
https://indico.in2p3.fr/e/simdet2023

SIMDET 2023

5th school on silicon detectors simulation

Use of Silvaco in HEP experiments

M. Bomben, APC & UPD - Paris

Université Paris Cité

cnrs IN2P3 Les deux infinis

Outline

- Silvaco TCAD tool
- Example: edgeless detectors
- From TCAD to Monte Carlo simulations
- Victory - From layout files to full 3D simulation
- Conclusion & Outlook

SILVACO TCAD TOOL

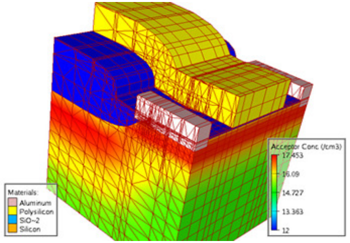
TCAD simulations

- Technology Computer Aided Design - TCAD
- Solve drift/diffusion & Poisson equations for electrons and holes:

$$\frac{\partial n}{\partial t} = \frac{1}{q}\frac{\partial J_n}{\partial x} + G_n - R_n \ ; \ J_n = qn\mu_n E + qD_n\frac{\partial n}{\partial x}$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q}\frac{\partial J_p}{\partial x} + G_p - R_p \ ; \ J_p = qn\mu_p E - qD_p\frac{\partial p}{\partial x}$$

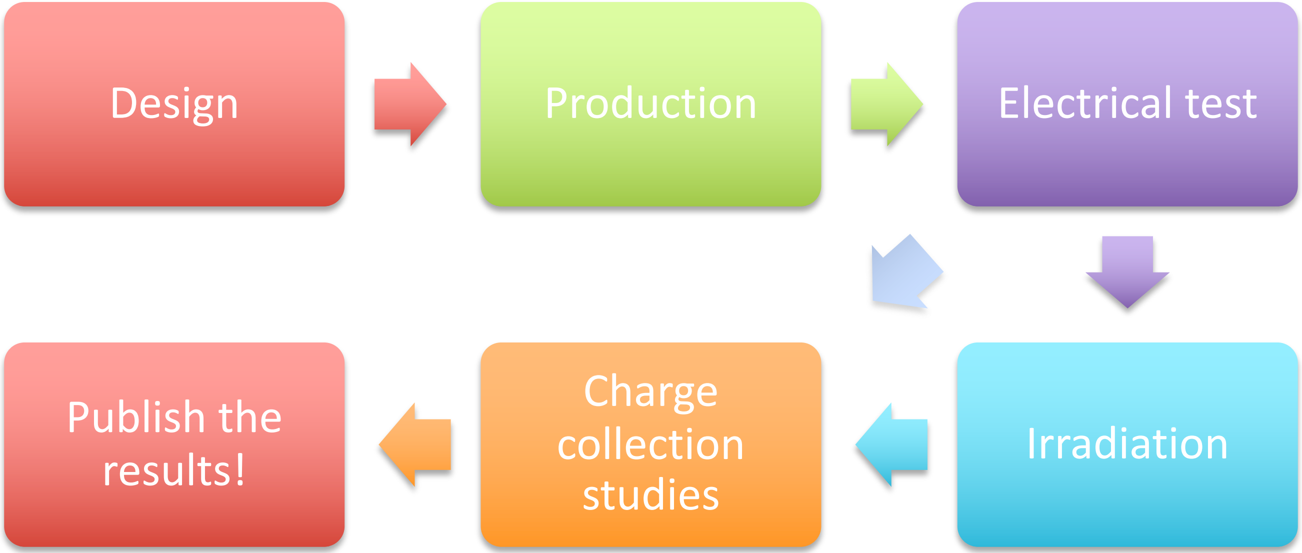
$$\frac{\partial^2\psi}{\partial x^2} = -\frac{q}{\epsilon_{Si}\epsilon_0}(N_D + p(x) - n(x) - N_A)$$



- taking into account boundary conditions
  - Electrodes’ potentials, interface charges, etc
- on a grid of points

SILVACO

Normal work flow for a HEP silicon sensors



Design

Production

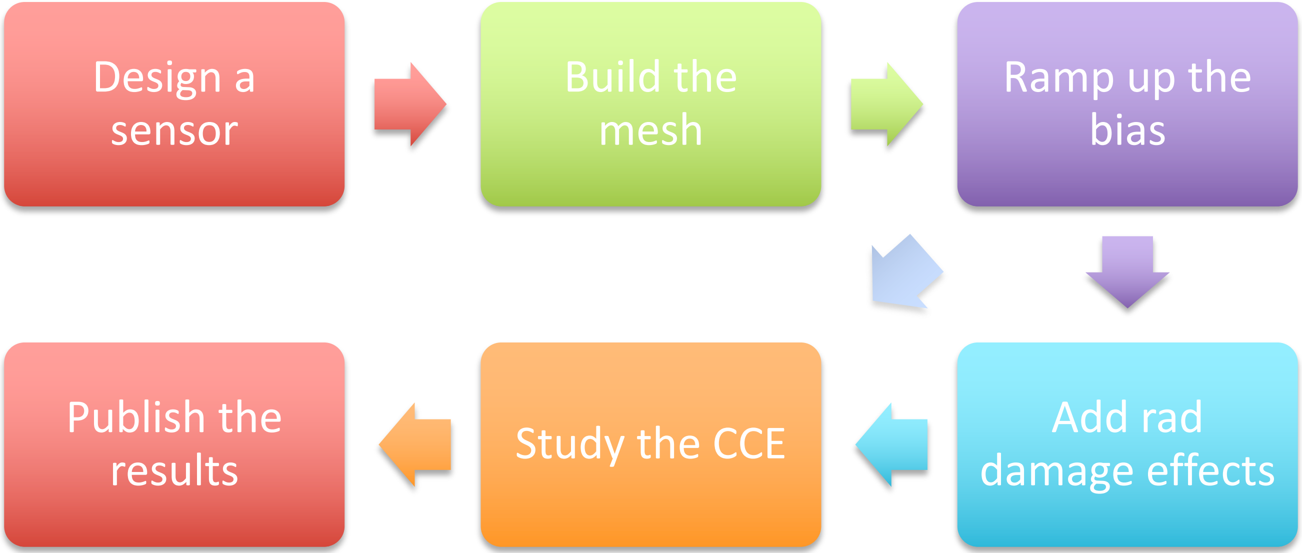
Electrical test

Irradiation

Charge collection studies

Publish the results!

TCAD simulation work flow



Design a sensor

Build the mesh

Ramp up the bias

Add rad damage effects

Study the CCE

Publish the results

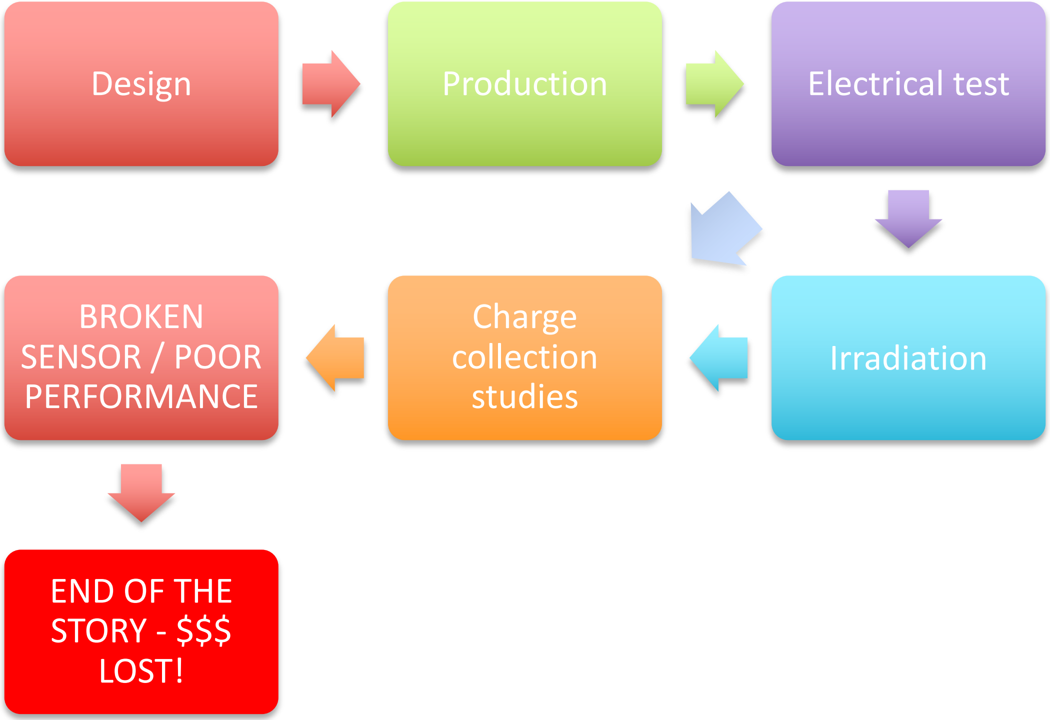
So why bother with simulations?

- You repeat all the “steps” of real sensors…

So why bother with simulations?

- You repeat all the “steps” of real sensors…
- It is not true!

Possible work flow for real sensors



Design

Production

Electrical test

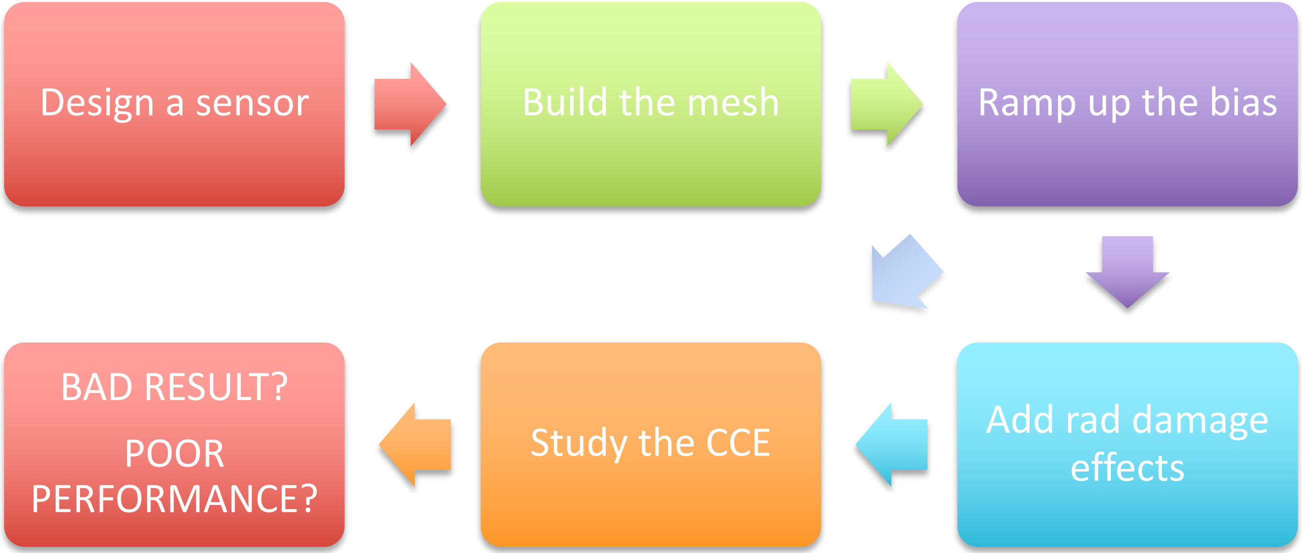
Irradiation

Charge collection studies

BROKEN SENSOR / POOR PERFORMANCE

END OF THE STORY - $$$ LOST!

TCAD simulation work flow



Design a sensor

Build the mesh

Ramp up the bias

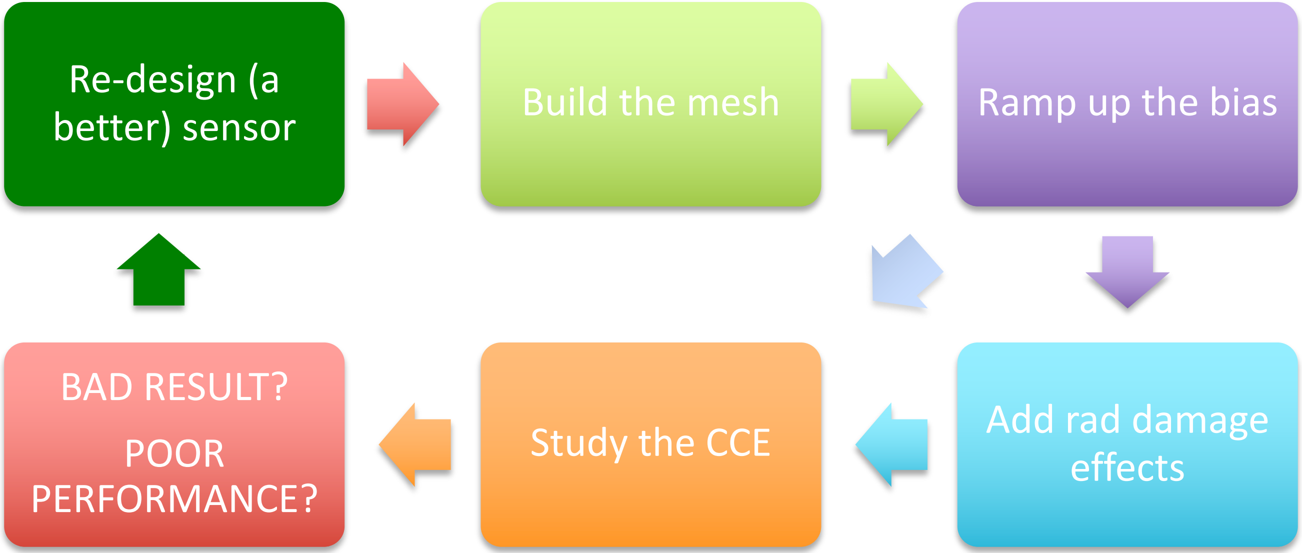
Add rad damage effects

Study the CCE

BAD RESULT?

POOR PERFORMANCE?

TCAD simulation work flow



Re-design (a better) sensor

Build the mesh

Ramp up the bias

Add rad damage effects

Study the CCE

BAD RESULT?

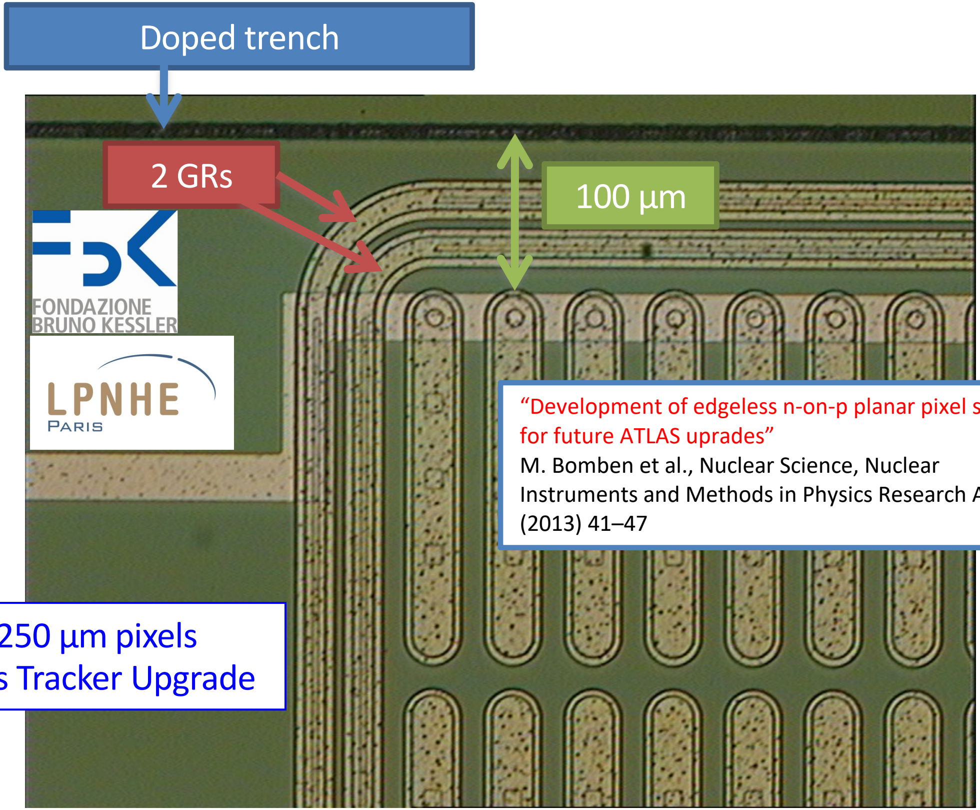
POOR PERFORMANCE?

