of STA3800 sample has been completed by EAG Laboratories in Sunnyvale, Ca.
- Cross sectional SEMs were taken here at UC Davis.

# SEM Cross-Section I



## SEM Cross-Section II

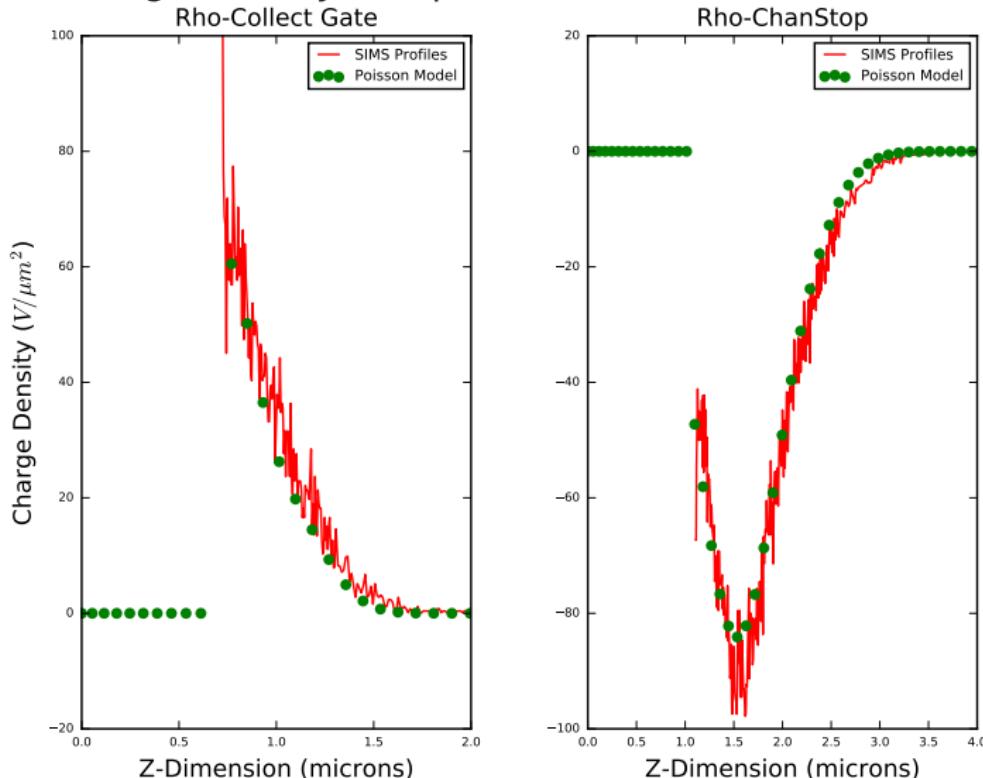


4/24/2017 | WD | HV | mag | spot | Lens Mode | mode | 3 μm |  
12:29:35 PM | 4.9 mm | 10.0 kV | 21 804 x | 2.0 | Immersion | SE |

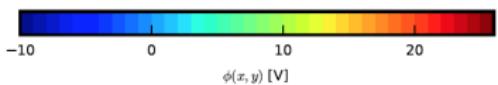
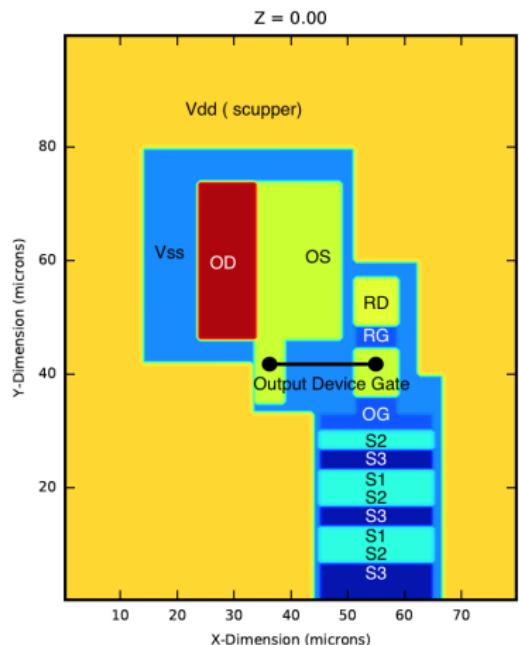
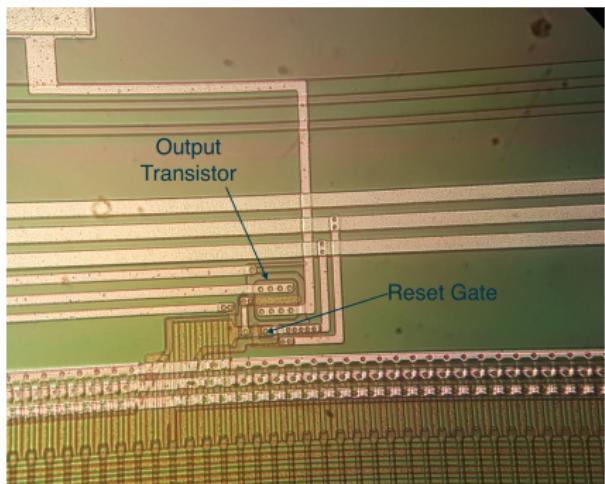
Simulation does not include small gaps between the polys. These appear small enough that this is justified.

# Fit to measured SIMs - two Gaussians

Charge Density Comparison. Grid = 320\*320\*320.

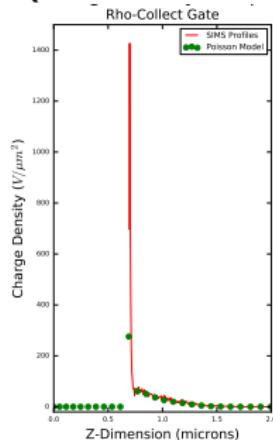


# Output Transistor Region

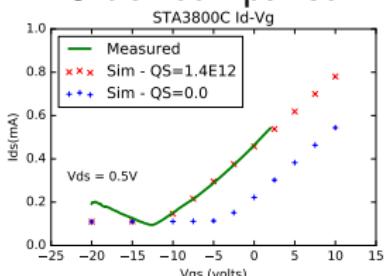


# Channel Charge Surface Spike needs to be included!

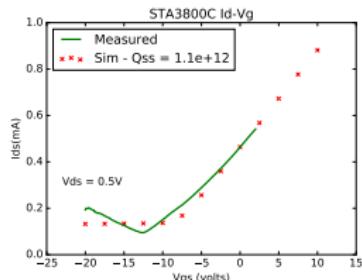
$$QS = 1.1E12$$



## Older comparison



## Current model

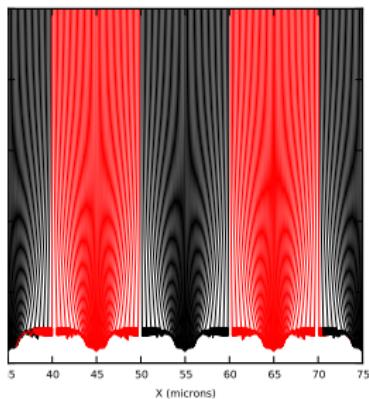


- Surface spike, since it is in a single simulation grid cell, needs to have the correct charge.
- Integrating SIMS -  $1.1E12 \text{ cm}^{-2}$ . Using this value in current model.
- Spike is probably due to phosphorous “pile-up”.

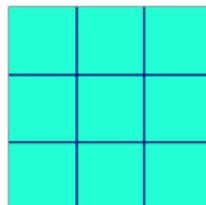
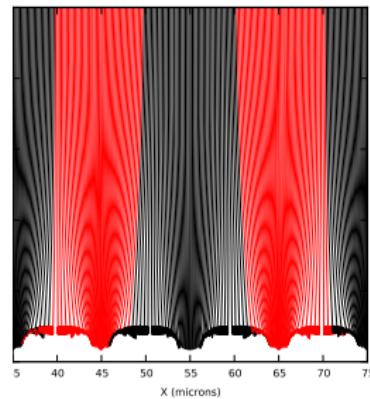
# Verification Brighter-Fatter Effect

# Basics of the Brighter-Fatter Effect

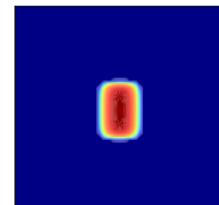
Diffusion turned off here.



Diffusion turned off here.



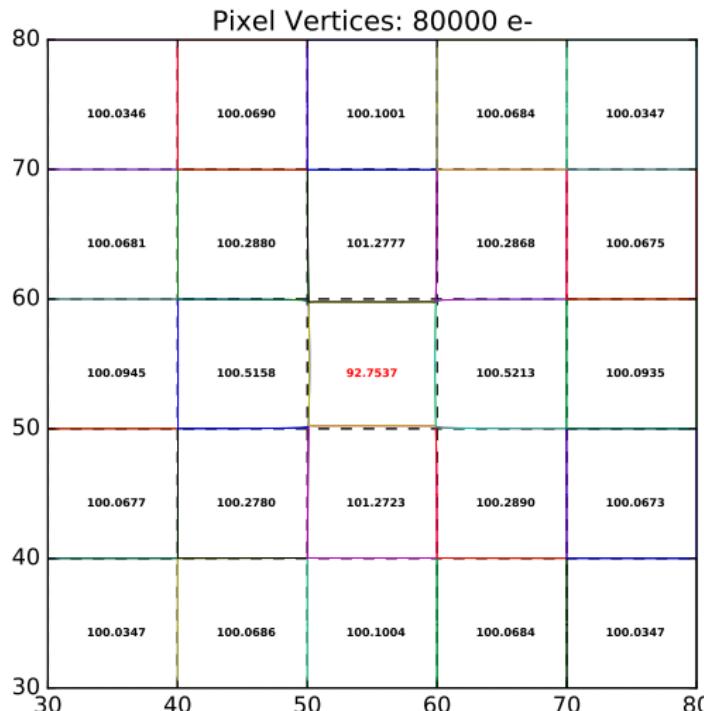
Pixel empty of charge



Pixel with 100K e-

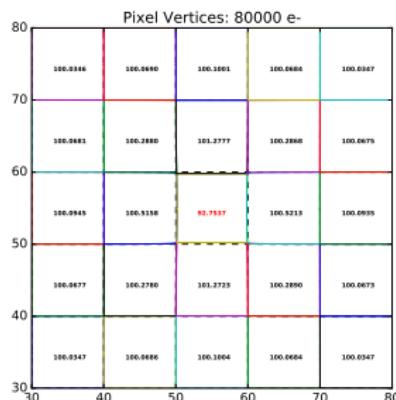
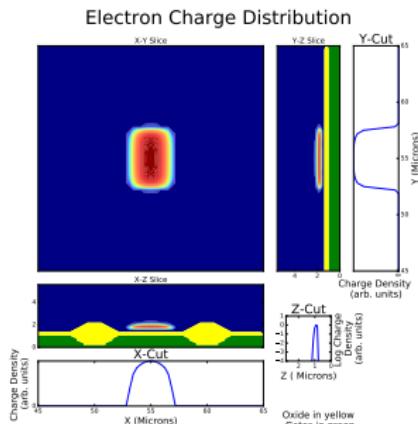
- Electrons stored in the potential well repel incoming electrons and push them into surrounding pixels.