Simulations benefits

- Simulating sensors helps in saving:
- ➢ Development time
- ➢ Number of submissions
- ➢ Money
- You can learn a lot in terms of:
- ❑ Physics
  - Study quantities otherwise not accessible!
  - Examples:
    - Carrier distribution
    - Electric field distribution
    - Current densities
    - Etc....

EXAMPLE: EDGELESS DETECTORS

Edgeless pixel detector

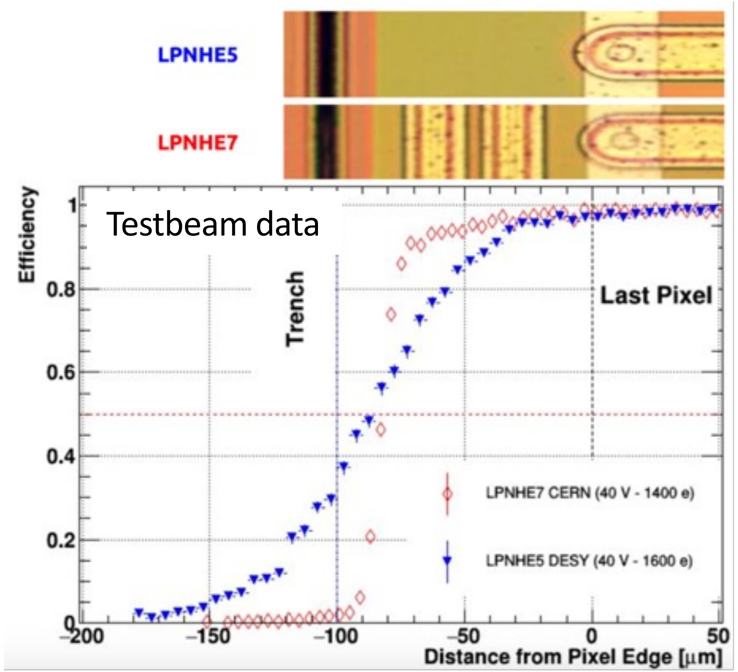


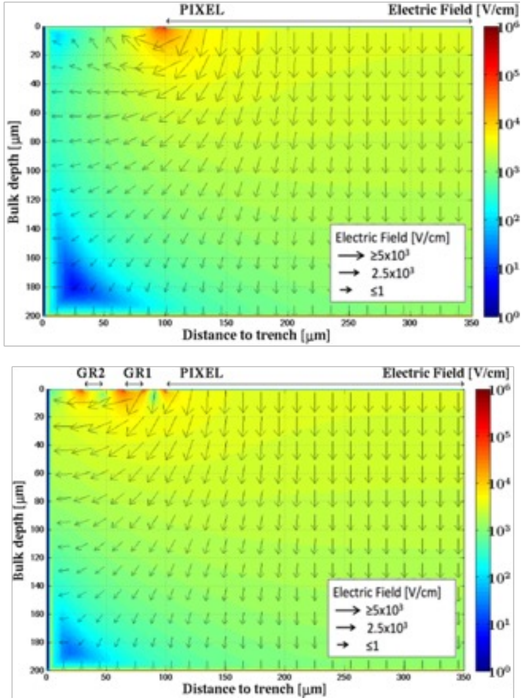
“Development of edgeless n-on-p planar pixel sensors for future ATLAS uprades”
M. Bomben et al., Nuclear Science, Nuclear Instruments and Methods in Physics Research A 712 (2013) 41–47

50 µm x 250 µm pixels
R&D for Atlas Tracker Upgrade

Hit efficiency at sensor edge

JINST 12 P05006 (2017)

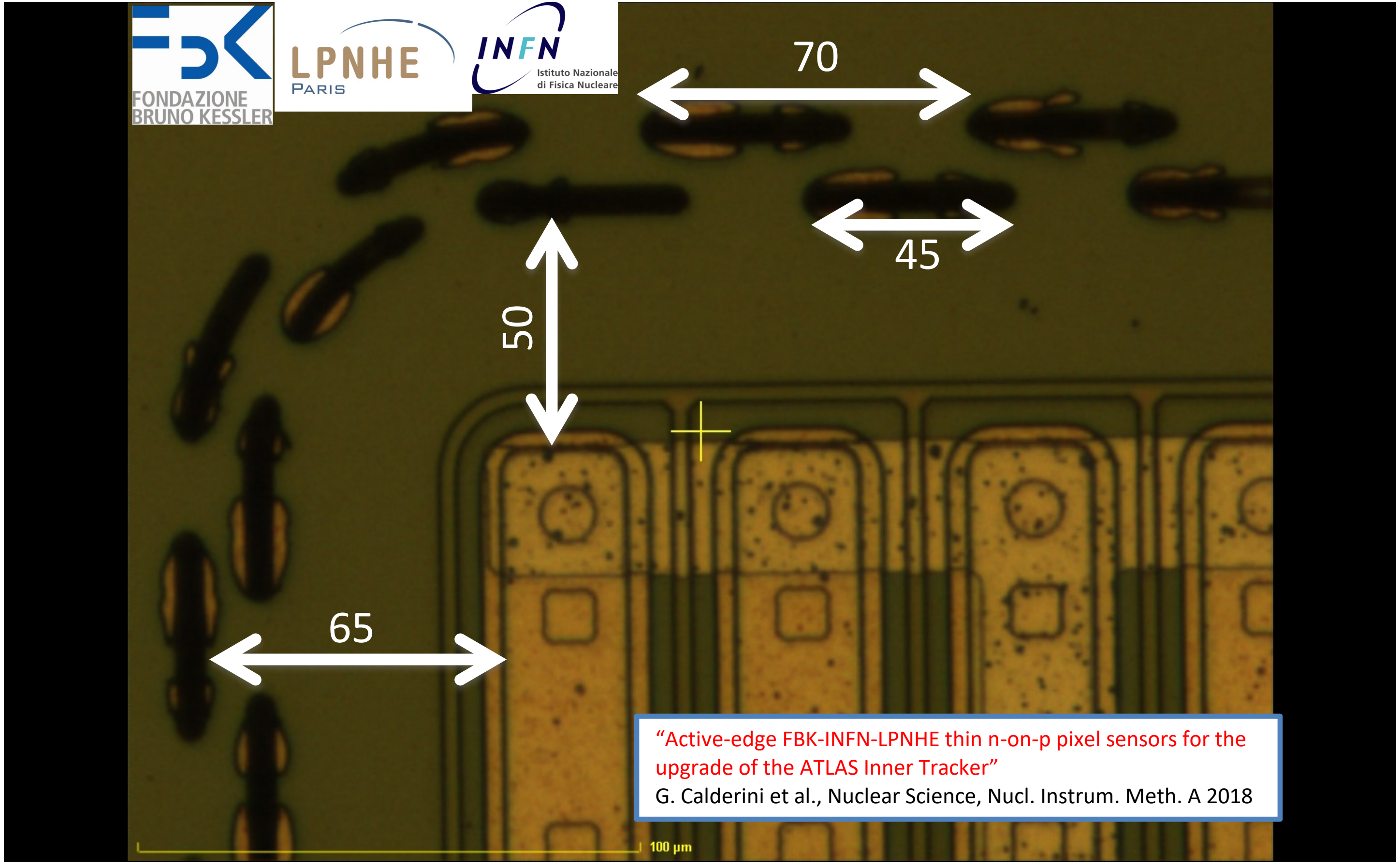




Pixel detector efficient beyond pixels area: > 80% up to 75 µm away from the last one

Reason: electric field lines closing on pixels and not on GRs!

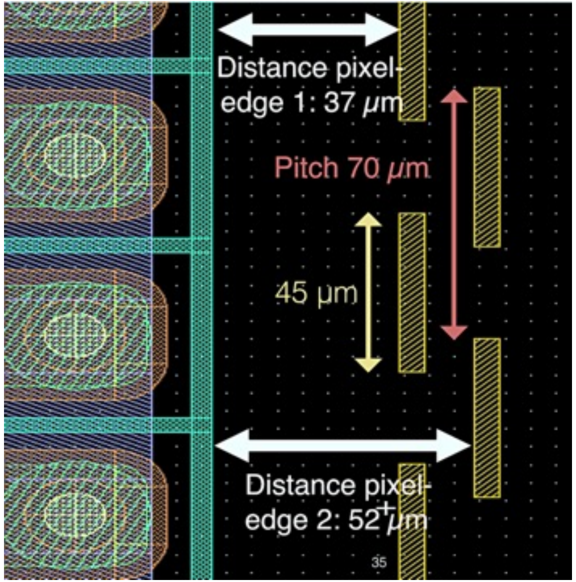
Novative edgeless production – staggered trenches

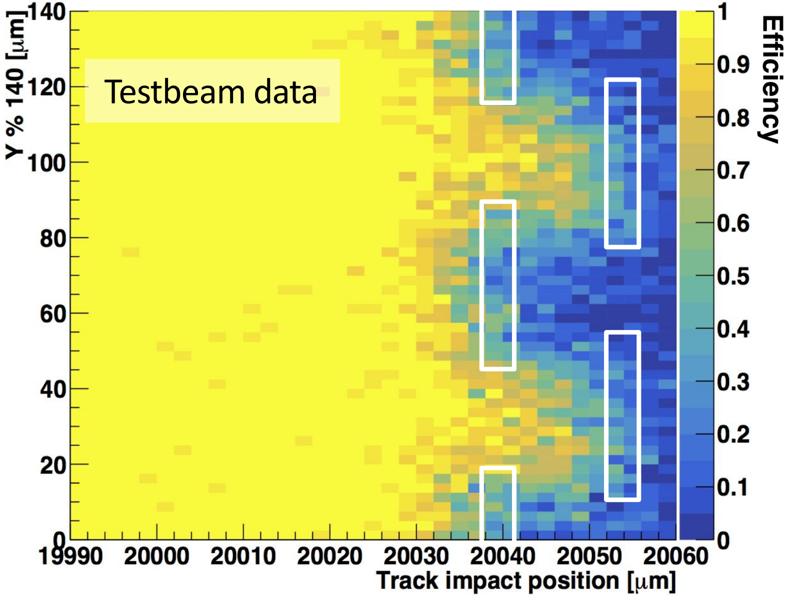


“Active-edge FBK-INFN-LPNHE thin n-on-p pixel sensors for the upgrade of the ATLAS Inner Tracker”
G. Calderini et al., Nuclear Science, Nucl. Instrum. Meth. A 2018

Hit efficiency at sensor edge

A. Ducourthial thesis
https://indico.in2p3.fr/e/18186/





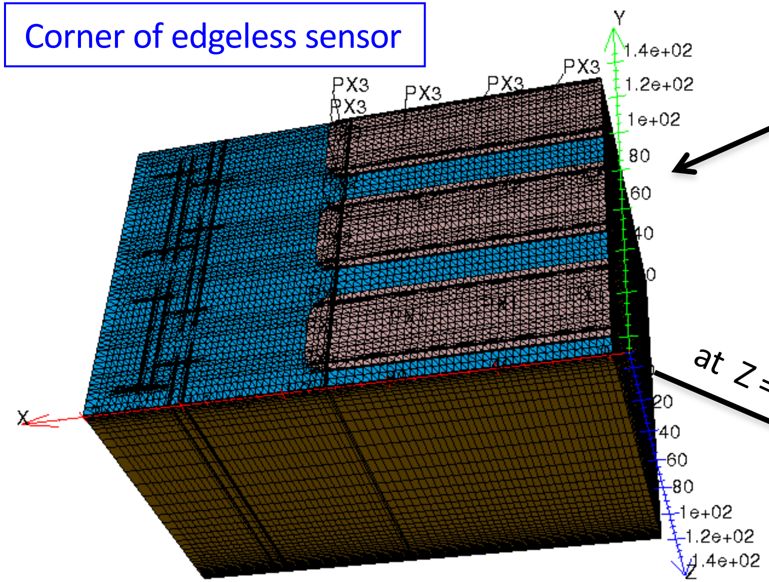
130 µm thick sensor with staggered trenches, no GRs, ~50 µm last pixel to last edge

The efficiency follows the edge pattern

The efficiency is higher than 50% up to 44 µm from the last pixel

Simulations in 3D

Corner of edgeless sensor



13439 points
26517 triangles

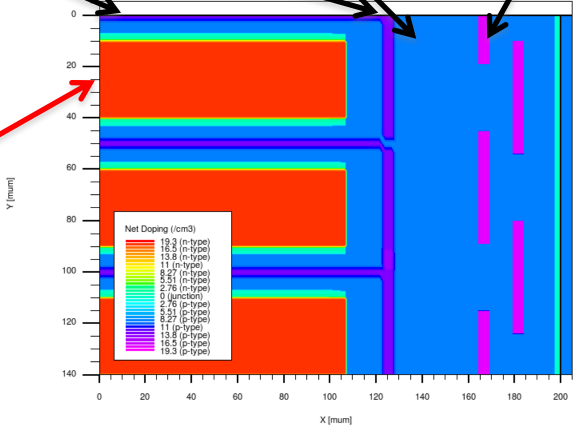
at Z = 0.2 µm

p-stop

p-spray

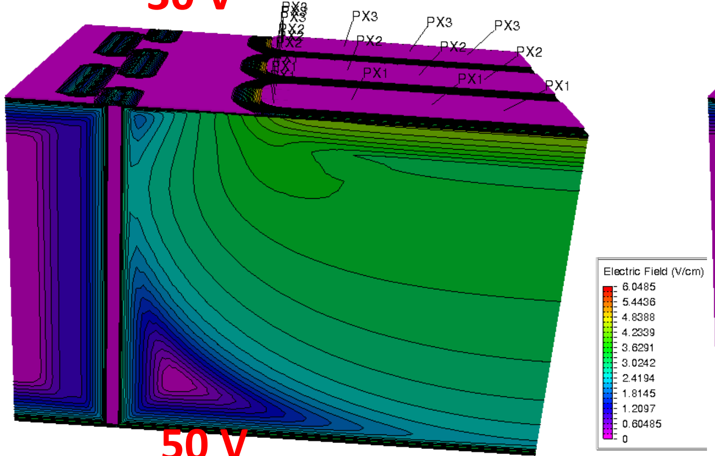
trenches

n$^+$ implant

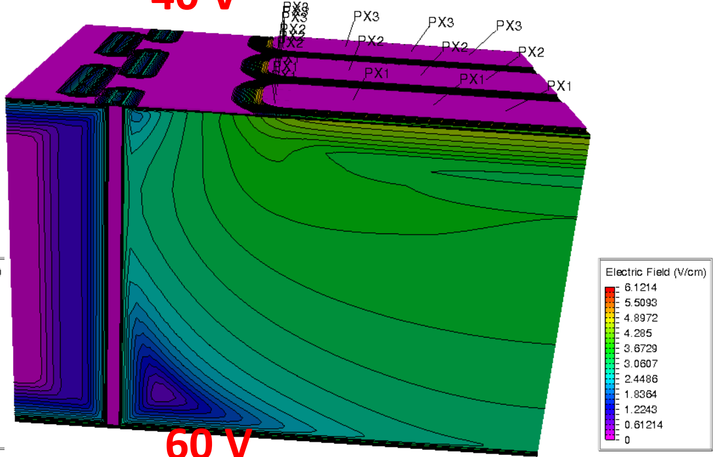


Electric field at sensor edge

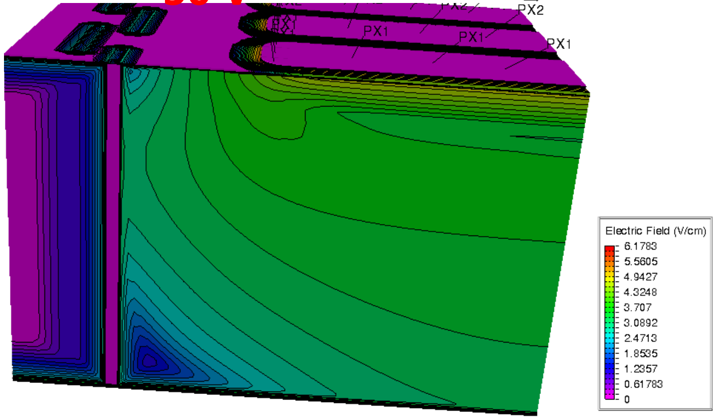
30 V



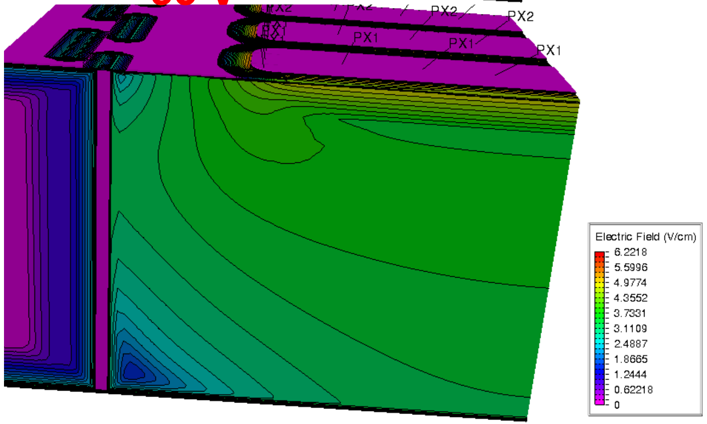
40 V



50 V



60 V

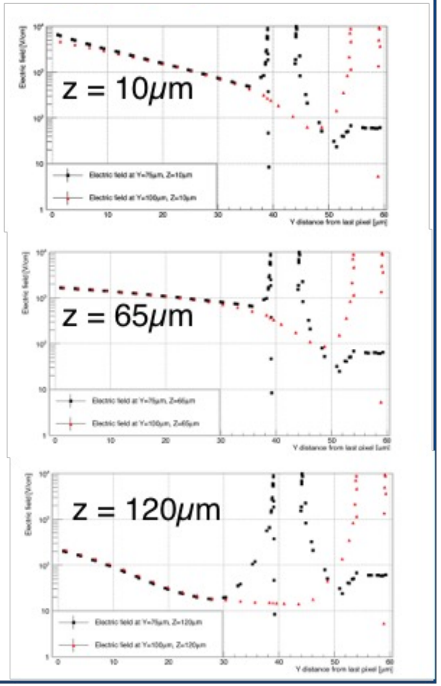


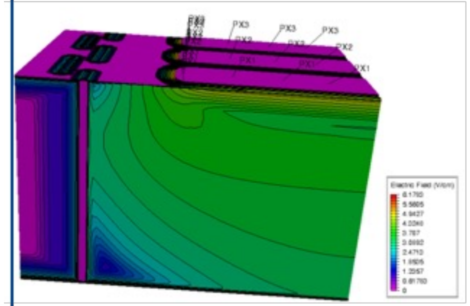
Hit efficiency at sensor edge - projections

TCAD Simulations - Electric field

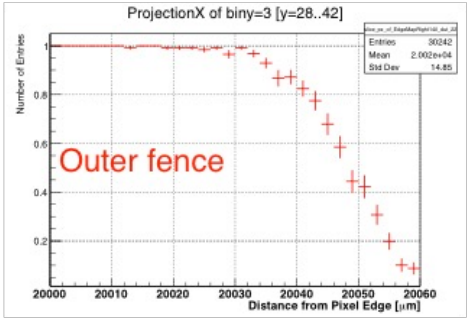
Simulation of the electric field for several depth z in the sensor:

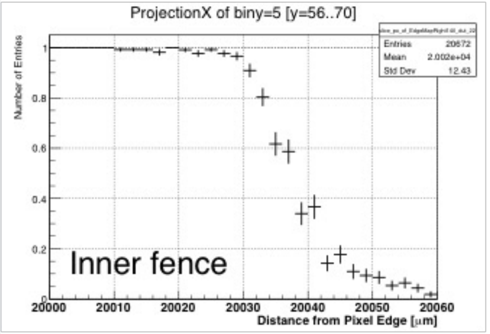
- E drops at 0 when at edge position
- low E in the bottom corner close to the edge.





Edge Efficiency



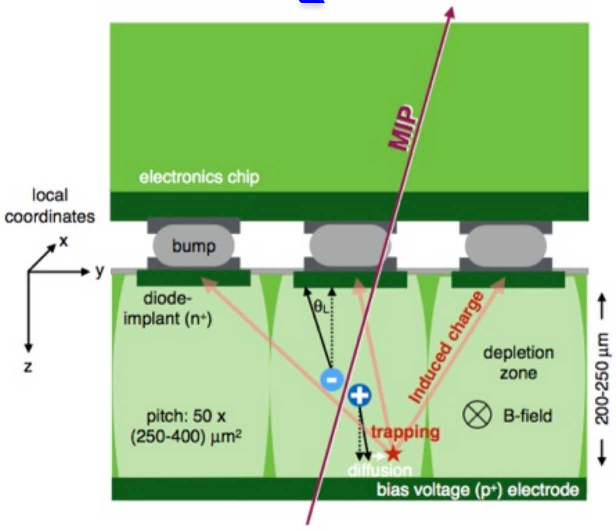


Efficiency drop matches the Electric field drop in the vicinity of the edge

FROM TCAD TO MONTE CARLO SIMULATIONS… AND BACK TO TCAD

Radiation damage effects in ATLAS MC sim.

Include all this in ATLAS MonteCarlo ✅



Digitization happens after simulated charge deposition and before space point reconstruction

JINST **14** P06012

Charge carriers will drift toward the collecting electrode due to **electric field**, which is deformed by **radiation damage**.

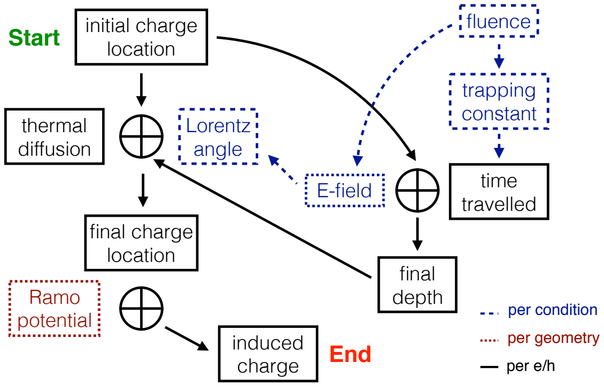
Their path will be deflected by magnetic field (**Lorentz angle**) and **diffusion**.

Due to **radiation damage** they can be **trapped** and induce/screen a fraction of their charge (**Ramo potential**).

Total induced charge is then digitized and clustered.

Implementation

As many quantities as possible are precalculated

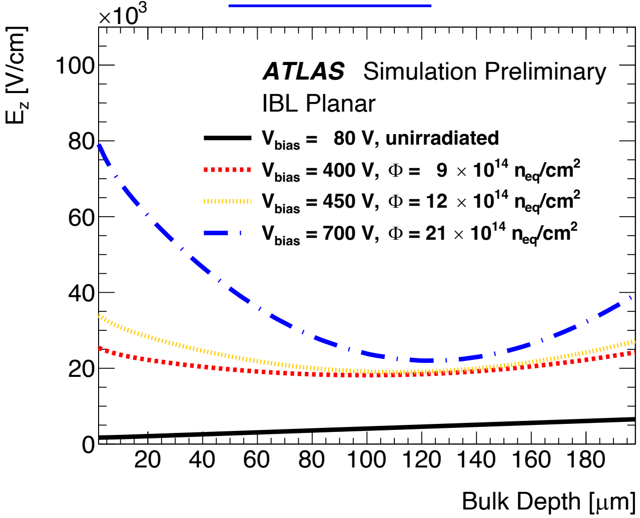


Now default in ATLAS MC!

Ingredients – TCAD simulations

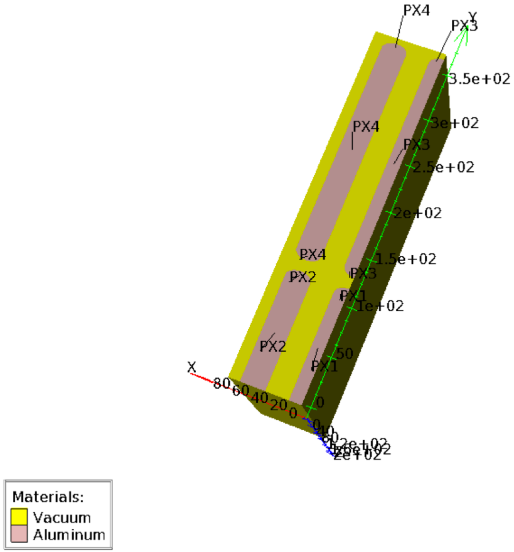
From fluence level
the electric field is evaluated
using TCAD tools

PIX-2023-006

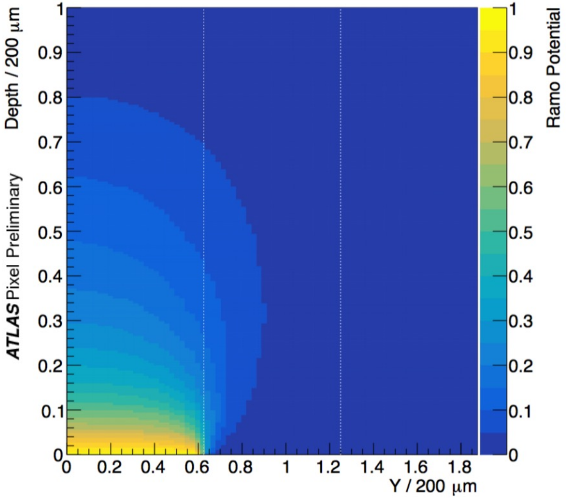


"Chiochia" model – NIM A 568 (2006)

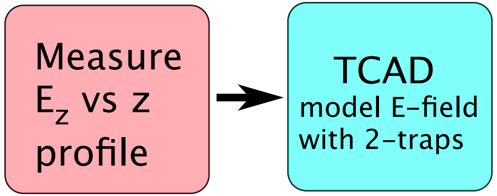
Ramo
potential
from
TCAD too



Ramo map:
projection



Radiation damage in TCAD simulations



Measure E_z vs z profile → TCAD model E-field with 2-traps

I. Pintilie (VERTEX 2016)

- Numerically impossible to simulate all measured defects
  - Plus: their properties are not all well known
  - Plus: there might be more defects to be identified

➢ **Instead use few (2-5) effective states**

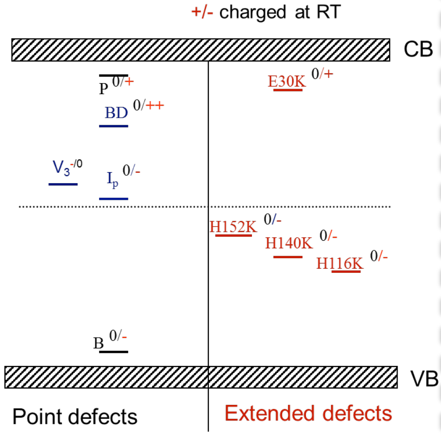
Measured defects

Point defects

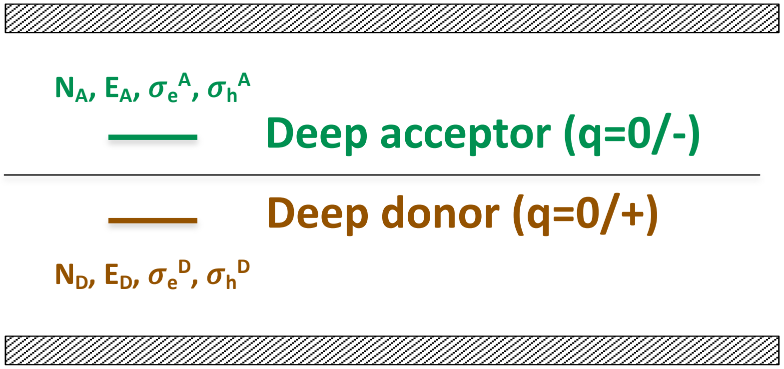
- $E_a^{BD} = E_c - 0.225$ eV
- $\sigma_n^{BD} = 2.3 \cdot 10^{-14}$ cm^2
- $E_a^{V3} = E_c - 0.545$ eV
  - ☐ $\sigma_n^{V3} = 1.7 \cdot 10^{-15}$ cm^2
  - ☐ $\sigma p^{V3} = 9 \cdot 10^{-14}$ cm^2
- $E_a^{Ip} = E_c - 0.545$ eV
  - ☐ $\sigma_n^{Ip} = 1.7 \cdot 10^{-15}$ cm^2
  - ☐ $\sigma p^{Ip} = 9 \cdot 10^{-14}$ cm^2

Extended defects

- ➢ $E_a^{H116K} = E_v + 0.33$eV
- ➢ $\sigma_p^{H116K} = 4 \cdot 10^{-14}$ cm^2
- ➢ $E_a^{H140K} = E_v + 0.36$eV
- ➢ $\sigma_p^{H140K} = 2.5 \cdot 10^{-15}$ cm^2
- ➢ $E_a^{H152K} = E_v + 0.42$eV
- ➢ $\sigma_p^{H152K} = 2.3 \cdot 10^{-14}$ cm^2
- ➢ $E_a^{E30K} = E_c - 0.1$eV
- ➢ $\sigma_n^{E30K} = 2.3 \cdot 10^{-14}$ cm^2



Simulated effective defects in TCAD



$N_A, E_A, \sigma_e^A, \sigma_h^A$

Deep acceptor (q=0/-)

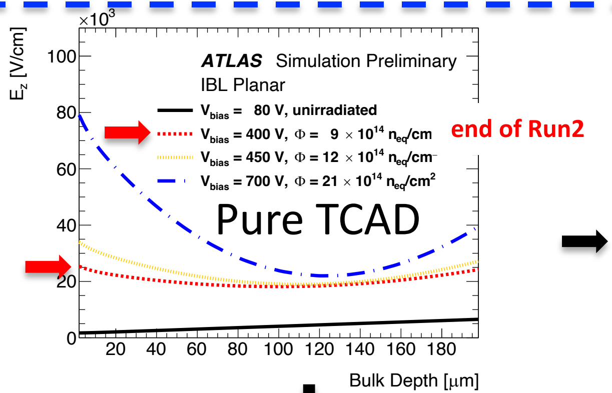
Deep donor (q=0/+)

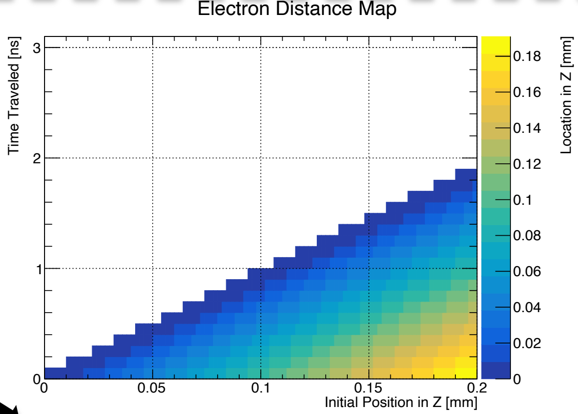
$N_D, E_D, \sigma_e^D, \sigma_h^D$

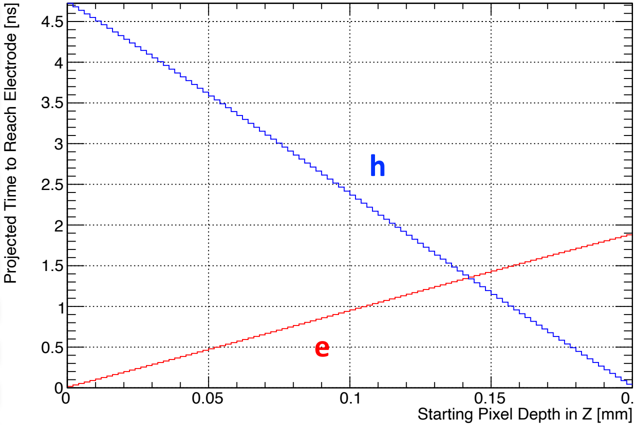
EVL (2002)

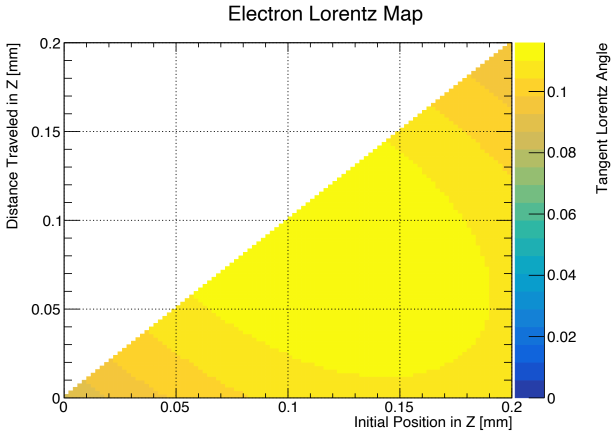
V. Chiochia et al. (2005)

What do we do with TCAD simulation?