# Pixel Shape Distortion due to Collected Charge

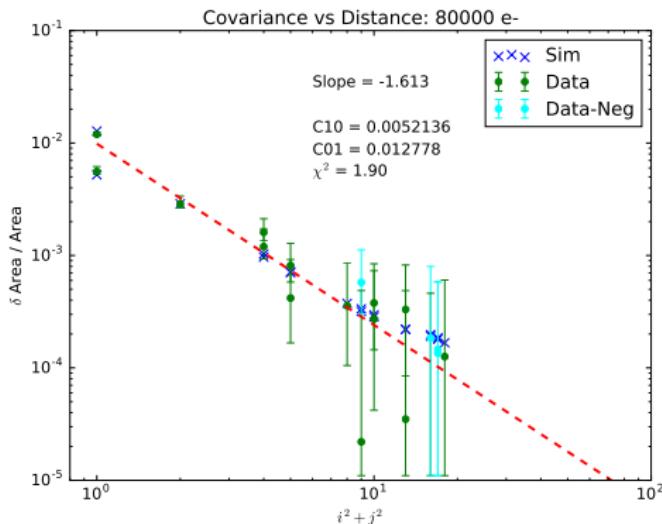


Pixel edges are found through binary search with diffusion off.

# Pixel Areas and Correlations

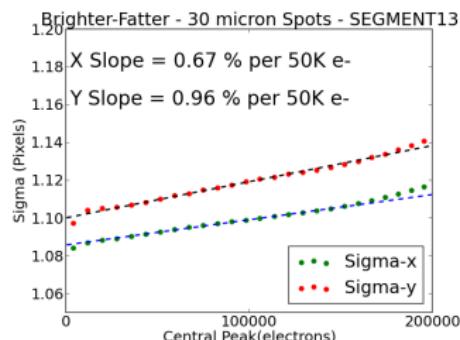
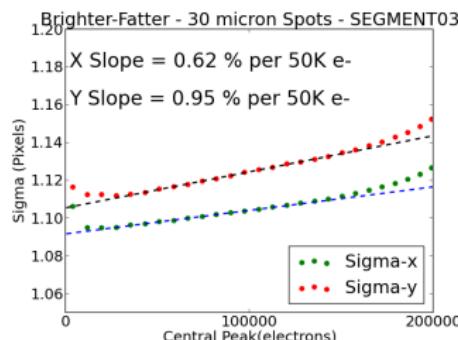
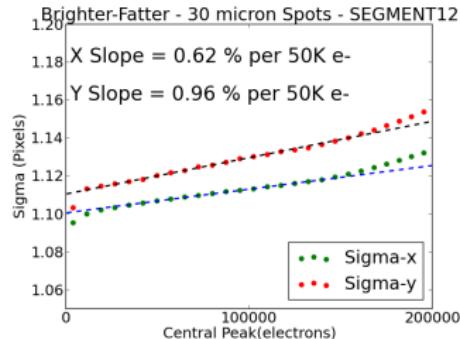
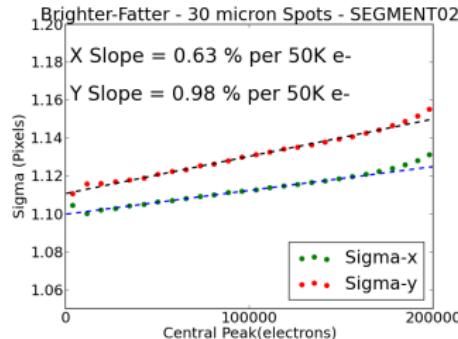


## Simulations vs STA3800 Measurements



- Antilogus, et al., JINST 9C3048 (2014), arXiv:1402.0725.
- Rasmussen, A., JINST 904027 (2014), arXiv:1403.3317.

# Typical Brighter-Fatter Effect Measurements - STA3800



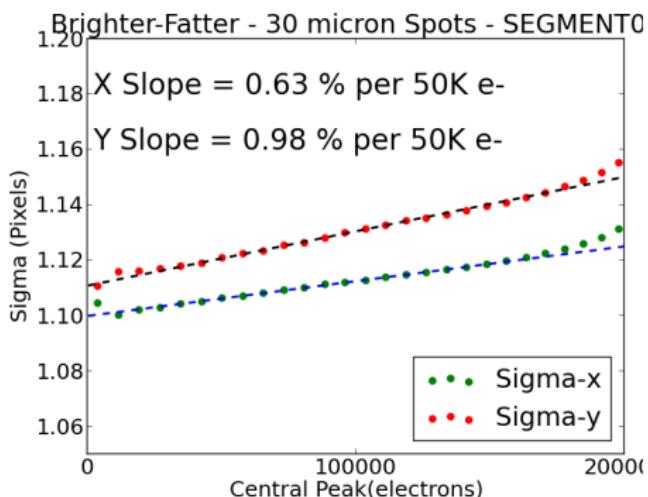
Many measurements have been made under different conditions.

## Simulation Strategy for B-F effect.

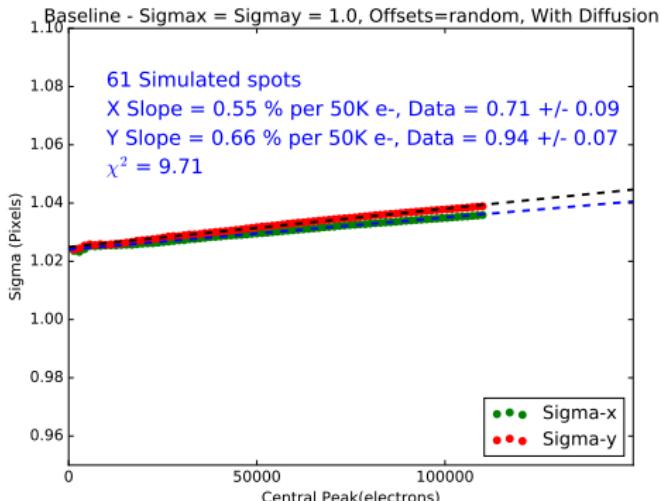
- Solve Poisson's equation for postage stamp with all pixels empty.
- Choose a random location within the central pixel.
- Determine starting locations for N electrons in a 2D Gaussian spot.
- Propagate these electrons down to their collecting gates.
- Re-solve Poisson's equation with these wells now containing the appropriate charge.
- Repeat with N more electrons.
- I have been using 10,000 electrons per step, which places about 1000 electrons in the central pixel, so about 100 iterations are needed to fill the central pixel.
- In practice, repeat for more than one spot (typically 64), each with a different central location.
- Typical run takes  $\approx$  6 hours.

# Measurements vs Simulations

## Measurements



## Simulations

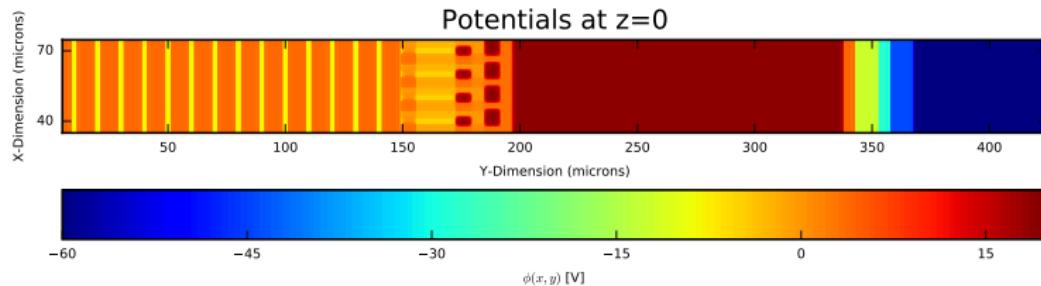
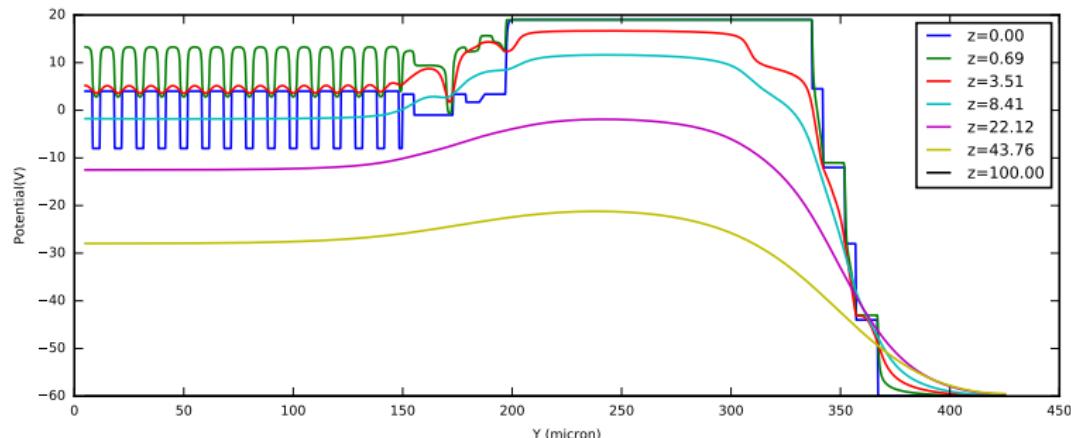


- Past simulations had a better agreement.
- Currently working on understanding the source of the discrepancy - simulations or measurement?

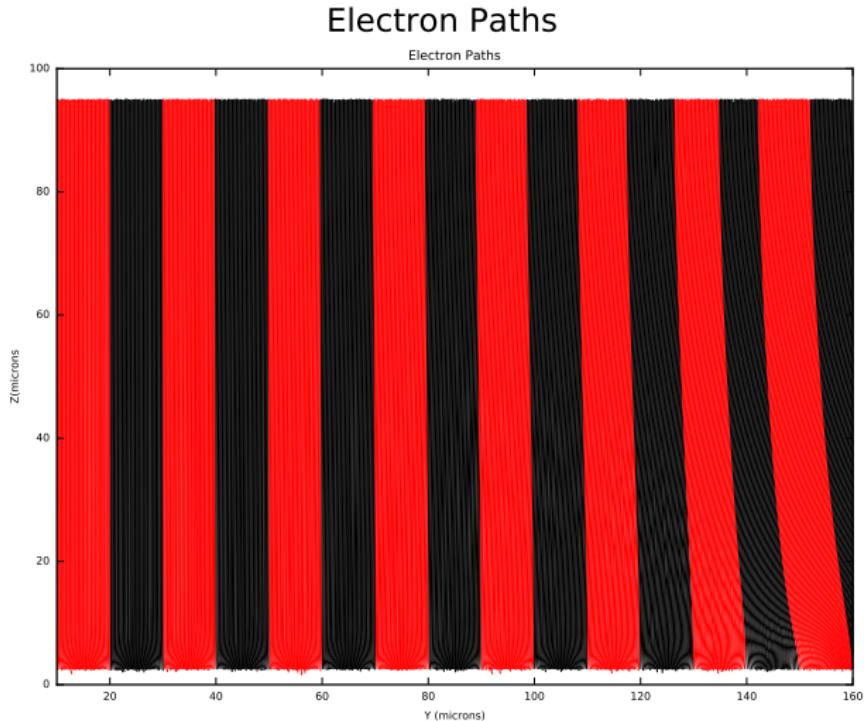
# Verification Astrometric Shift at Array Edge

# Potential Simulation at Array Edge

Potentials. Grid = 128\*1344\*320.

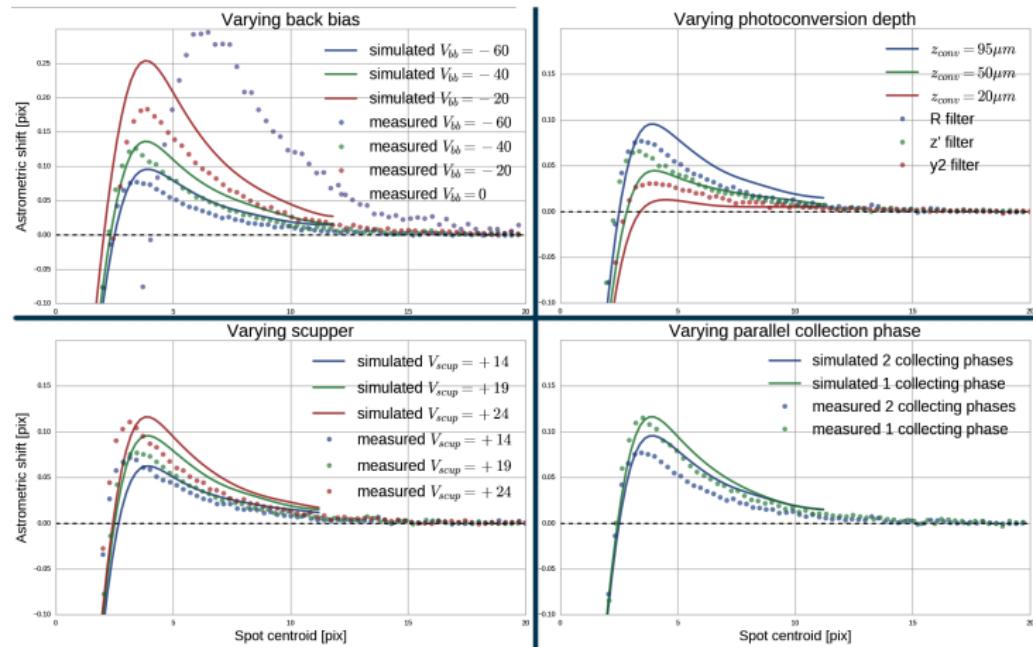


# Array Edge Electron Paths



Shift at edge of array is large!

# Astrometric Shift at Array Edge



Simulation captures shape, location, and variation with voltages.  
Acknowledgment to Andrew Bradshaw for this figure.

# Verification Saturation

# Bloomed vs Surface Full Well

Janesick

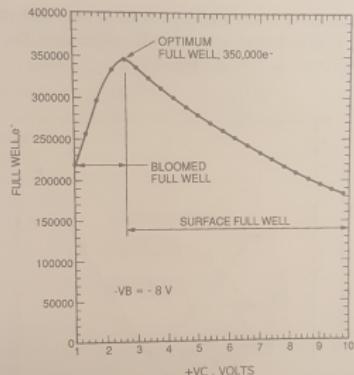
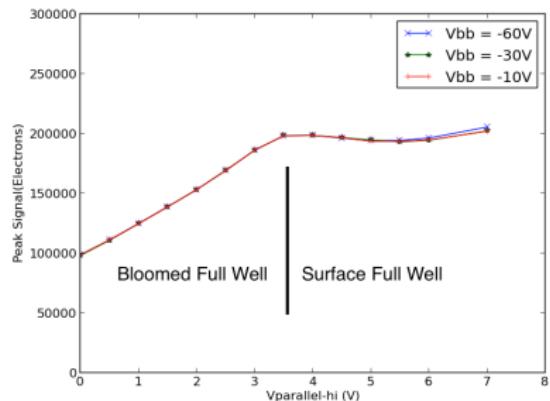


Figure 4.4(a) Full well transfer curve showing BFW and SFW regimes and the optimum full well bias point.

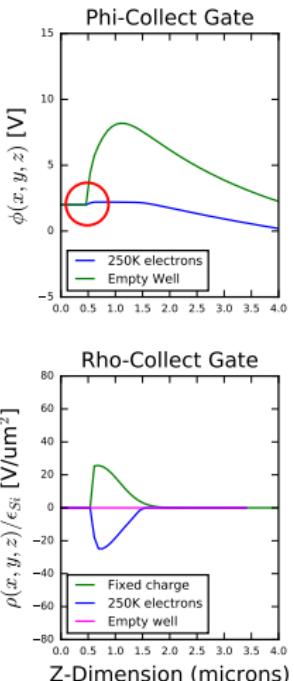
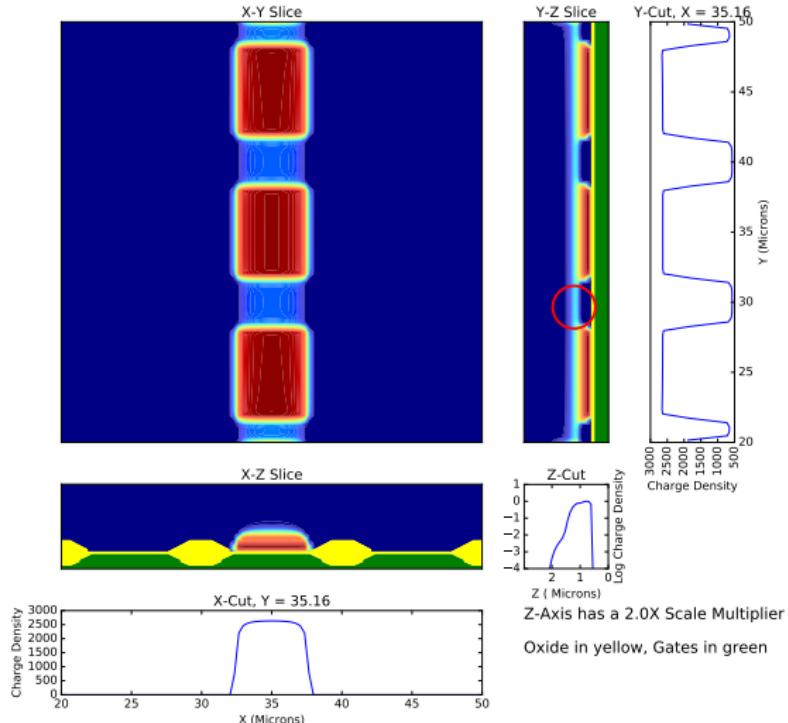
ITL Measurements

Saturation Curve - Surface vs Bloomed Full Well - ITL STA3800 - 033



# Simulations - 3x250K electrons - Vparallel-high = 2.0V

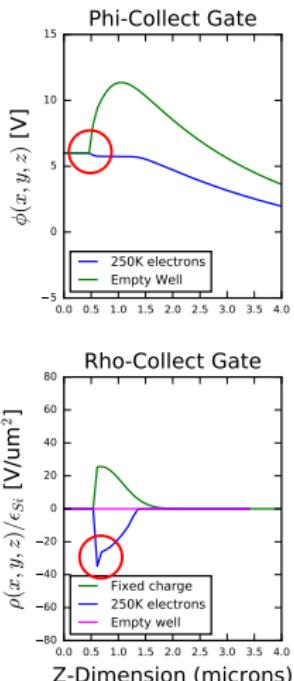
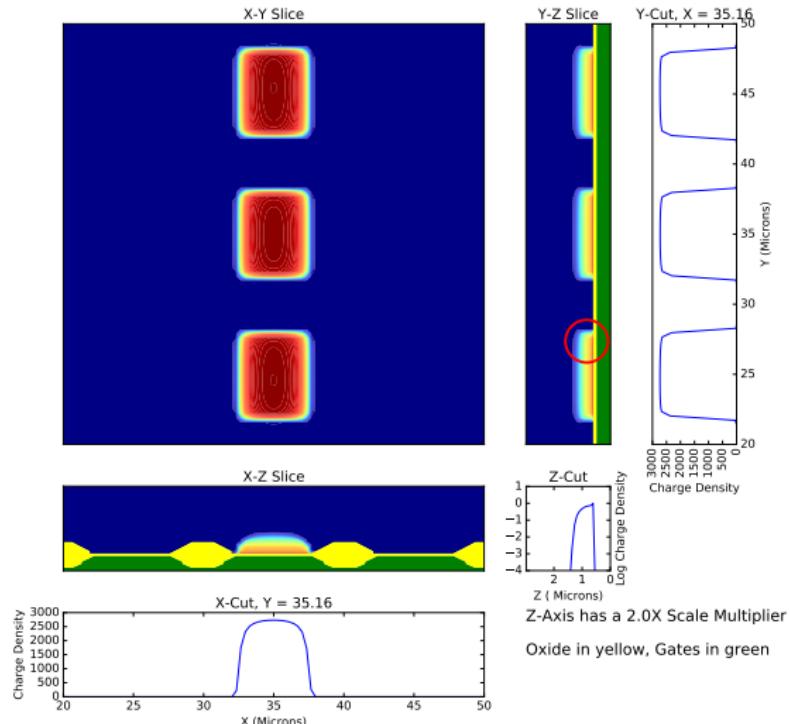
## Electron Charge Distribution



At 2.0V we are in the BFW condition. The pixels merge at the top.