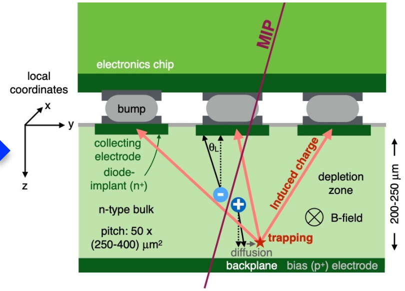


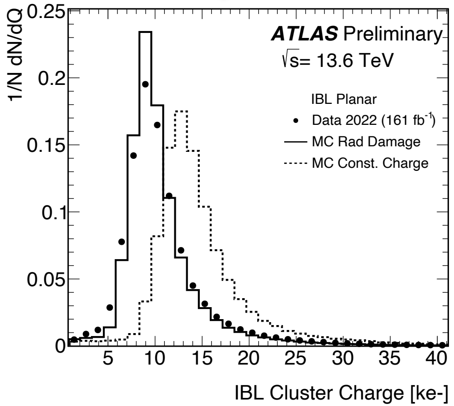






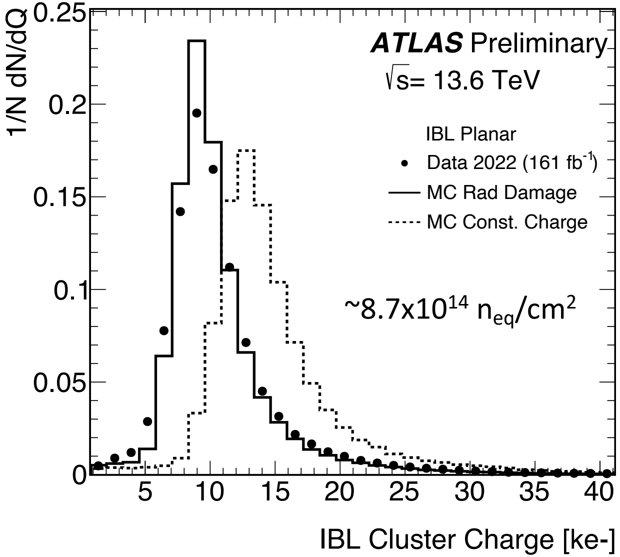
Rad. Damage Digi



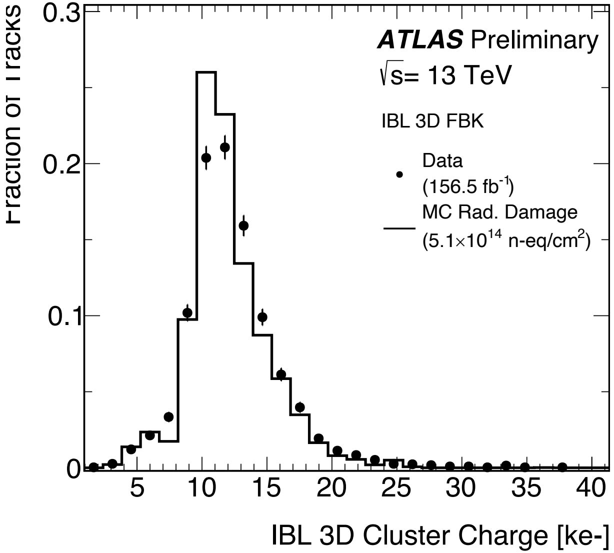


Run3 data vs MonteCarlo

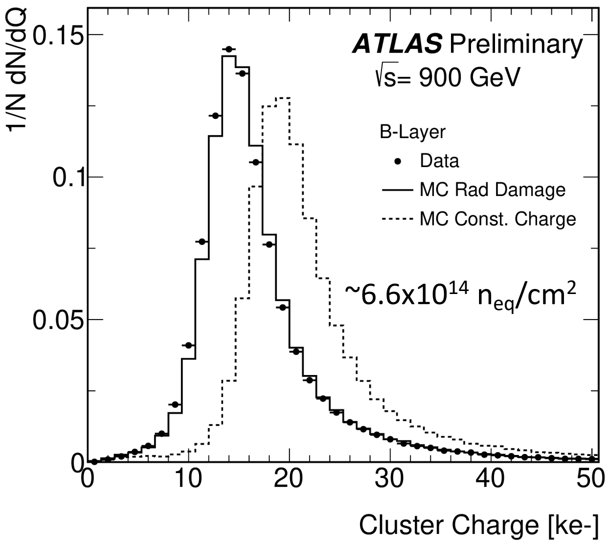
ATL-COM-INDET-2022-027



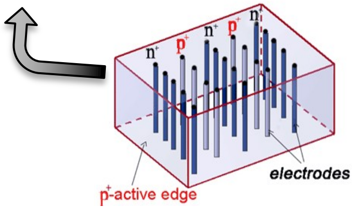
ATL-COM-INDET-2023-011



ATL-PHYS-PUB-2022-033

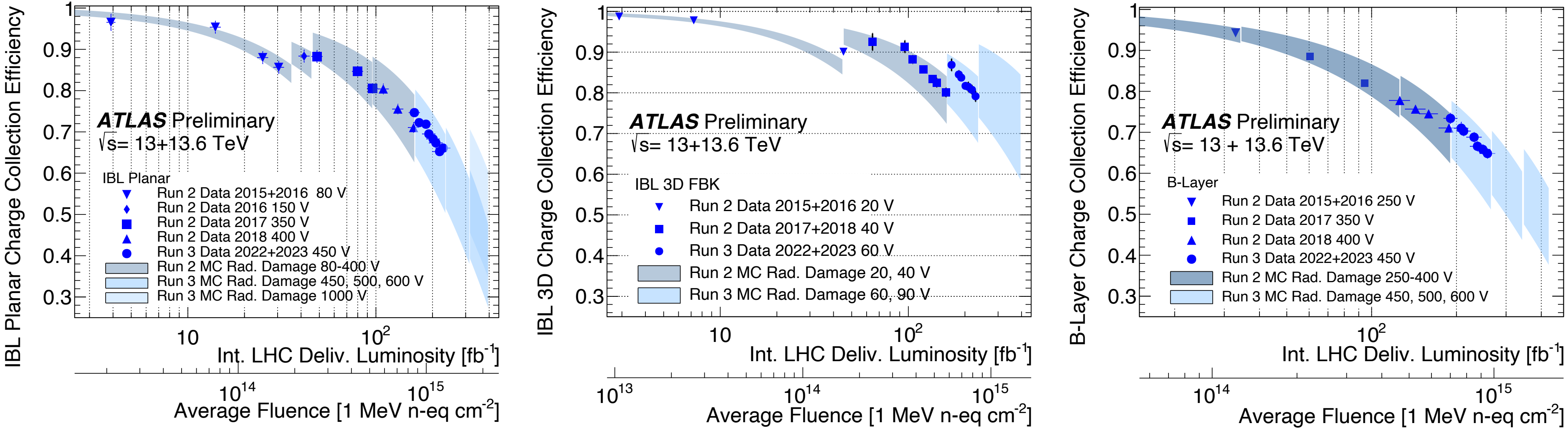


Most Probable Values match at 1 % level



Charge collection efficiency vs luminosity

ATL-COM-INDET-2023-008



- ✓ **Excellent agreement over almost two order of magnitudes of fluence**
- ✓ Predictions indicate enough charge till the end of Run3
- ✓ Nice agreement for 3D sensors too!
- ➢ *N.B. different material, device and radiation damage model (Folkestad et al., NIM A (2017))*

Once the modeling validated…

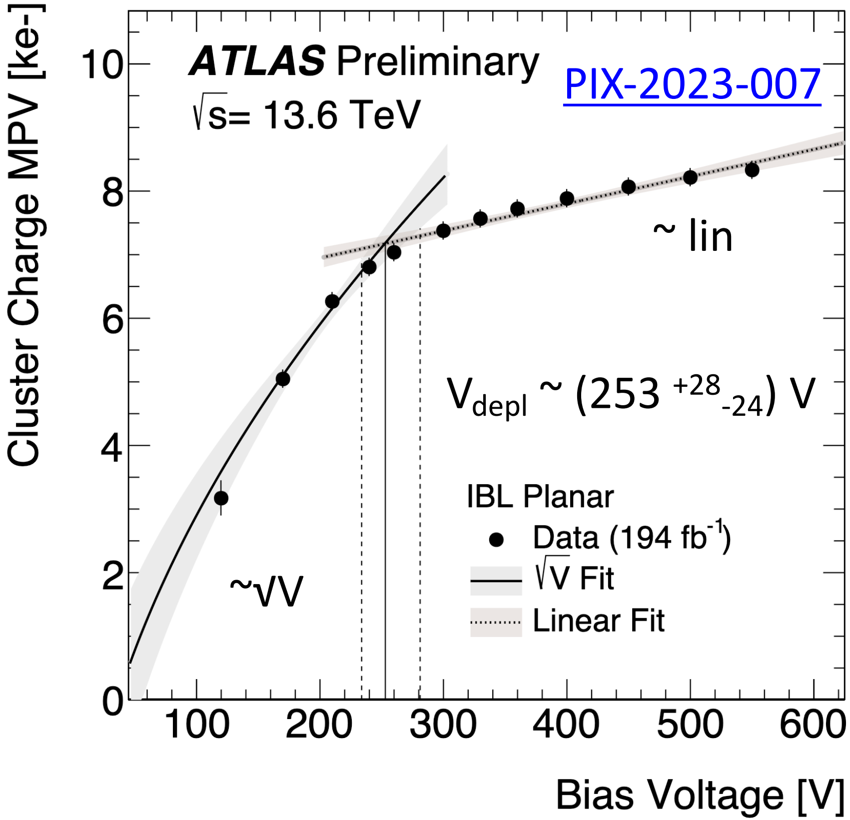
- We can make predictions
  - and of course we do!

➢ **but we also get insight into observables otherwise difficult/impossible to access**

- In the following I will focus on ’’depletion voltage’’ and use TCAD results to try to shed light on the Q vs V dependence and indeed on ’’V_{depl}’’

- All results for a n-in-n planar pixel 200 µm thick at 1.0×10^{15} n_{eq}/cm^2 (end 2022)

Q vs V

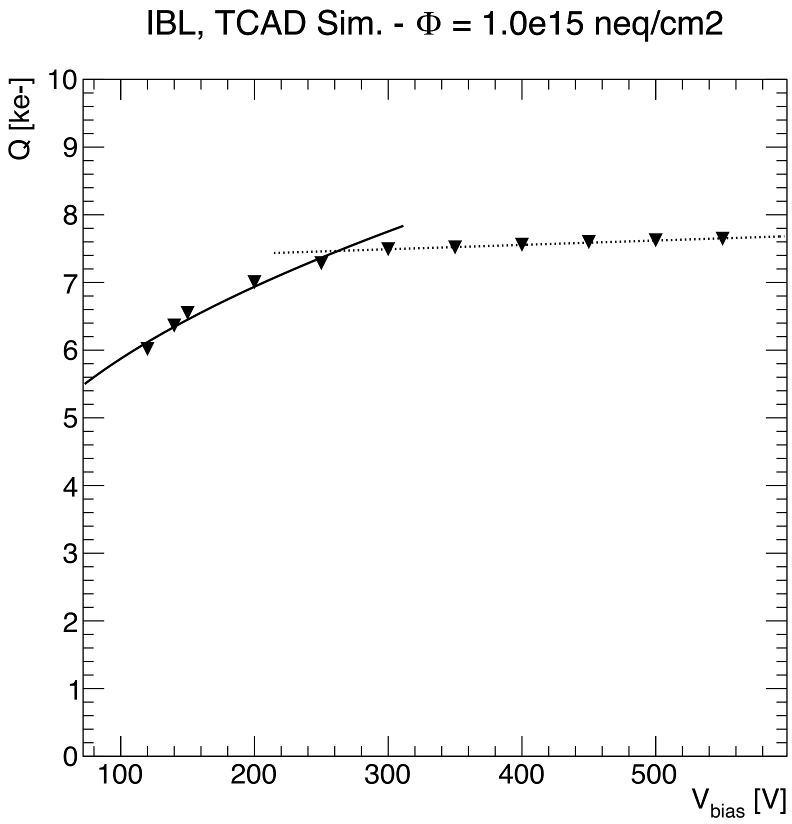


Now well established behaviour of Q vs V

- below ‘‘depletion’’ -> Q ~ √V
- above ‘‘depletion’’ -> Q ~ lin(V)

… but why?

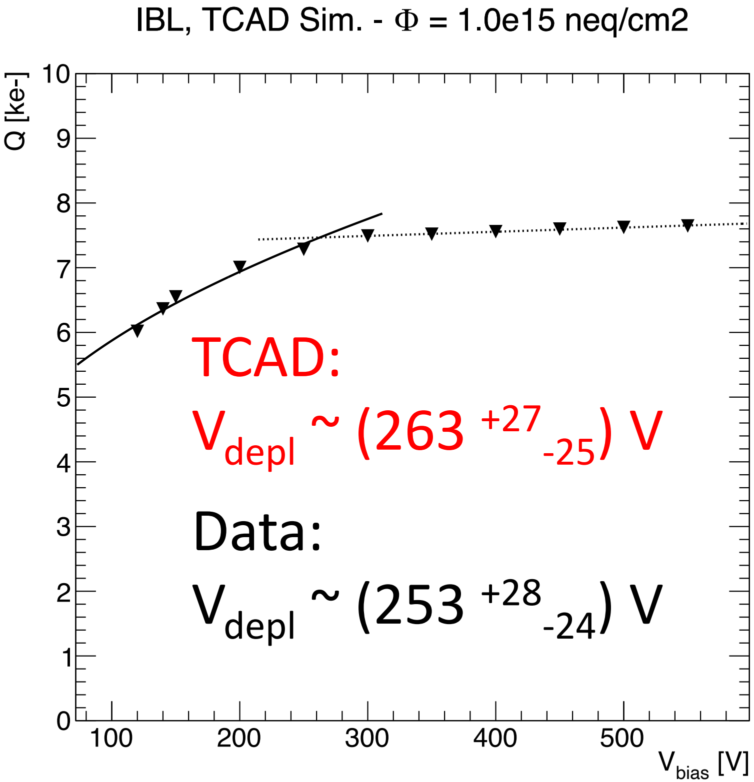
Do we see the same in TCAD?