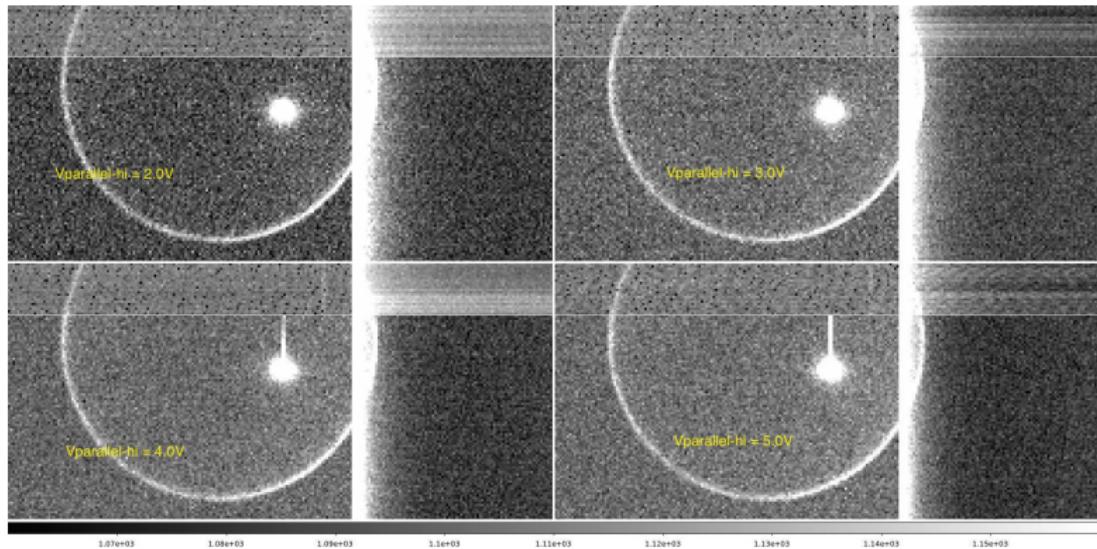
# Simulations - 3x250K electrons - Vparallel-high = 6.0V

## Electron Charge Distribution



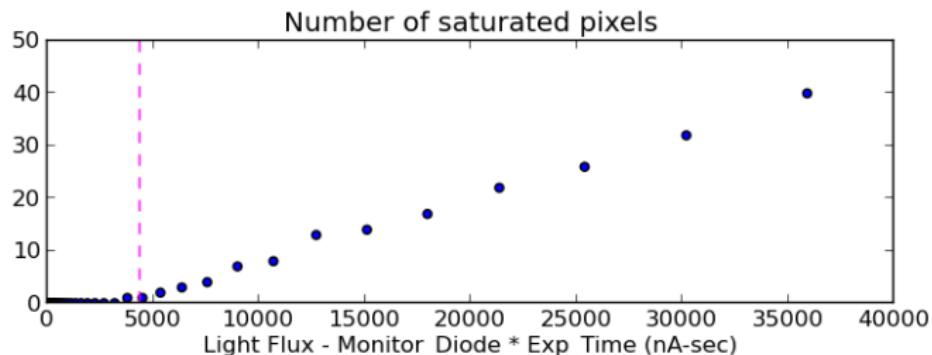
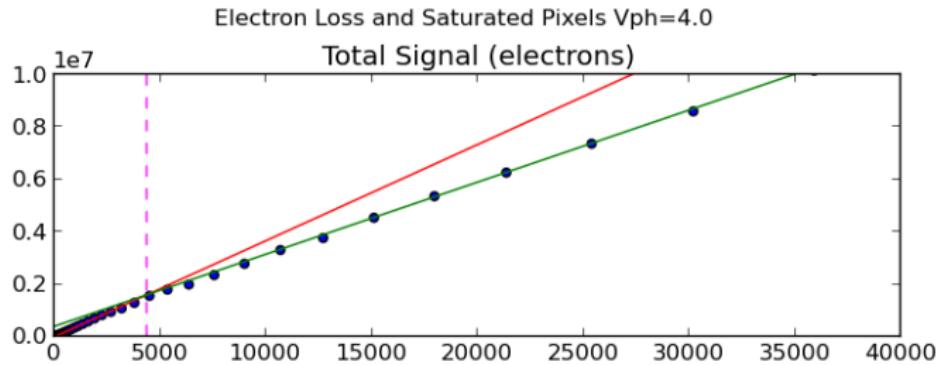
At 6.0V we are in the SFW condition. Charge builds up at the interface.

## “Trailing “ is seen in the SFW condition



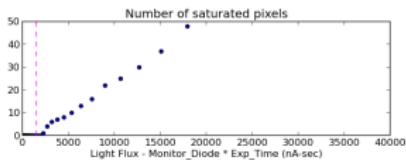
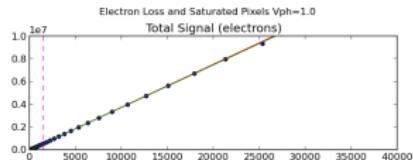
Charge building up at the surface is trapped in surface traps.

# Review of Charge loss seen in saturation

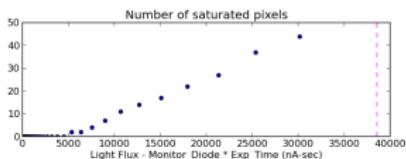
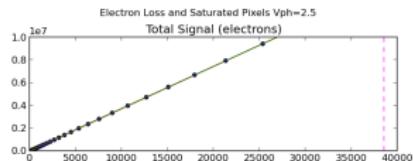


# Charge loss only occurs in SFW condition.

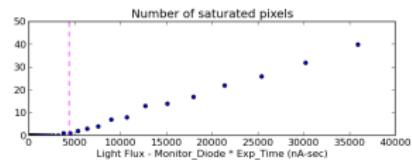
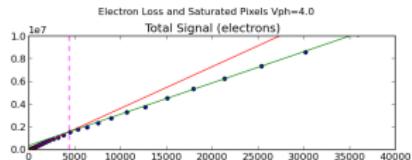
$V_{parallel\_hi} = 1.0V$



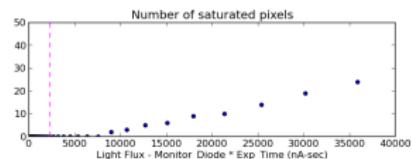
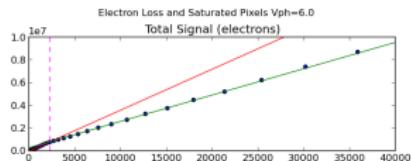
$V_{parallel\_hi} = 2.5V$



$V_{parallel\_hi} = 4.0V$

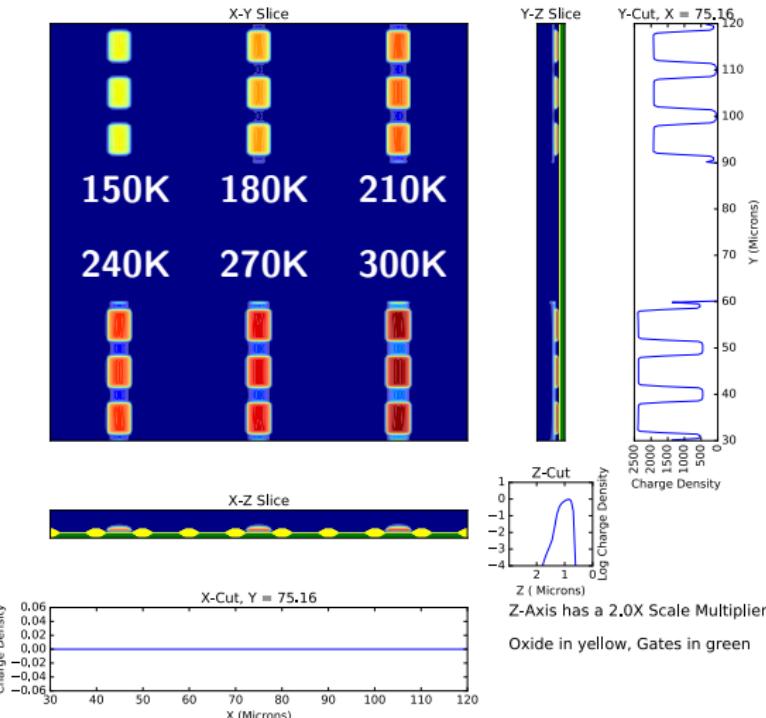


$V_{parallel\_hi} = 6.0V$



# $V_{\text{parallel\_hi}} = 1.0V$ - Multiple Fluxes

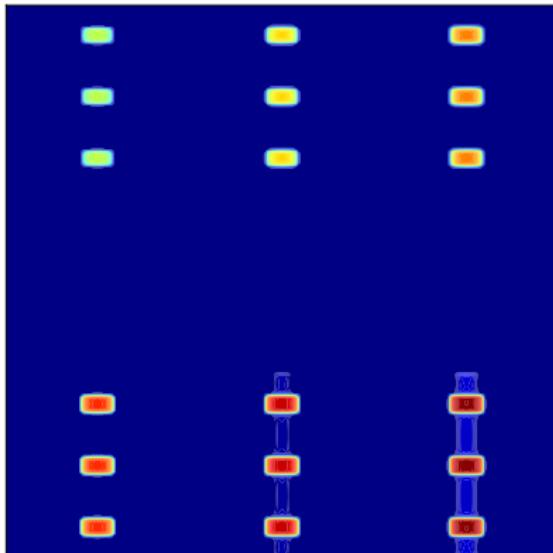
## Electron Charge Distribution



# Blooming occurs during readout with One Phase High!

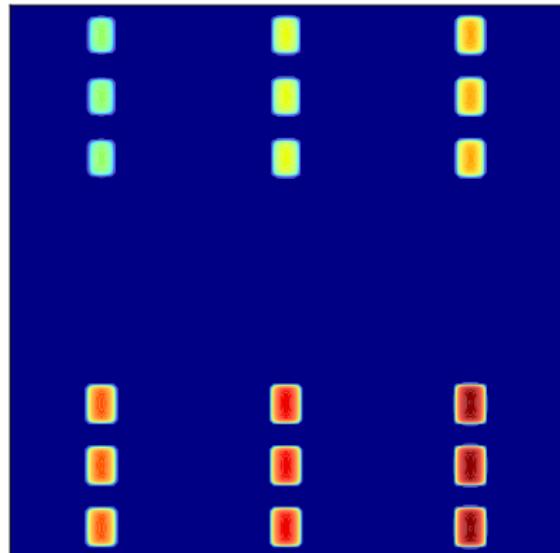
One Phase High

X-Y Slice



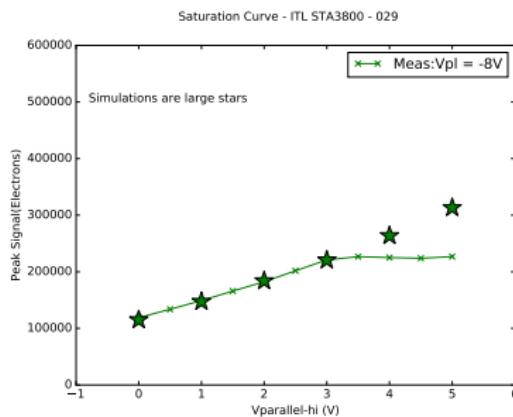
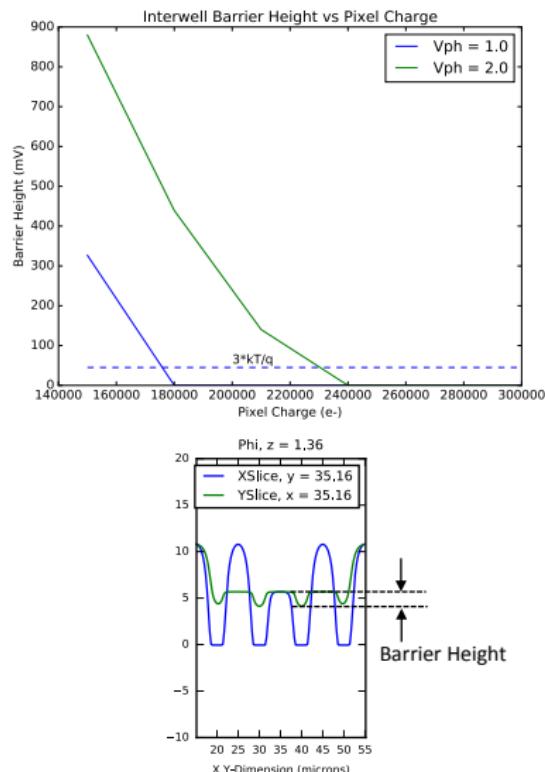
Two Phases High

X-Y Slice



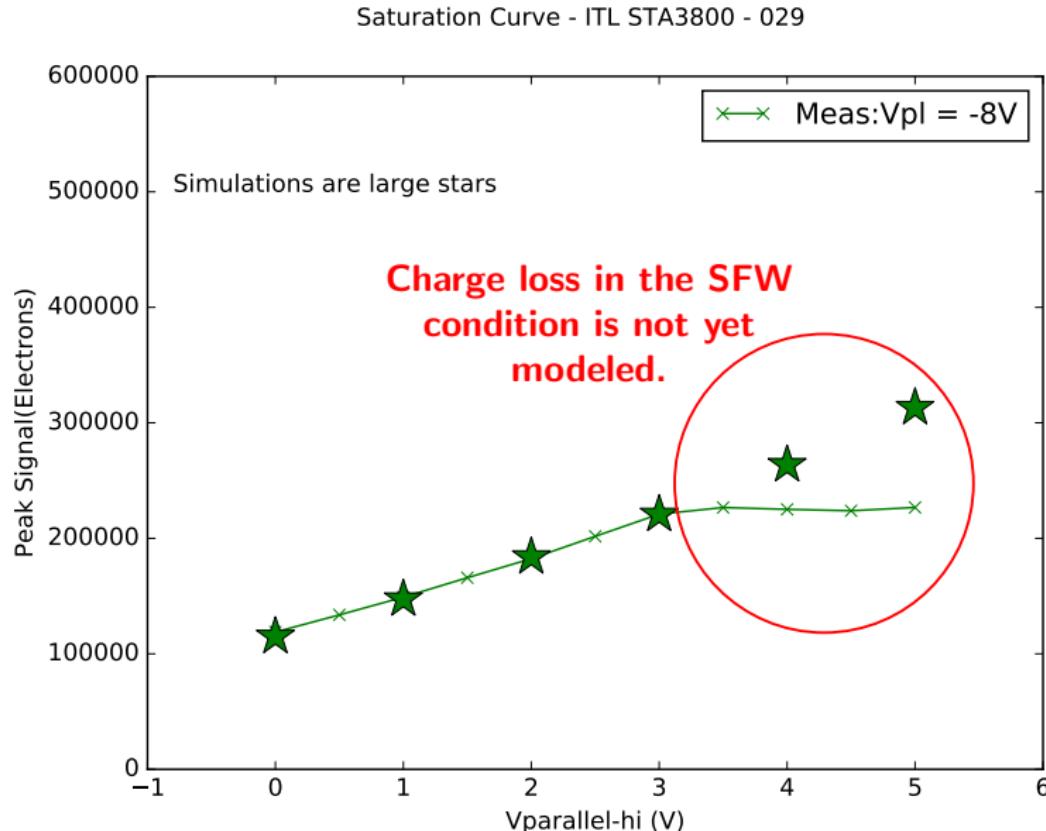
- Image integration is done with 2/3 phases high.
- However, to simulate the full well condition, we must simulate with one phase high, because blooming happens during readout when one phase is high and the charge is compressed into a smaller volume.

# Barrier Height reduction vs Vparallel\_hi

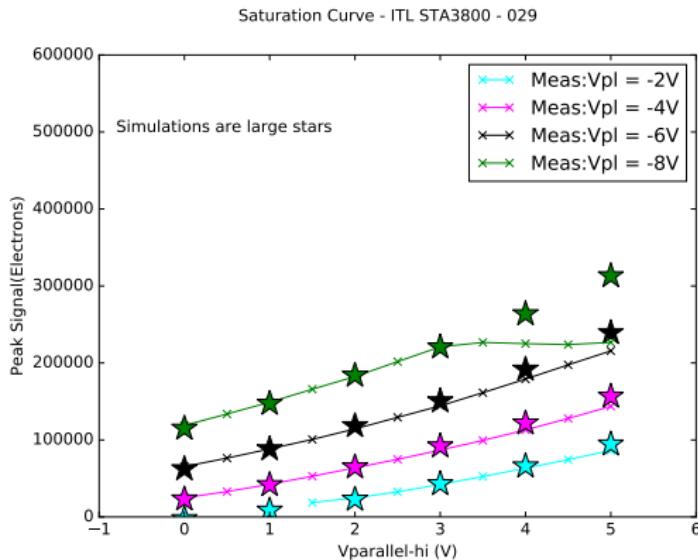


- When the barrier height is less than some level, the wells merge.
- This process allows us to simulate the saturation level.

# Measurements vs Simulation - Single Phase High



# Full Variation of Vparallel high and low



- This agreement assumes the pixel merging happens when the barrier height is less than 1.1V
- This is higher than expected - noise?, Vp not reaching full voltage?, or ?.

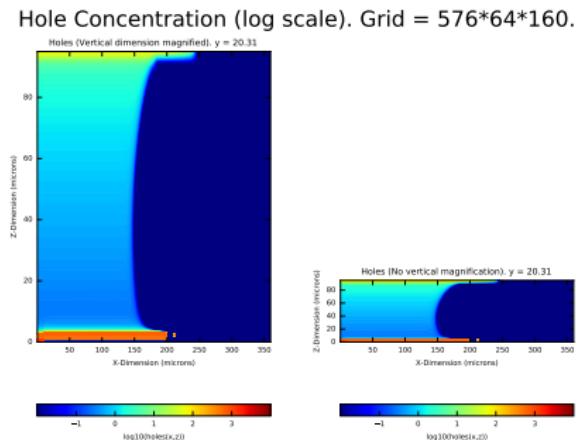
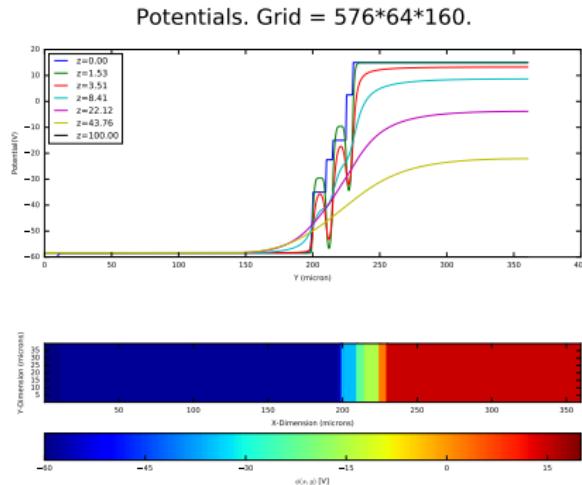
## Conclusions

- BFW and SFW conditions clearly seen in measurements and simulations.
- Charge loss is only seen in the SFW condition.
- Saturation levels across parallel voltages are well fit by the simulations.

# Verification Other Tests

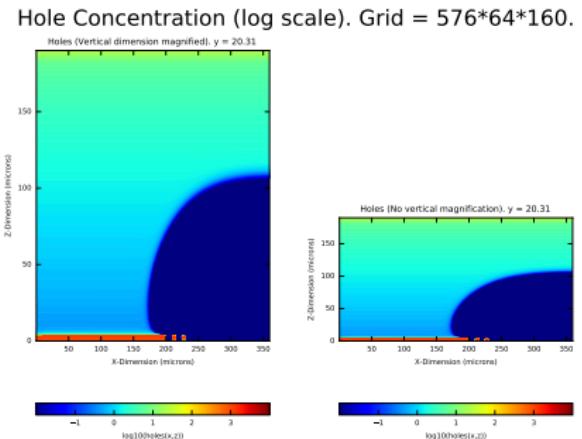
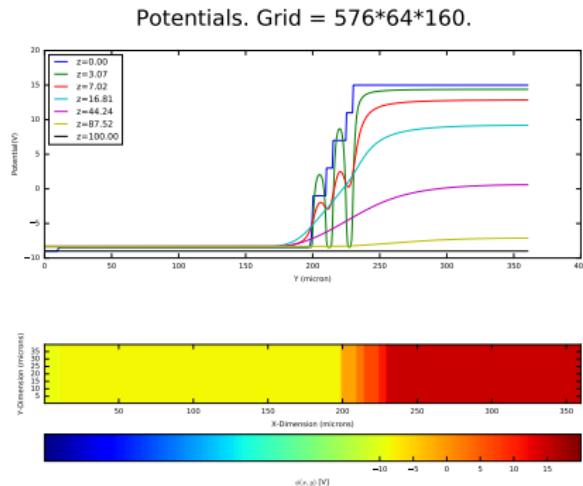
# Guard Ring at Chip Edge - I