…yes ☺

This confirms the effect is due to evolution of the electric field profile with bias voltage

Do we see the same in TCAD?



TCAD:

$V_{depl} \sim (263\ ^{+27}_{-25})$ V

Data:

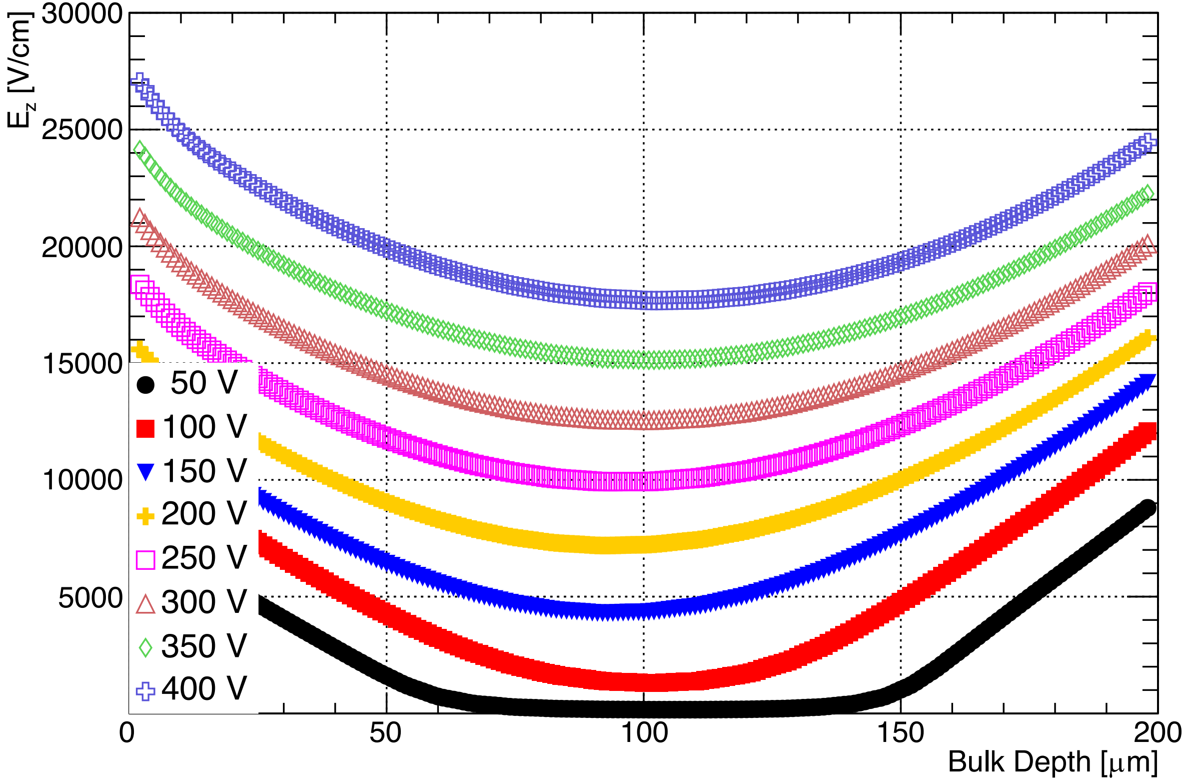
$V_{depl} \sim (253\ ^{+28}_{-24})$ V

…yes ☺

This confirms the effect is due to evolution of the electric field profile with bias voltage

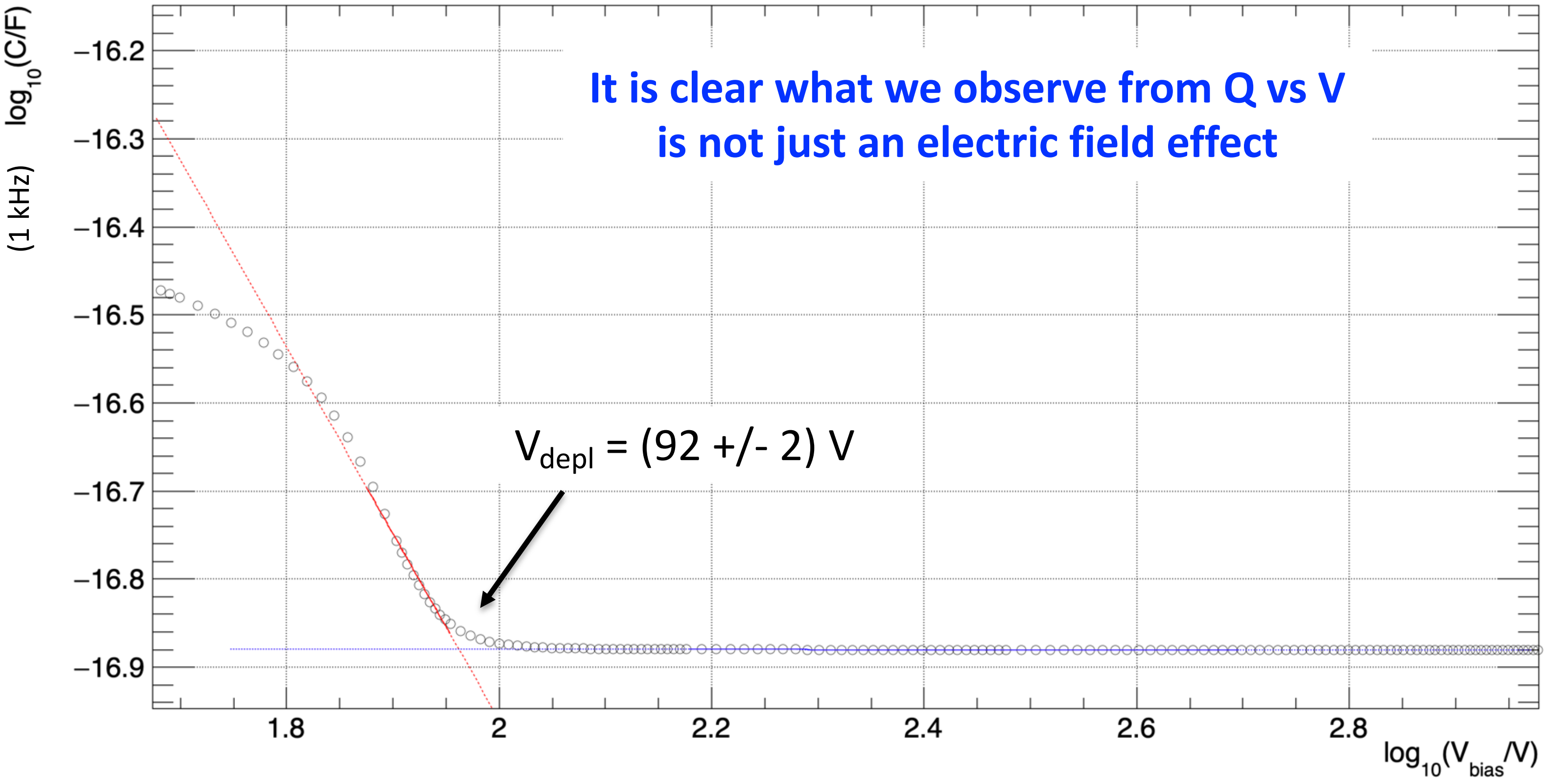
And TCAD alone is rather precise in predictions!

Electric field profiles



No major effect visible going from below 250 V to above that value

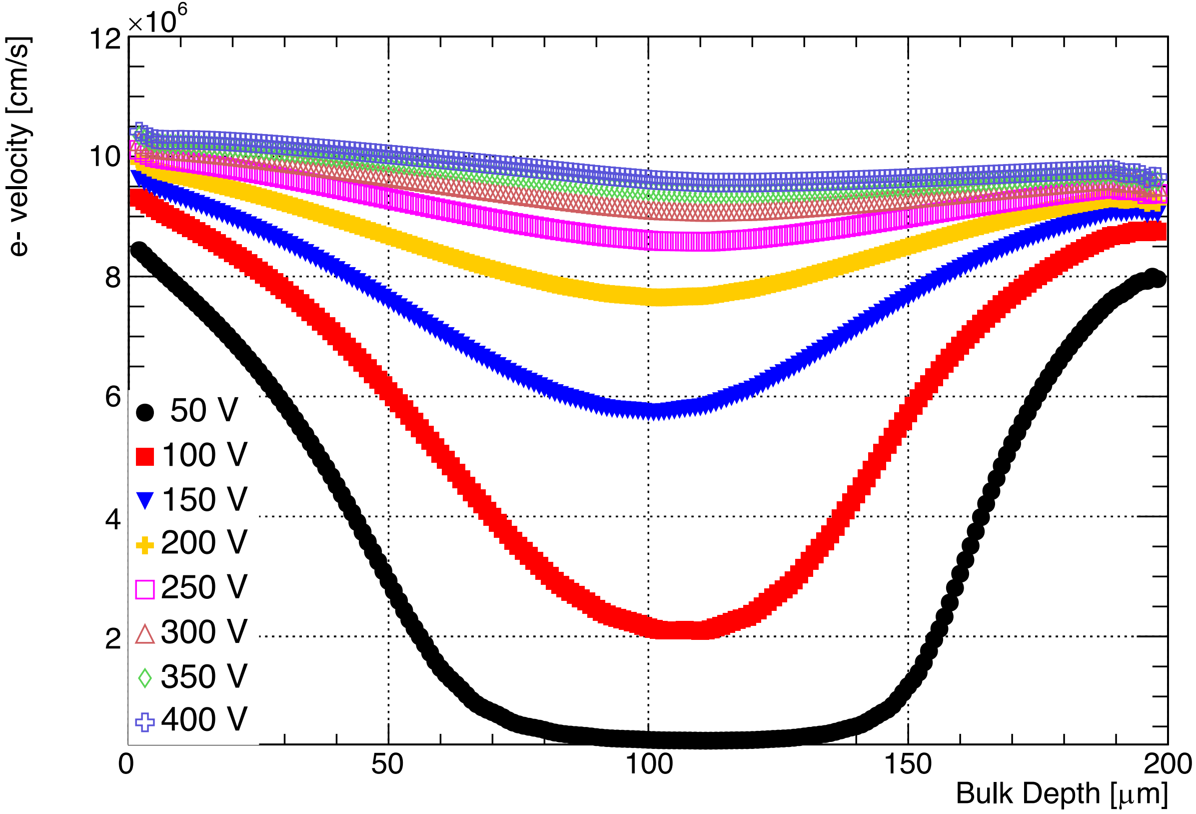
CV curve



It is clear what we observe from Q vs V is not just an electric field effect

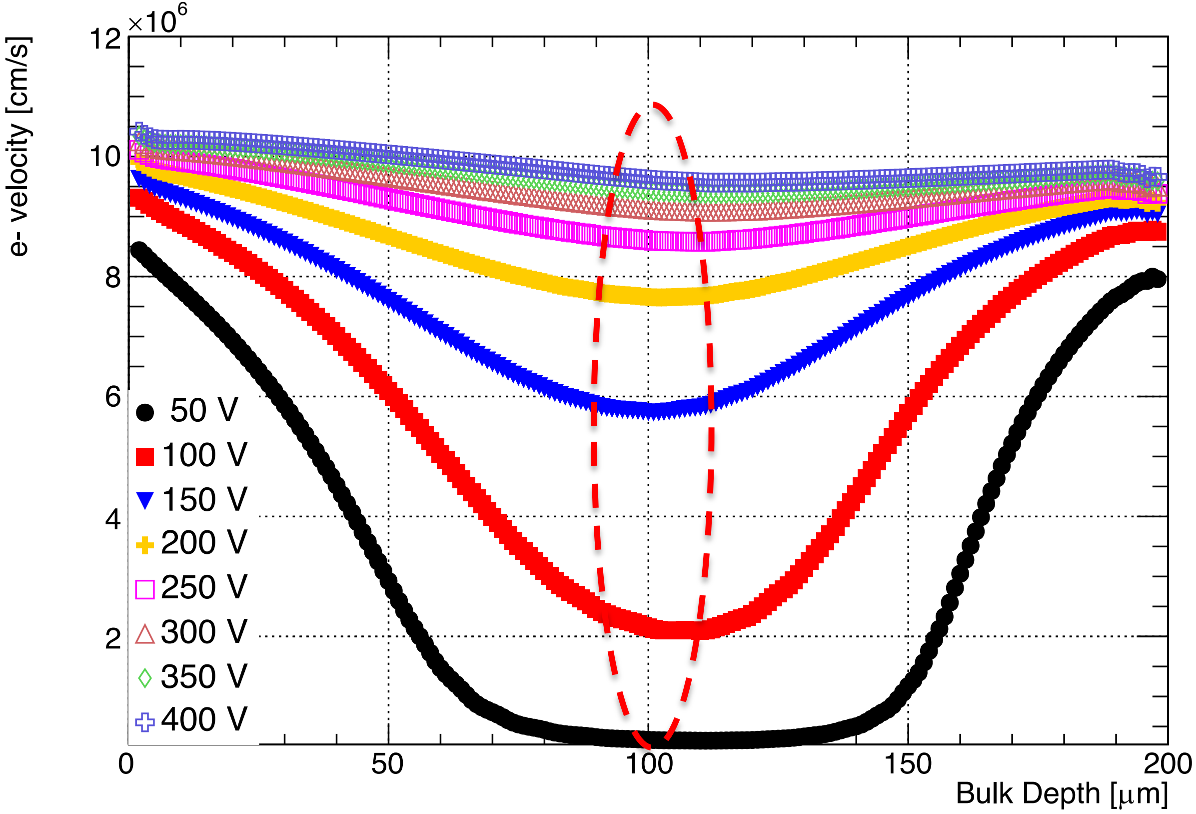
V_{depl} = (92 +/- 2) V

From electric field we calculate e- velocities



It seems the gradient is significantly reduced beyond 250 V

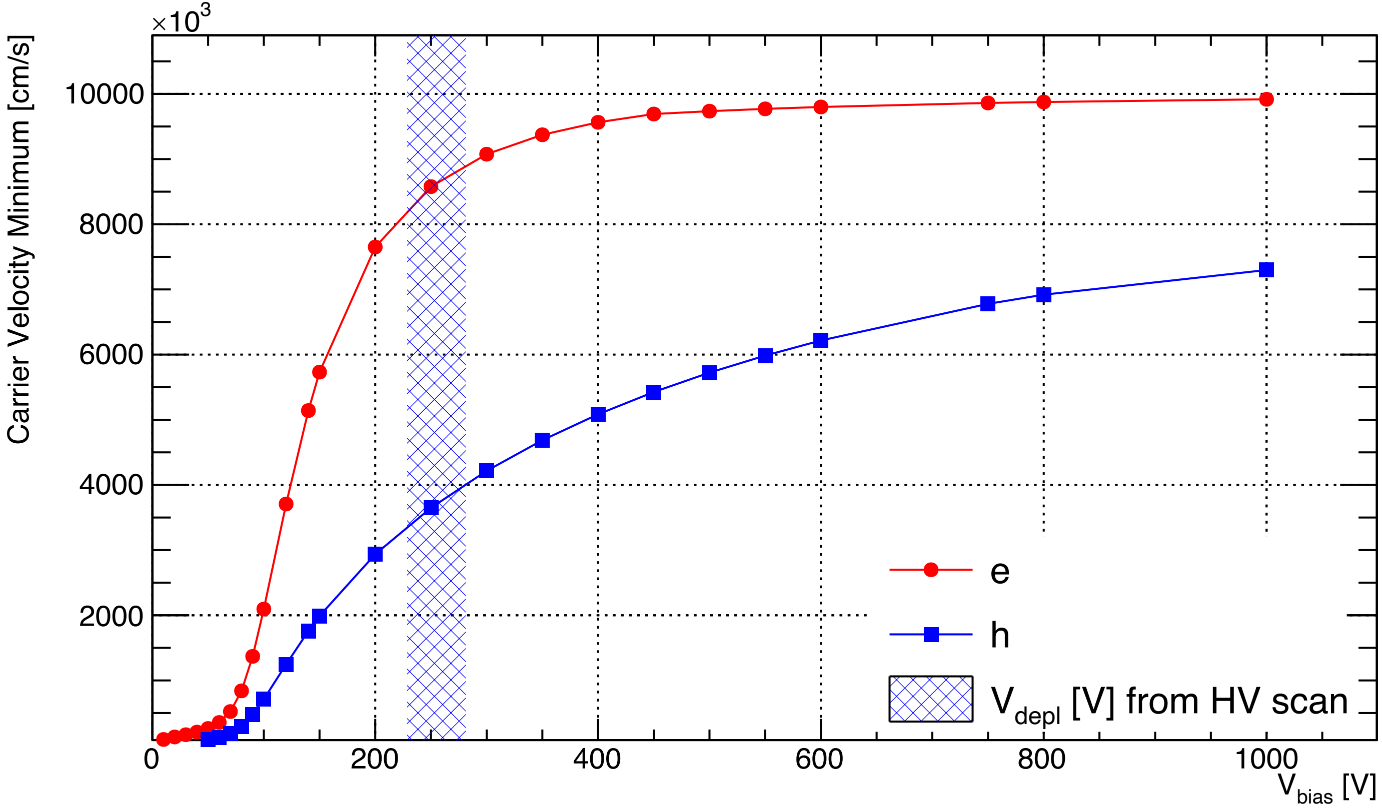
From electric field we calculate e- velocities



It seems the gradient is significantly reduced beyond 250 V

Let's focus on minima

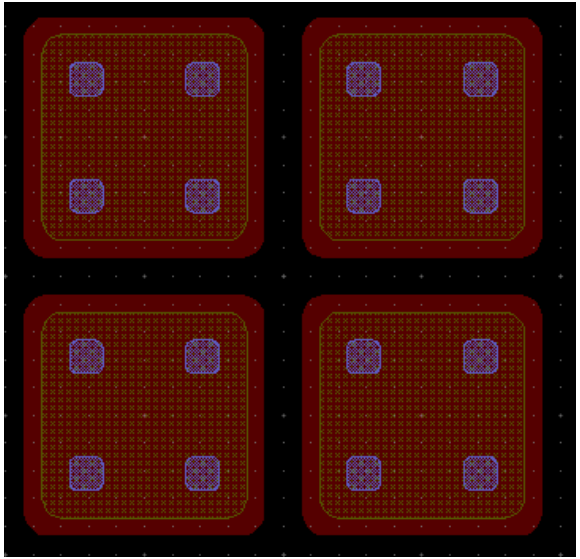
Carrier velocity minimum vs bias

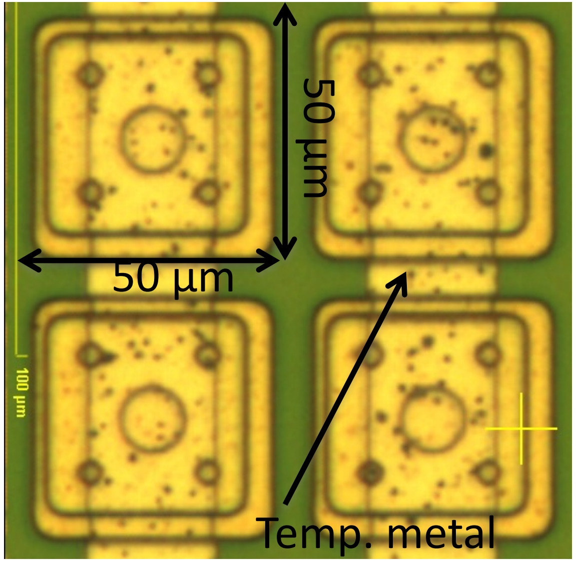


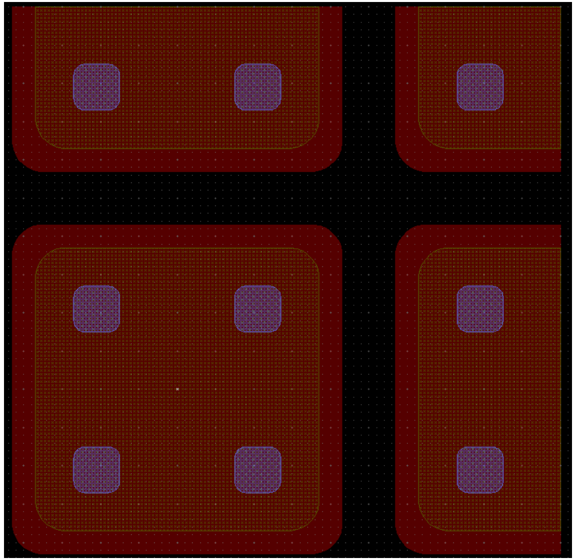
Depletion voltage is related to electron velocity saturation

VICTORY - FROM LAYOUT FILES TO FULL 3D SIMULATION

Fine pitch pixels



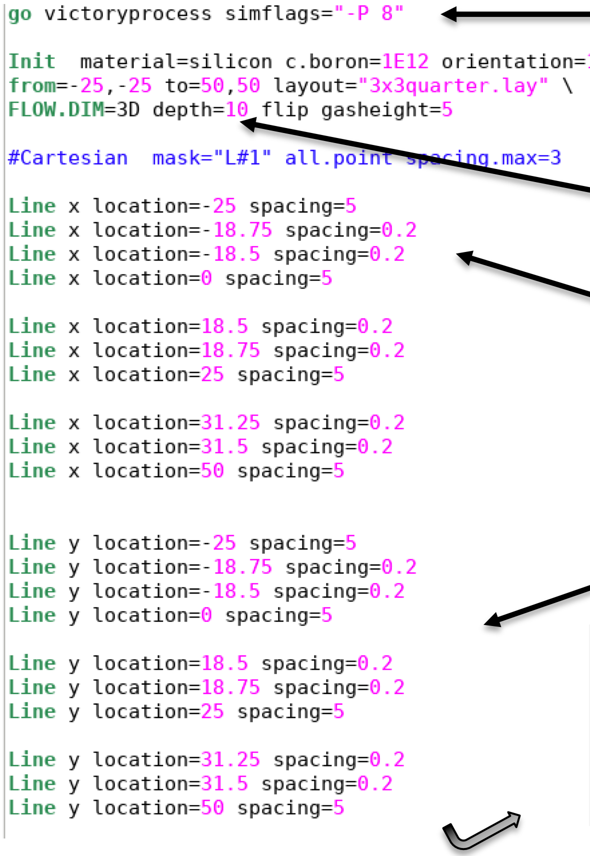




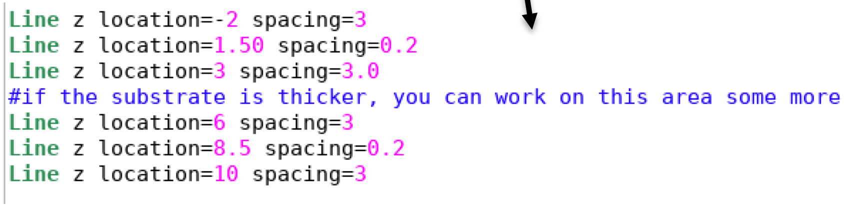
¼ of 3x3 pixels matrix

Wafer thickness: 100 µm

Victoryprocess – structure and mesh definition



```
go victoryprocess simflags="-P 8"

Init  material=silicon c.boron=1E12 orientation=100 \
from=-25,-25 to=50,50 layout="3x3quarter.lay" \
FLOW.DIM=3D depth=10 flip gasheight=5

#Cartesian  mask="L#1" all.point spacing.max=3

Line x location=-25 spacing=5
Line x location=-18.75 spacing=0.2
Line x location=-18.5 spacing=0.2
Line x location=0 spacing=5

Line x location=18.5 spacing=0.2
Line x location=18.75 spacing=0.2
Line x location=25 spacing=5

Line x location=31.25 spacing=0.2
Line x location=31.5 spacing=0.2
Line x location=50 spacing=5


Line y location=-25 spacing=5
Line y location=-18.75 spacing=0.2
Line y location=-18.5 spacing=0.2
Line y location=0 spacing=5

Line y location=18.5 spacing=0.2
Line y location=18.75 spacing=0.2
Line y location=25 spacing=5

Line y location=31.25 spacing=0.2
Line y location=31.5 spacing=0.2
Line y location=50 spacing=5
```



```
Line z location=-2 spacing=3
Line z location=1.50 spacing=0.2
Line z location=3 spacing=3.0
#if the substrate is thicker, you can work on this area some more
Line z location=6 spacing=3
Line z location=8.5 spacing=0.2
Line z location=10 spacing=3
```

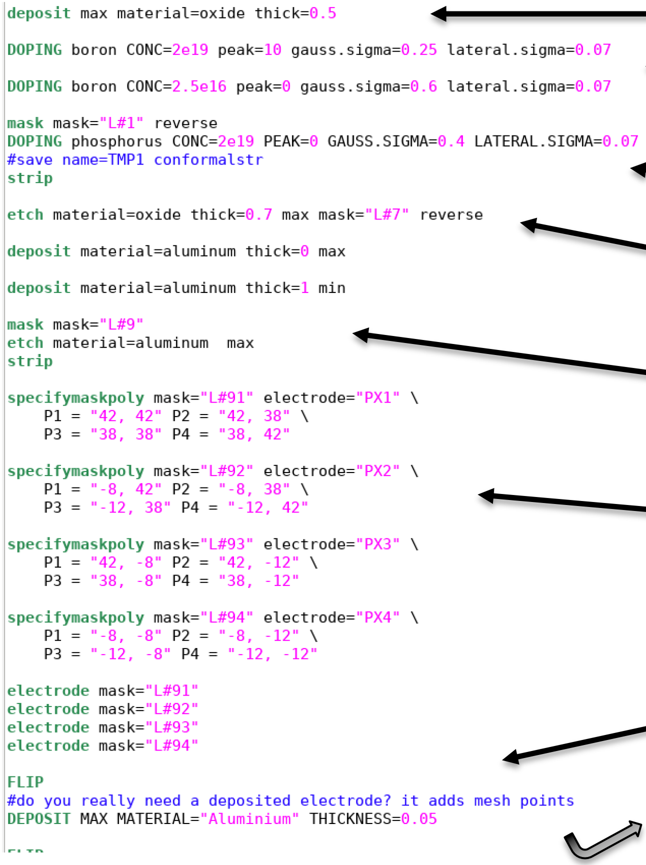
Use victoryprocess to build the structure

Define bulk material, orientation, doping, size, space on top and the layout file to be used

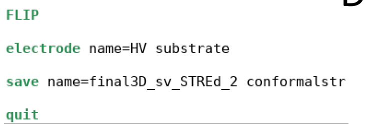
Simulate 10 µm thickness is enough

Add mesh planes

Victoryprocess – doping, etching, deposition



```
deposit max material=oxide thick=0.5

DOPING boron CONC=2e19 peak=10 gauss.sigma=0.25 lateral.sigma=0.07

DOPING boron CONC=2.5e16 peak=0 gauss.sigma=0.6 lateral.sigma=0.07

mask mask="L#1" reverse
DOPING phosphorus CONC=2e19 PEAK=0 GAUSS.SIGMA=0.4 LATERAL.SIGMA=0.07
#save name=TMP1 conformalstr
strip

etch material=oxide thick=0.7 max mask="L#7" reverse

deposit material=aluminum thick=0 max

deposit material=aluminum thick=1 min

mask mask="L#9"
etch material=aluminum  max
strip

specifymaskpoly mask="L#91" electrode="PX1" \
    P1 = "42, 42" P2 = "42, 38" \
    P3 = "38, 38" P4 = "38, 42"

specifymaskpoly mask="L#92" electrode="PX2" \
    P1 = "-8, 42" P2 = "-8, 38" \
    P3 = "-12, 38" P4 = "-12, 42"

specifymaskpoly mask="L#93" electrode="PX3" \
    P1 = "42, -8" P2 = "42, -12" \
    P3 = "38, -8" P4 = "38, -12"

specifymaskpoly mask="L#94" electrode="PX4" \
    P1 = "-8, -8" P2 = "-8, -12" \
    P3 = "-12, -8" P4 = "-12, -12"

electrode mask="L#91"
electrode mask="L#92"
electrode mask="L#93"
electrode mask="L#94"

FLIP
#do you really need a deposited electrode? it adds mesh points
DEPOSIT MAX MATERIAL="Aluminium" THICKNESS=0.05
```



```
FLIP

electrode name=HV substrate

save name=final3D_sv_STREd_2 conformalstr

quit
```

Deposit oxide

Uniform doping (backside/p-spray)