Silicon Thickness = 100 microns,  $V_{bb} = -60V$



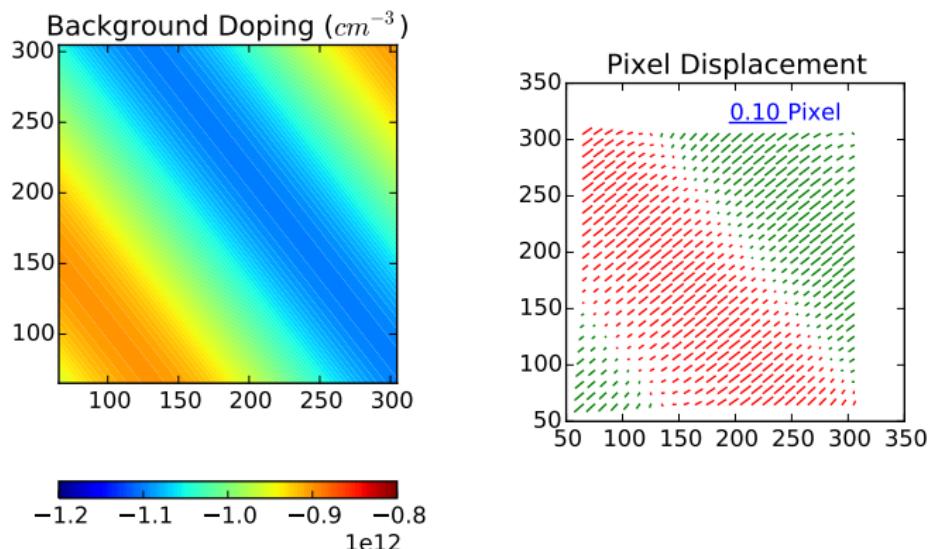
# Guard Ring at Chip Edge - II

Silicon Thickness = 200 microns,  $V_{bb} = -9V$



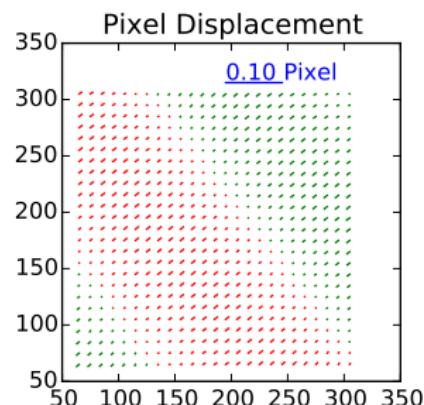
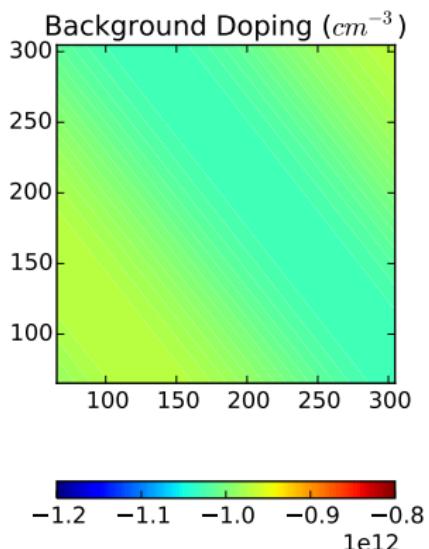
# Tree Rings - 10% Dopant Variation

Tree Rings: Amplitude = 0.10, Angle = 38.00 degrees, Period = 46.00 microns



# Tree Rings - 3% Dopant Variation

Tree Rings: Amplitude = 0.03, Angle = 38.00 degrees, Period = 46.00 microns



# Numerical Methods

# Solving Poisson's Equation on a Grid - I

$$\nabla^2 \varphi = \rho$$

$$\frac{\partial^2 \varphi_{i,j,k}}{\partial x^2} = \frac{(\varphi_{i+1,j,k} - \varphi_{i,j,k}) - (\varphi_{i,j,k} - \varphi_{i-1,j,k})}{h^2}$$

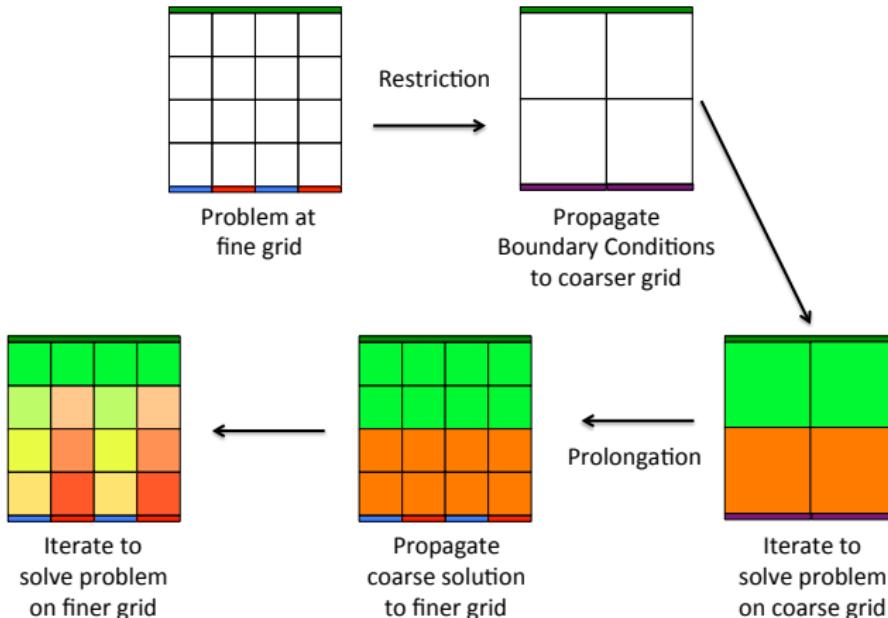
$$(\varphi_{i+1,j,k} + \varphi_{i-1,j,k} + \varphi_{i,j+1,k} + \varphi_{i,j-1,k} + \varphi_{i,j,k+1} + \varphi_{i,j,k-1} - 6 * \varphi_{i,j,k}) = h^2 * \rho_{i,j,k}$$

$$\varphi_{i,j,k} = \frac{1}{6} * (\varphi_{i+1,j,k} + \varphi_{i-1,j,k} + \varphi_{i,j+1,k} + \varphi_{i,j-1,k} + \varphi_{i,j,k+1} + \varphi_{i,j,k-1} - h^2 * \rho_{i,j,k})$$

$$\varphi_{i,j,k}^{(n+1)} = \frac{1}{6} * (\varphi_{i+1,j,k}^{(n)} + \varphi_{i-1,j,k}^{(n)} + \varphi_{i,j+1,k}^{(n)} + \varphi_{i,j-1,k}^{(n)} + \varphi_{i,j,k+1}^{(n)} + \varphi_{i,j,k-1}^{(n)} - h^2 * \rho_{i,j,k})$$

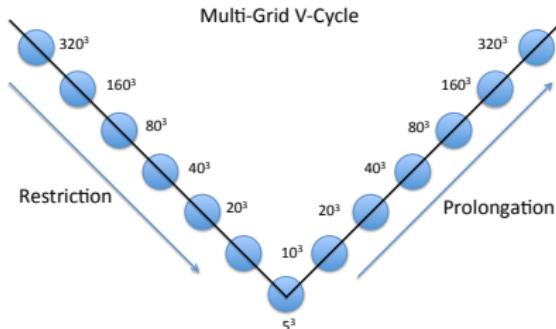
- Conceptually, we simply iterate until convergence.
- In practice, it converges very slowly - millions of iterations are required.

# Multi-Grid Methods to the Rescue - I



- Long wavelength modes are determined at the coarse grid.
- Iterations at each finer grid only need to be long enough to determine the short wavelength modes.

# Multi-Grid Methods to the Rescue - II

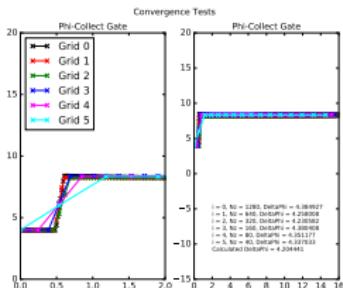


Finest Grid	Cells/Pixel	Grid Spacing	Time (laptop)
$160^3$	16	0.625 micron	60 sec.
$320^3$	32	0.3125 micron	8 min.
$640^3$	64	0.15625 micron	1 hr.

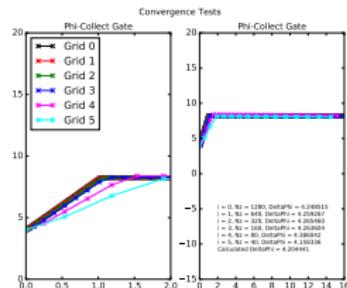
- Each successive step down is  $\approx 8$  times faster than the next larger grid.
- In practice, I use a coarsest grid of 4 grid cells per pixel, then 4X fewer iterations at each finer grid, ending with 64 iterations at the finest grid.

# Verifying Convergence

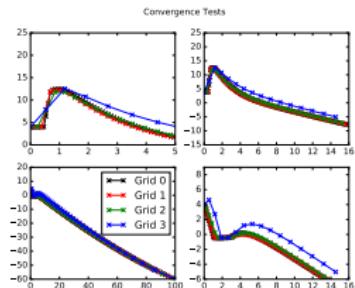
## Gate Capacitor



## Field Capacitor



## Single Pixel



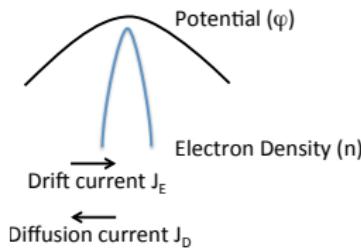
- The effective oxide thicknesses differ from what is requested due to finite grid resolution. The epsilon values on the coarser grids are adjusted to compensate for this error. This speeds convergence considerably and makes sure that the effective capacitance matches what it should be. These plots verify that the effective oxide thicknesses match what is requested within some error.