Doping through a mask

Etch oxide

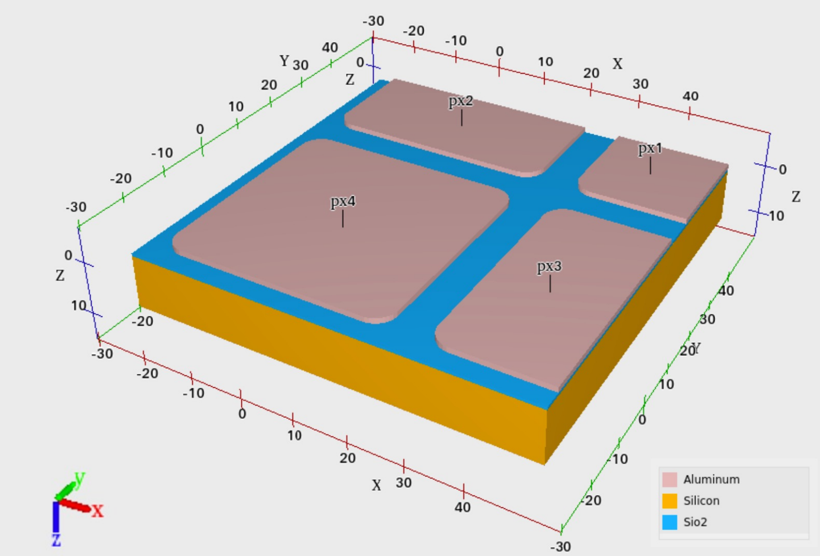
Deposit aluminium using mask

Define front side electrodes

Deposit aluminium on the backside

Declare backside electrode and save

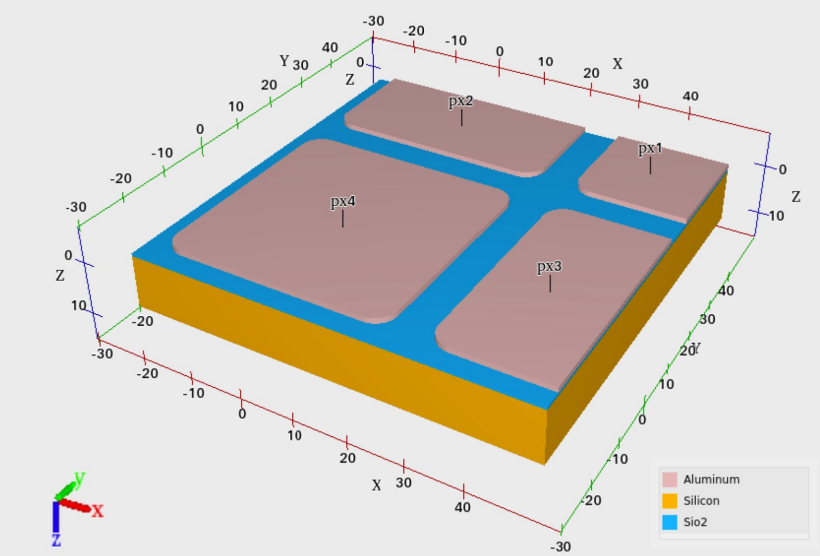
Stretching structure

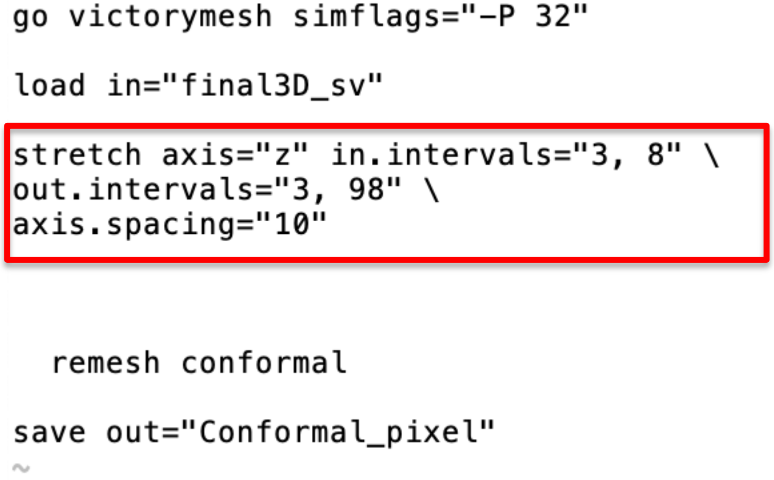


So far we “built” only 10 µm

Victorymesh - Stretching structure

We can stretch the bulk to get the desired thickness

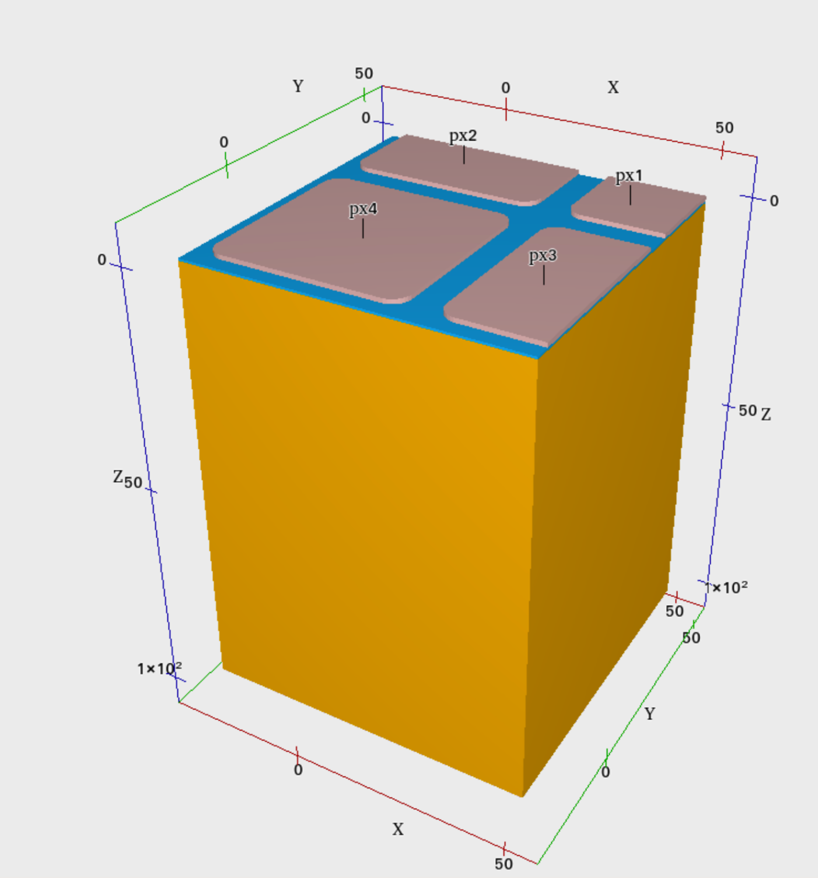




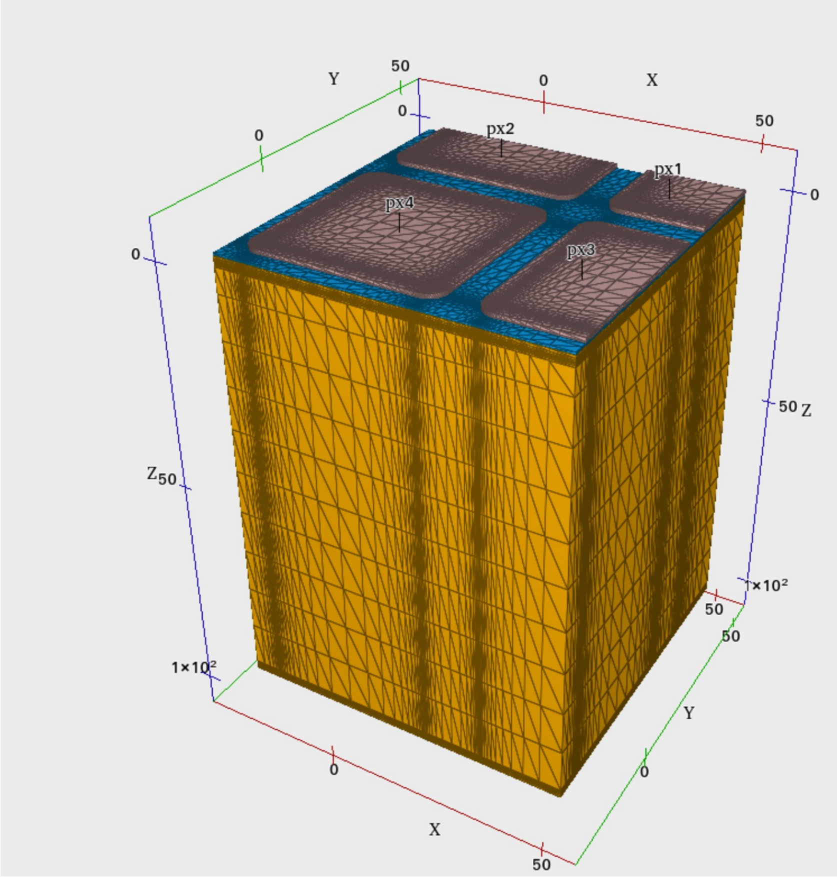
```
go victorymesh simflags="-P 32"

load in="final3D_sv"

stretch axis="z" in.intervals="3, 8" \
out.intervals="3, 98" \
axis.spacing="10"


  remesh conformal

save out="Conformal_pixel"
~
```

So far we “built” only 10 µm

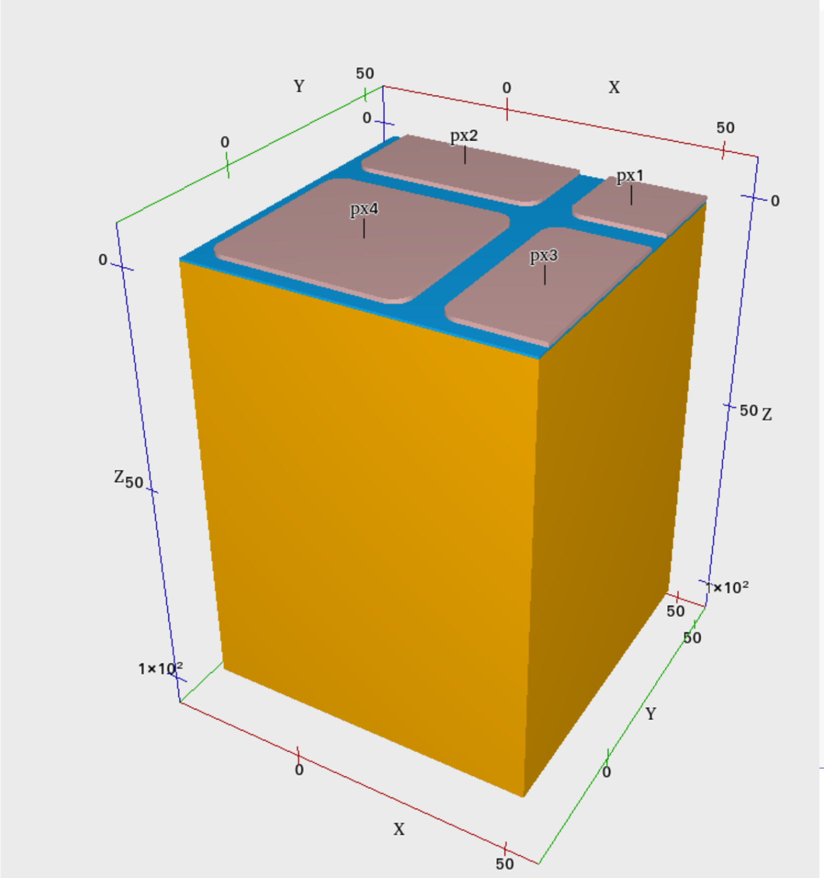
VictoryVisual - The final structure

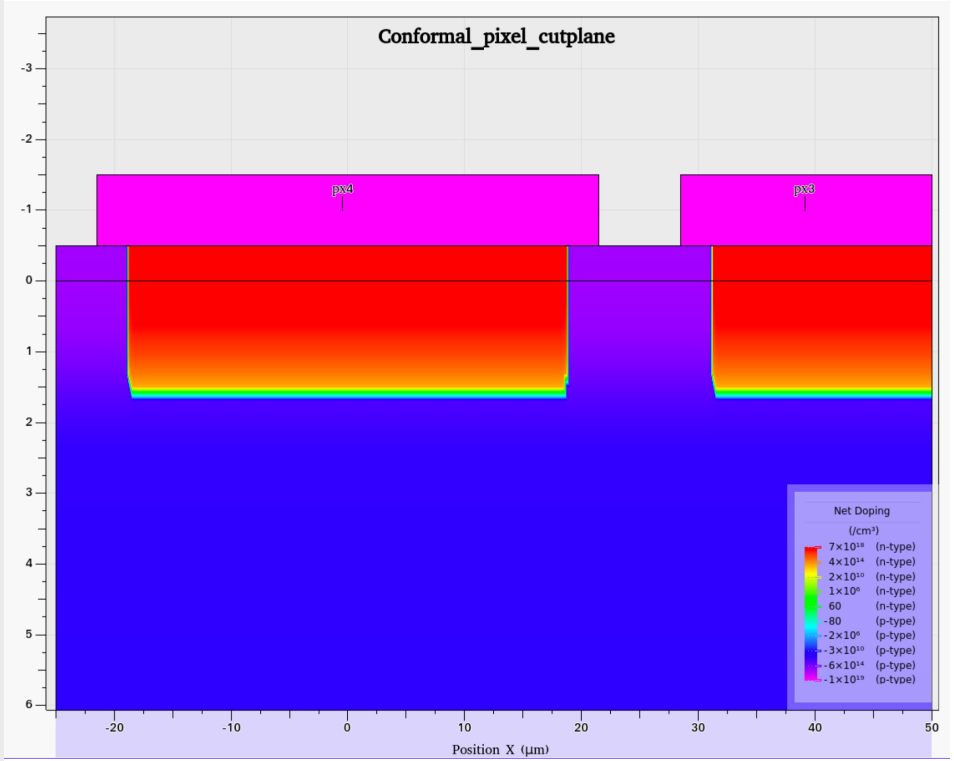


VictoryVisual - The mesh

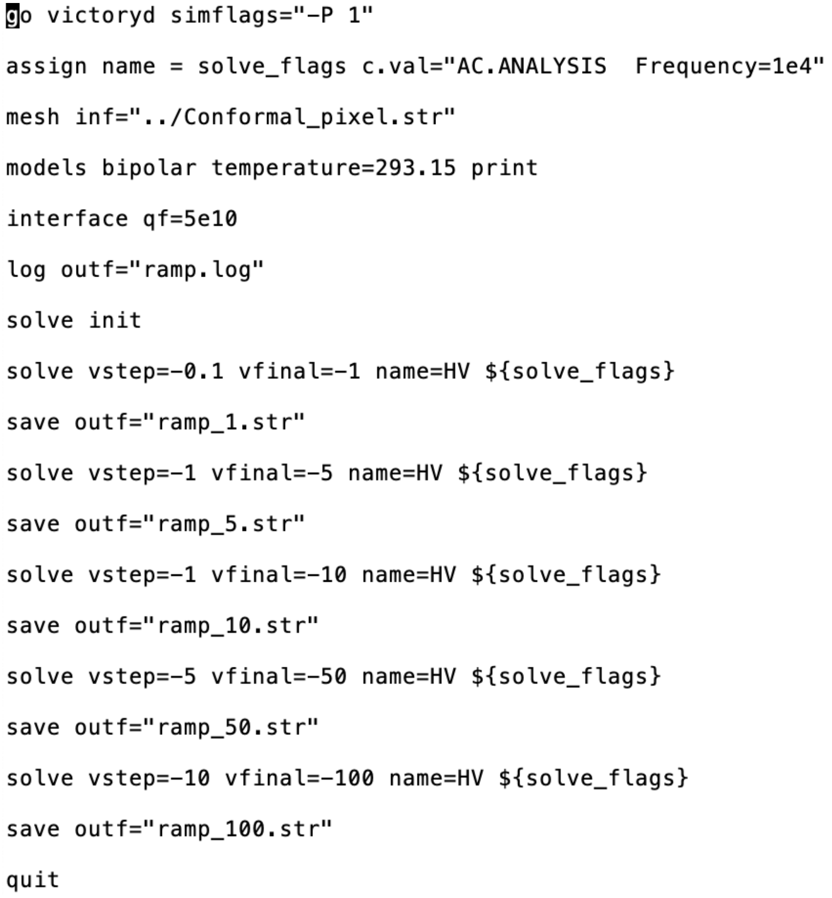


VictoryVisual - Slices





Victorydevice – device simulation



```
go victoryd simflags="-P 1"

assign name = solve_flags c.val="AC.ANALYSIS  Frequency=1e4"

mesh inf="../Conformal_pixel.str"

models bipolar temperature=293.15 print

interface qf=5e10

log outf="ramp.log"

solve init

solve vstep=-0.1 vfinal=-1 name=HV ${solve_flags}

save outf="ramp_1.str"

solve vstep=-1 vfinal=-5 name=HV ${solve_flags}

save outf="ramp_5.str"

solve vstep=-1 vfinal=-10 name=HV ${solve_flags}

save outf="ramp_10.str"

solve vstep=-5 vfinal=-50 name=HV ${solve_flags}

save outf="ramp_50.str"

solve vstep=-10 vfinal=-100 name=HV ${solve_flags}

save outf="ramp_100.str"

quit
```

Declare variables

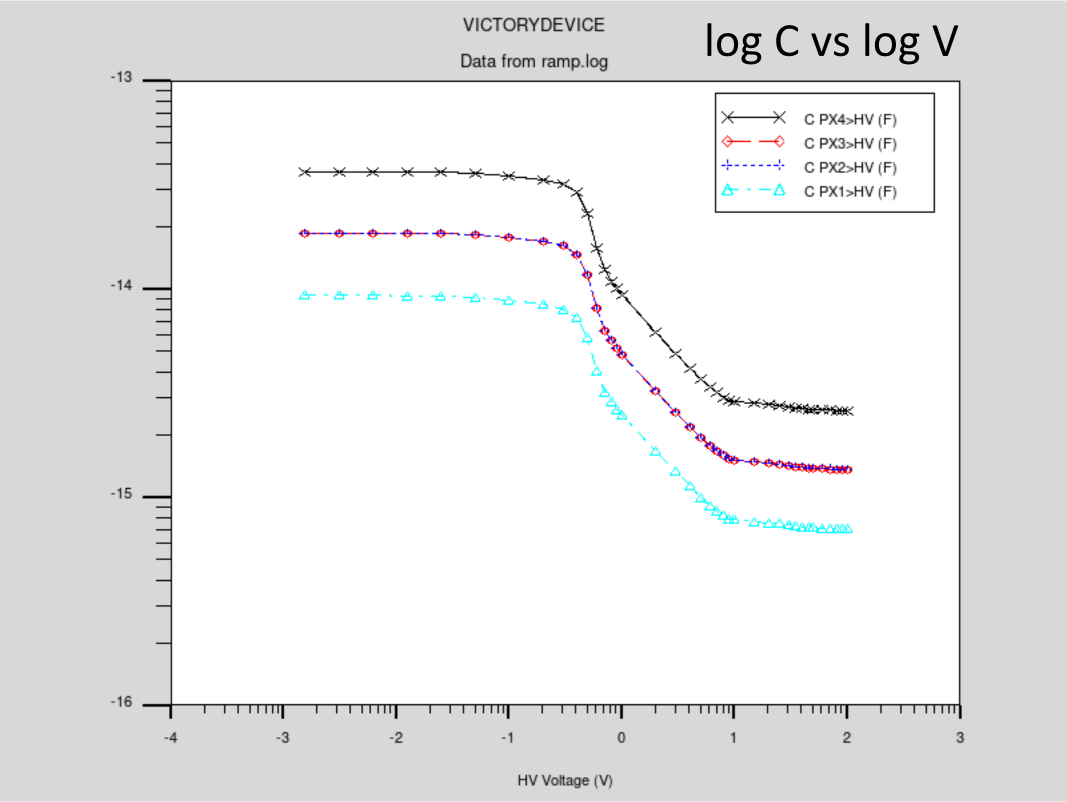
Load structure, define physics models and temperature