# Numerical Methods Mobile Carriers

# Using Quasi-Fermi Levels to Solve for Mobile Carrier Density

- In Quasi-Equilibrium:

$$J_E = q_e \mu_n n \frac{d\varphi}{dx} = -J_D = -q_e D_n \frac{dn}{dx} \quad (1)$$



$$\mu_n d\varphi = -D_n \frac{dn}{n} \quad (2)$$

$$\frac{\mu_n}{D_n} = \frac{q_e}{kT} \quad (\text{Einstein Relation}) \quad (3)$$

- So:

$$\frac{q_e \varphi}{kT} = \log(n) + C \quad (4)$$

$$n = n_i \exp\left(\frac{q_e(\varphi - \varphi_F)}{kT}\right) \quad (5)$$

$$\frac{kT}{q_e} \approx 15 \text{mV at } -100 \text{C}$$

- So we need to solve the following equation for  $\varphi$ :

$$\nabla^2 \varphi = \frac{1}{\epsilon_{Si}} (\rho_{\text{Fixed}} + q_e n_i \exp\left(\frac{q_e(\varphi - \varphi_F)}{kT}\right)) \quad (6)$$

## Solving Poisson's Equation on a Grid - II

$$\nabla^2 \varphi = \rho$$

$$\frac{\partial^2 \varphi_{i,j,k}}{\partial x^2} = \frac{(\varphi_{i+1,j,k} - \varphi_{i,j,k}) - (\varphi_{i,j,k} - \varphi_{i-1,j,k})}{h^2}$$

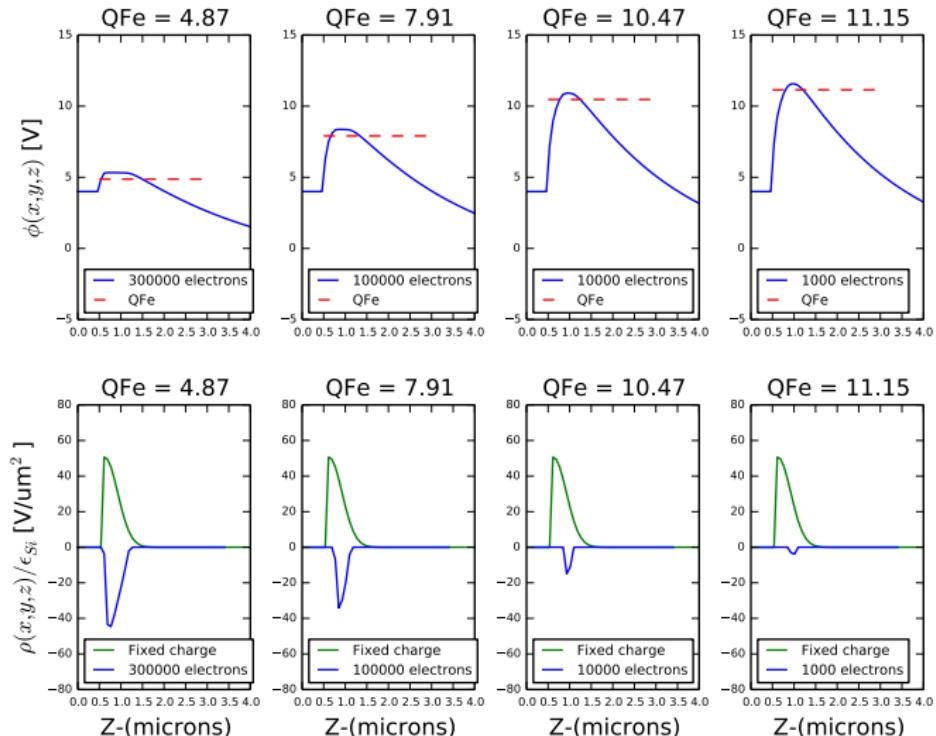
$$(\varphi_{i+1,j,k} + \varphi_{i-1,j,k} + \varphi_{i,j+1,k} + \varphi_{i,j-1,k} + \varphi_{i,j,k+1} + \varphi_{i,j,k-1} - 6 * \varphi_{i,j,k}) = h^2 * \rho_{i,j,k}$$

$$\varphi_{i,j,k}^{(n+1)} = \frac{1}{6} * (\varphi_{i+1,j,k}^{(n)} + \varphi_{i-1,j,k}^{(n)} + \varphi_{i,j+1,k}^{(n)} + \varphi_{i,j-1,k}^{(n)} + \varphi_{i,j,k+1}^{(n)} + \varphi_{i,j,k-1}^{(n)} - h^2 * \rho_{i,j,k})$$

$$\varphi^{(n+1)} = \frac{1}{6} * (\varphi_{pm}^{(n)} - h^2 * \rho_f - h^2 K \exp(\frac{q_e(\varphi^{(n+1)} - \varphi_F)}{kT}))$$

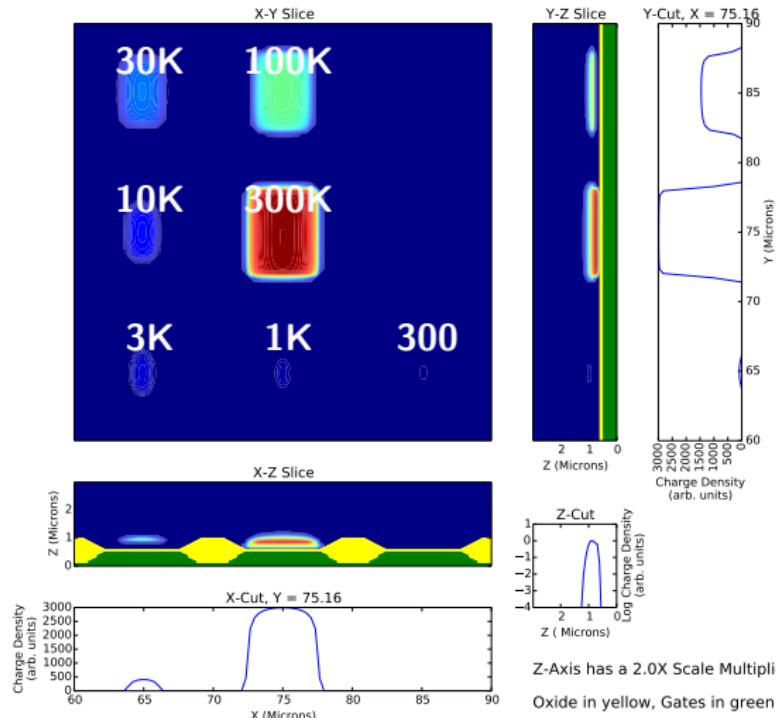
- We take this last equation as a non-linear equation for  $\varphi^{(n+1)}$  and run a Newton's method "inner loop" at each grid point.
- Then we iterate to convergence as before.
- This allows us to simultaneously solve for the potential and the carrier density.
- Similar equation for holes, but with opposite signs.

# 1D Profiles as QFe is varied



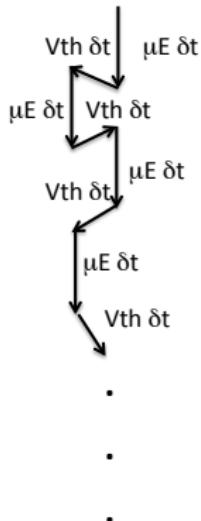
# Electron Density as QFe is varied

## Electron Charge Distribution



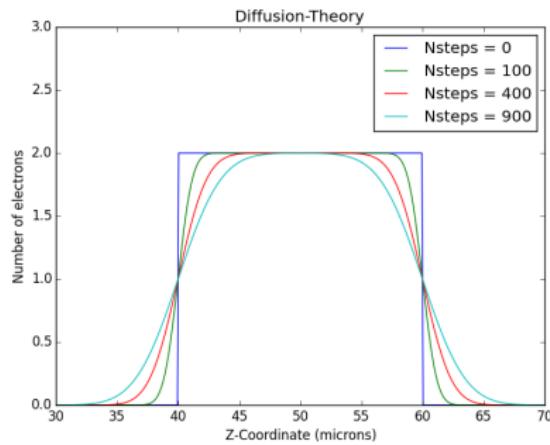
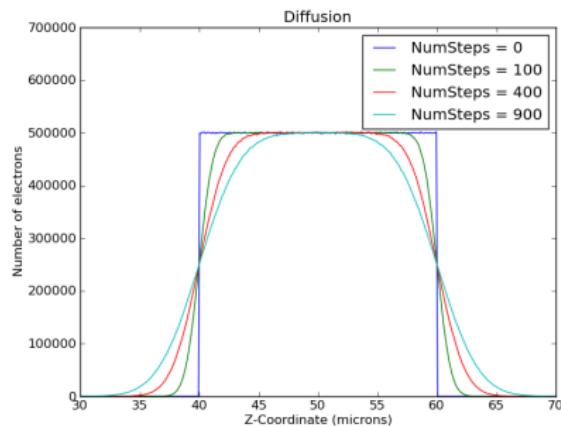
# Numerical Methods Electron Diffusion and Tracking

# Diffusion Model



- Mobility:  $\mu(E, T)$  calculated from Jacobini model
- $\mu = 1584 \frac{\text{cm}^2}{\text{V}\cdot\text{sec}}$  at  $E = 6000 \frac{\text{V}}{\text{cm}}$
- Collision time:
  - $\tau = \frac{m_e^*}{q_e} \mu$
  - $\tau$  typically about 0.9 ps.
- $\delta t$  drawn from exponential distribution with mean of  $\tau$
- $V_{th} = \sqrt{\frac{3kT}{2m_e^*}}$
- $V_{th} \approx \mu E$
- Each thermal step in a random direction in 3 dimensions.
- Typically about 1000 steps to propagate to the collecting well.

# Diffusion Model Check-out - Step Function

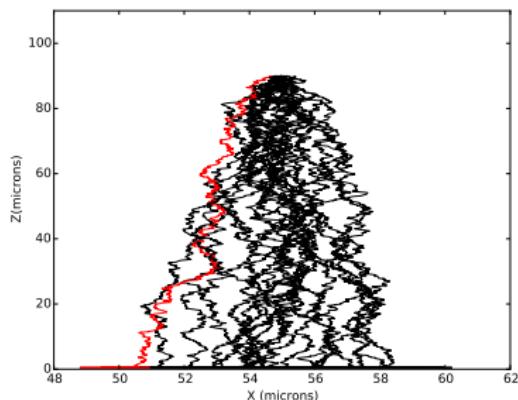


$10^8$  electrons in initial step function  
- no E-field.

$$\text{erf}\left(\frac{x-x_1}{\sqrt{4D\tau N_{\text{steps}}}}\right) - \text{erf}\left(\frac{x-x_2}{\sqrt{4D\tau N_{\text{steps}}}}\right)$$
$$D = \frac{kT}{q} \mu$$

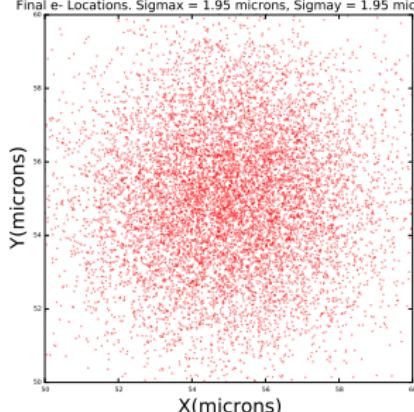
# Diffusion Model Check-out - Small (0.1 micron) Spot

Electron Path Plot - Vertical Zoom = 0.1



Electron Paths

CCD Pixel Plots. Grid = 320\*320\*320.  
Final e- Locations. Sigmmax = 1.95 microns, Sigmay = 1.95 microns

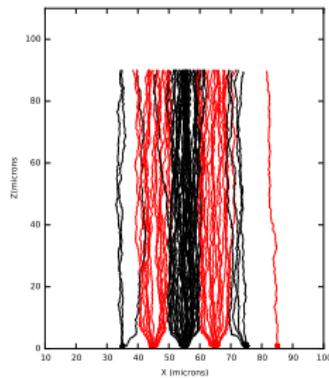
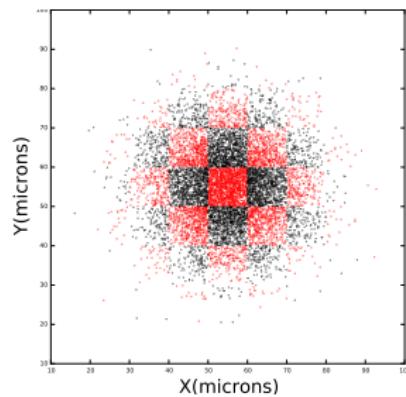
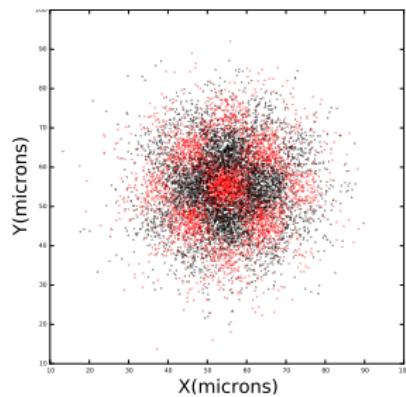


Spot size at collection.

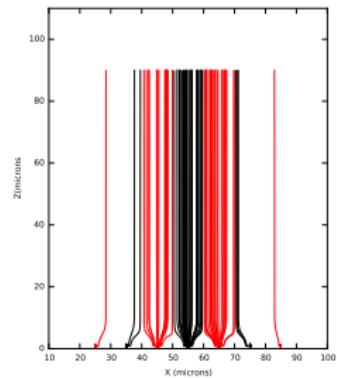
$$\sigma = \sqrt{2 * D * T_{\text{transit}}} = \sqrt{2 * \frac{kT}{q} \mu * \frac{T_{\text{Si}}^2}{\mu V}} = T_{\text{Si}} \sqrt{\frac{2 \frac{kT}{q}}{V}} = 1.95 \mu$$

FWHM = 4.6 microns, in agreement with Fe measurements.

# Impact of electron diffusion



Theoretical Diffusion



Diffusion turned off

# Numerical Methods

## Electron Methods

# Electron Methods

- Quasi-Fermi level works well, and it is clearly the right way to calculate the hole density, since we know the potential in the hole region.
- It is more problematic for calculating the electrons. We know the Quasi-Fermi level is constant, but we don't know its value. Setting the Q-F level to give the right number of electrons is an iterative process that takes a lot of time.
- New procedure is to require the Q-F level to be constant in each well, but not to explicitly know its value. If we add the constraint that electrons in each well are conserved, we can use the Q-F equations to move electrons around until the Q-F level is constant.
- This is faster in several ways. It removes the need to iterate to find the Q-F value, and it reduces the steps required when tracking electrons. We only need to know which well they are in, then use the above procedure to find their equilibrium position.
- The code is working, and the results are basically the same as the old (see the following slides). All three methods are now in the Poisson\_CCD code.

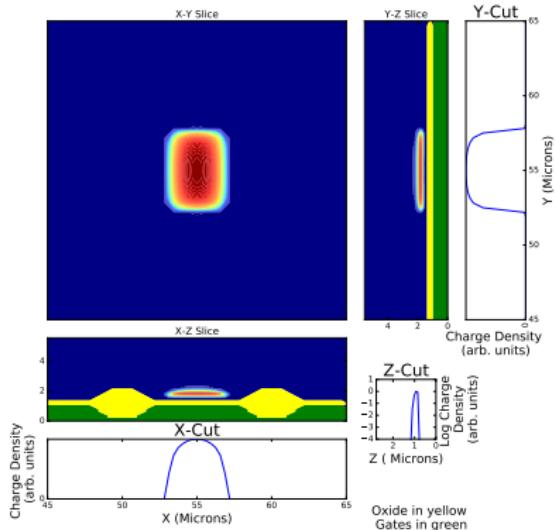
# Three Different Methods for Electron Density

Hole Density is always calculated by fixing the Quasi-Fermi level, but there are three different methods for calculating the electron density.

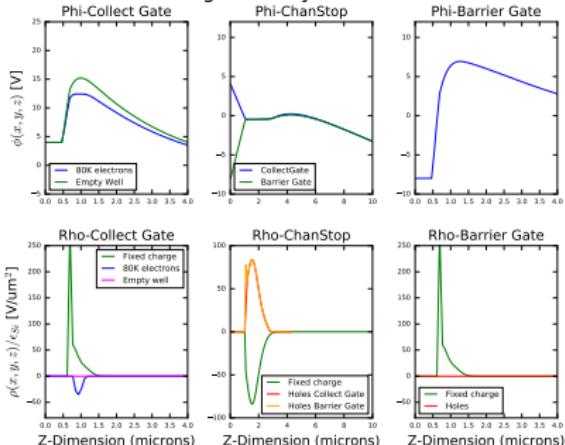
Electron Tracking	Fix QFe	Move e-
ElectronMethod = 0	ElectronMethod = 1	ElectronMethod = 2
Track e- to a final location	Set a value for QFe	Move e- to keep QFe constant. Exact QFe value not known
Pros:	Pros:	Pros:
Conceptually simple.	Most accurate. Best for large e- count	Most accurate. Best for small e- count
Cons:	Cons:	Cons:
Slowest Electrons not re-equilibrated	Slow Must iterate to find QFe	Large e- count can “leak out”

# Old (QFe) approach. One well with 80K e-.

Electron Charge Distribution

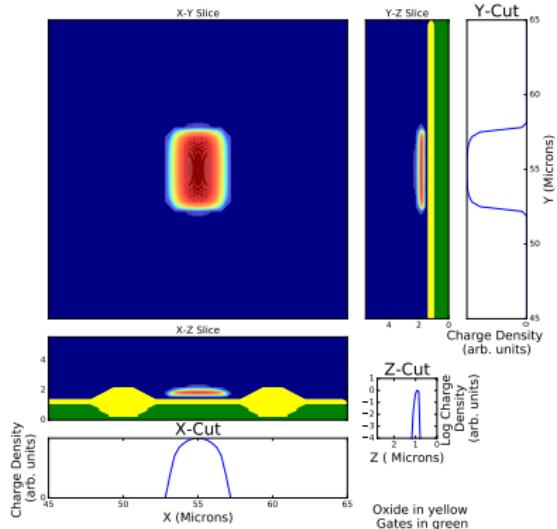


1D Potential and Charge Density Slices. Grid = 320\*320\*320.

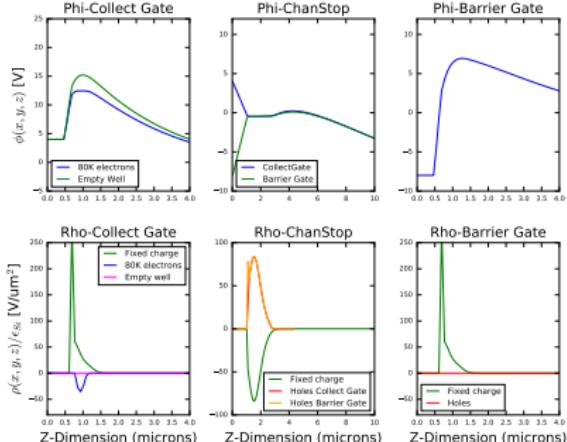


# New (Move e-) approach. One well with 80K e-.

Electron Charge Distribution

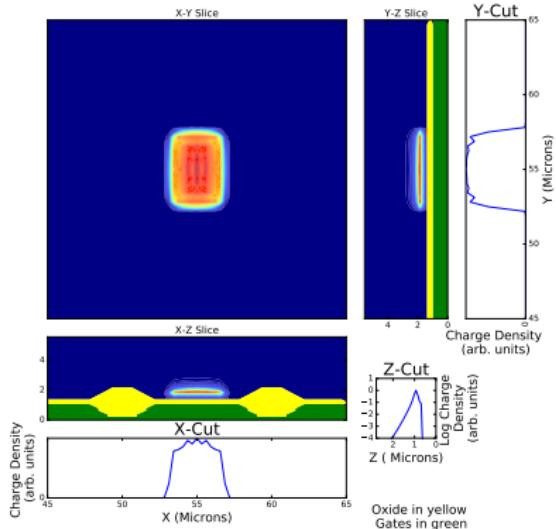


1D Potential and Charge Density Slices. Grid = 320\*320\*320.

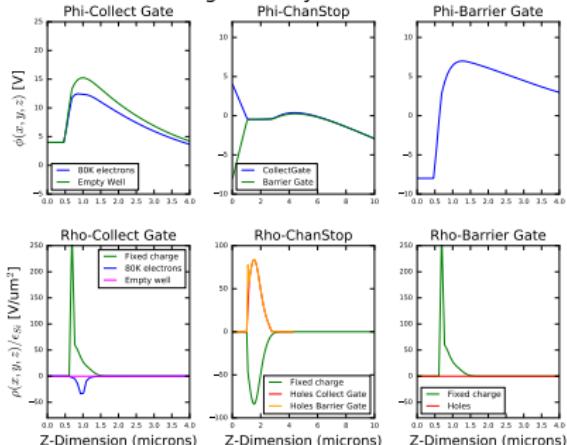


# Older (electron tracking) approach

## Electron Charge Distribution



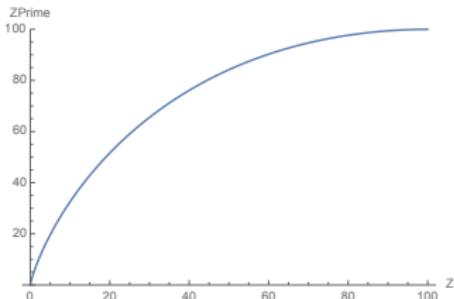
1D Potential and Charge Density Slices. Grid = 320\*320\*320.



# Numerical Methods

## Non-Linear Z-Axis

# “Stretched” Z-Axis



- $zp(z)$ :

$$zp = -T_{Si} * (NZExp - 1.0) * (z/T_{Si})^{(NZExp+1.0)/NZExp} + NZExp * z; \quad (7)$$

- $NZExp = 10$ : Slope = 10 at  $z = 0$ ; Slope = 1/10 at  $z = 100$ .

- Linear:

$$\nabla^2 \varphi = \frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} + \frac{\partial^2 \varphi}{\partial z^2} \quad (8)$$

- Non-Linear:

$$\nabla^2 \varphi = \frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} + \frac{\partial^2 \varphi}{\partial z^2} \left( \frac{\partial z'}{\partial z} \right)^2 + \frac{\partial \varphi}{\partial z'} \frac{\partial^2 z'}{\partial z^2} \quad (9)$$

- The added partial derivatives can be pre-computed.

## Summary

- The Poisson\_CCD simulation tool is useful for simulating many different aspects of the CCD.
- The code has been validated with a variety of measurements.
- All of the plots shown here were run with the 'hole20' branch of Poisson\_CCD22 at  
[https://github.com/craiglagegit/Poisson\\_CCD22](https://github.com/craiglagegit/Poisson_CCD22)