Add interface charge

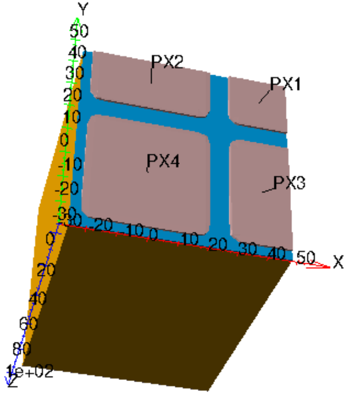
Start simulating for V=0 on all electrodes

Ramp voltage, perform AC simulation and save solutions each time you want
(Later you can restart simulating from such solution files)

Tonyplot(3D) – depletion capacitance

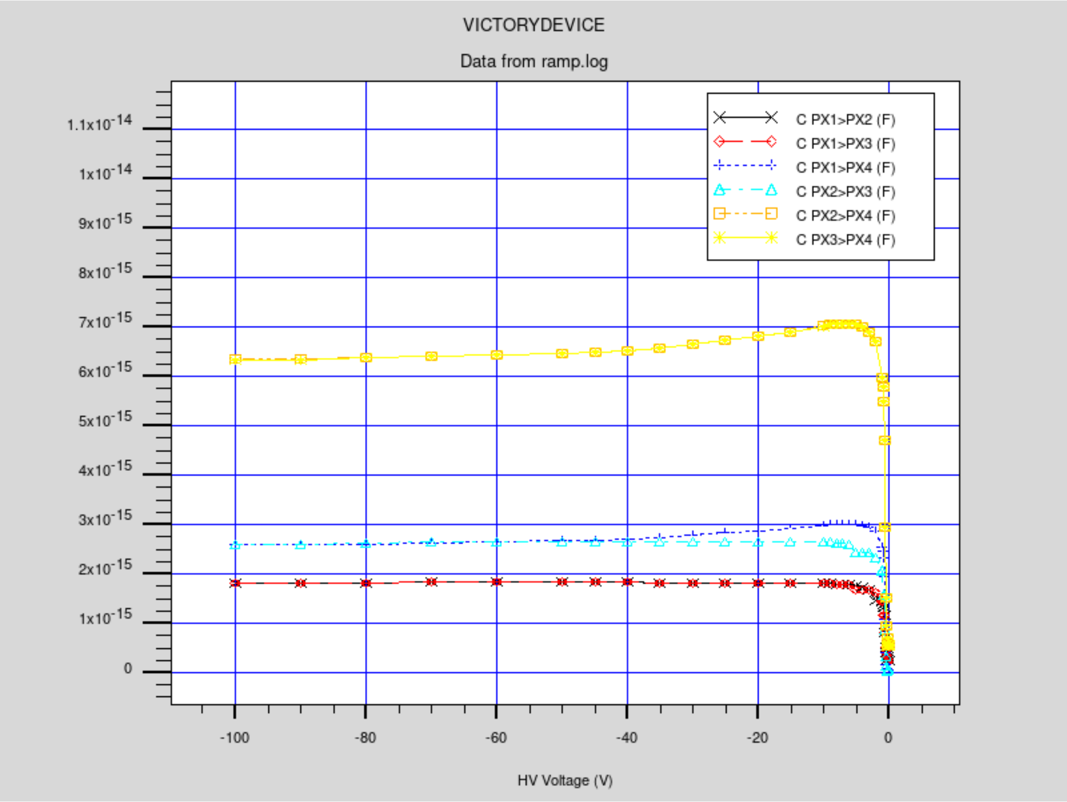


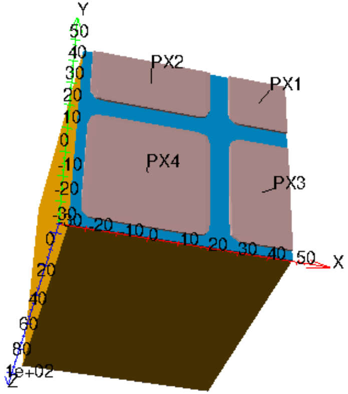
log C vs log V



Depletion voltage and capacitance at depletion in agreement with expectations

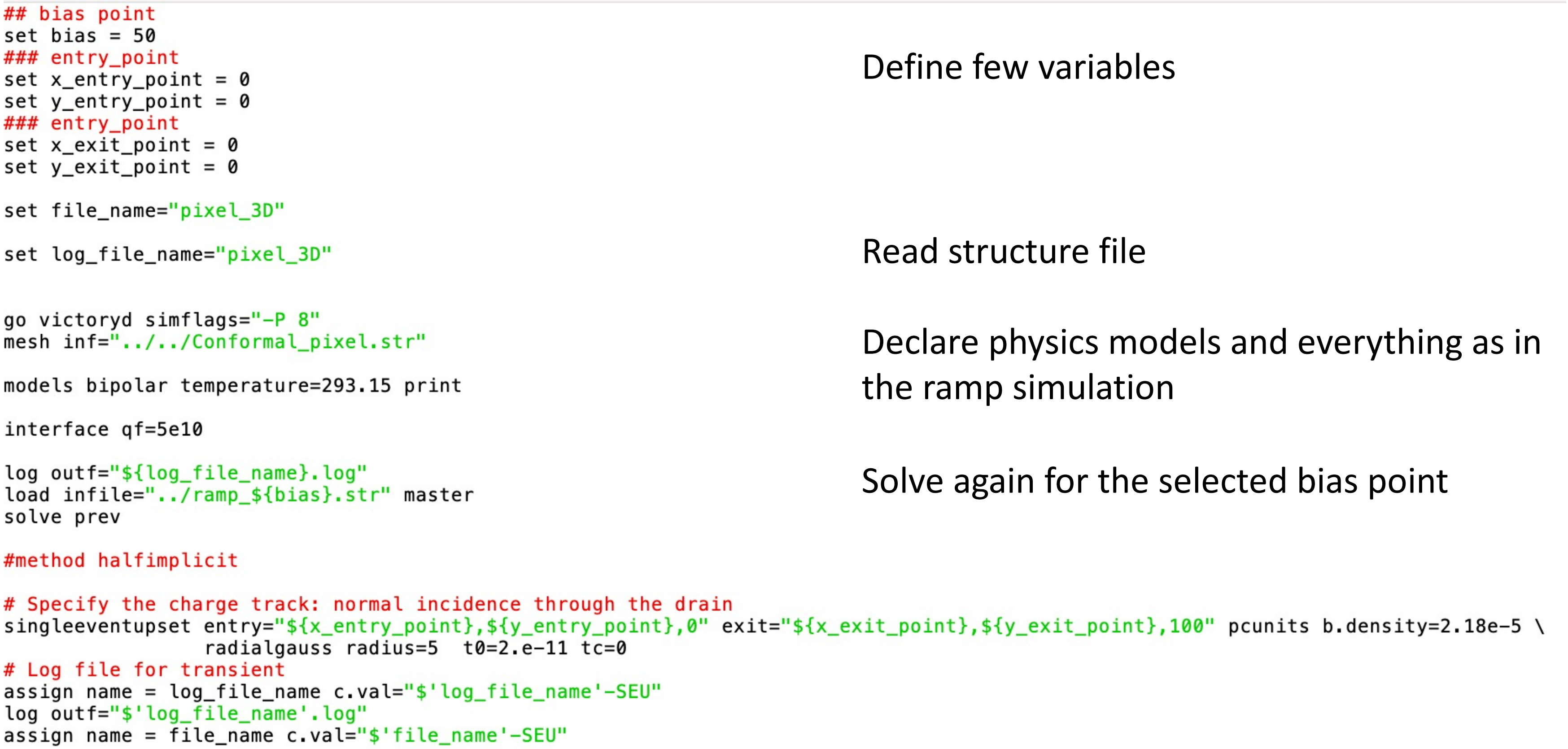
Tonyplot(3D) – Interpixel capacitance





Nice scaling with shared perimeter

Victorydevice – Transient signal simulation



```
## bias point
set bias = 50
### entry_point
set x_entry_point = 0
set y_entry_point = 0
### entry_point
set x_exit_point = 0
set y_exit_point = 0

set file_name="pixel_3D"

set log_file_name="pixel_3D"


go victoryd simflags="-P 8"
mesh inf="../../Conformal_pixel.str"

models bipolar temperature=293.15 print

interface qf=5e10

log outf="${log_file_name}.log"
load infile="../ramp_${bias}.str" master
solve prev

#method halfimplicit

# Specify the charge track: normal incidence through the drain
singleeventupset entry="${x_entry_point},${y_entry_point},0" exit="${x_exit_point},${y_exit_point},100" pcunits b.density=2.18e-5 \
                 radialgauss radius=5  t0=2.e-11 tc=0
# Log file for transient
assign name = log_file_name c.val="$'log_file_name'-SEU"
log outf="$'log_file_name'.log"
assign name = file_name c.val="$'file_name'-SEU"
```

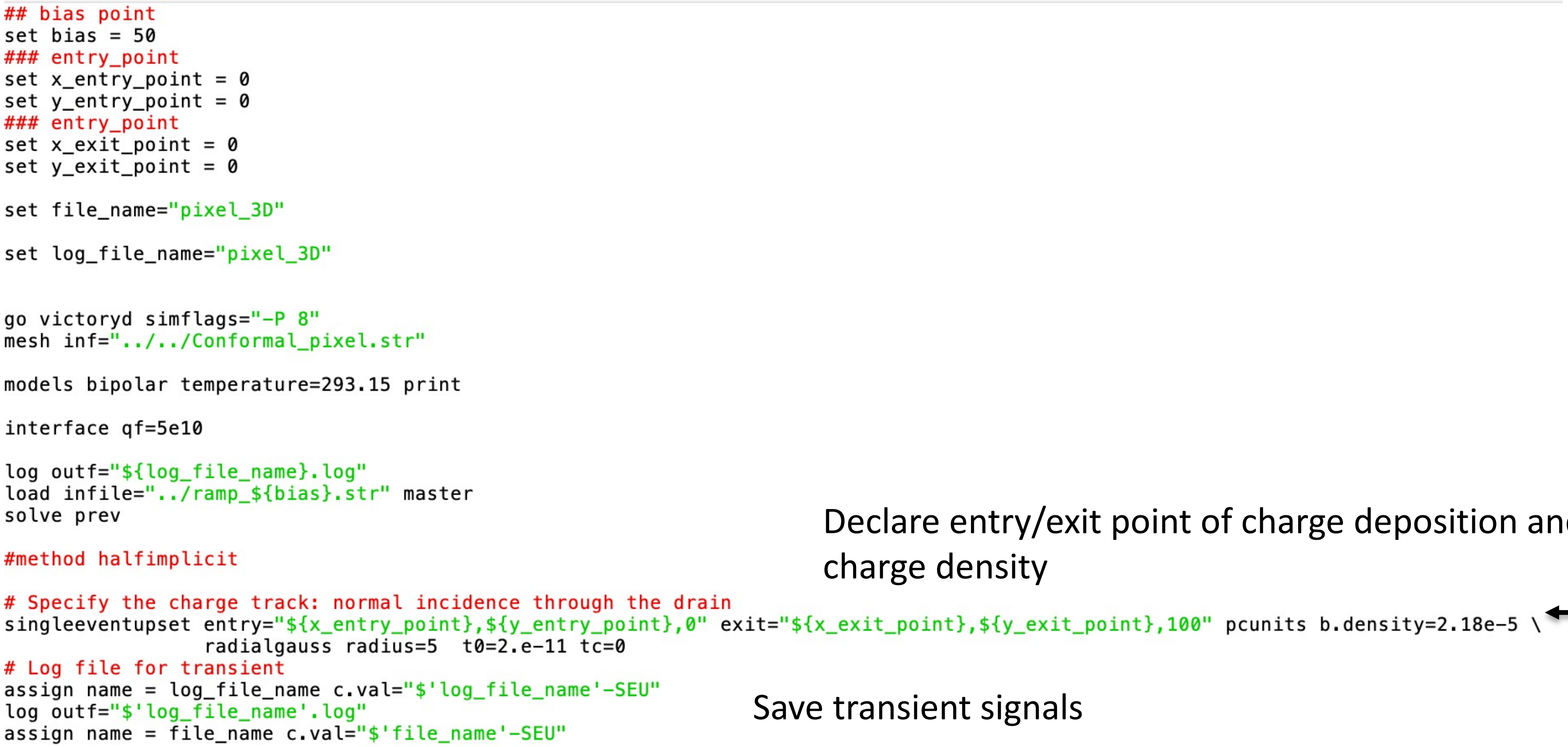
Define few variables

Read structure file

Declare physics models and everything as in the ramp simulation

Solve again for the selected bias point

Victorydevice – Transient signal simulation

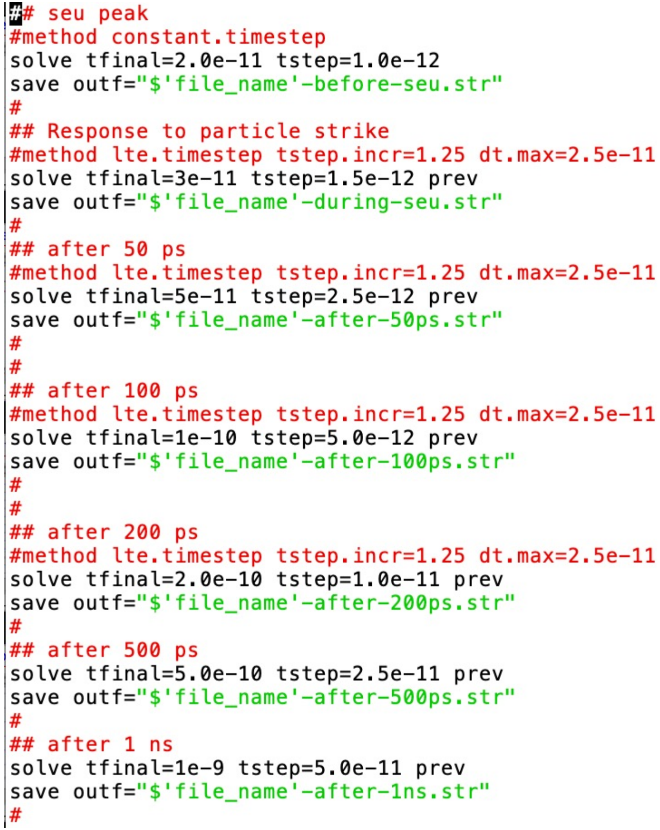


```
## bias point
set bias = 50
### entry_point
set x_entry_point = 0
set y_entry_point = 0
### entry_point
set x_exit_point = 0
set y_exit_point = 0

set file_name="pixel_3D"

set log_file_name="pixel_3D"


go victoryd simflags="-P 8"
mesh inf="../../Conformal_pixel.str"

models bipolar temperature=293.15 print

interface qf=5e10

log outf="${log_file_name}.log"
load infile="../ramp_${bias}.str" master
solve prev

#method halfimplicit

# Specify the charge track: normal incidence through the drain
singleeventupset entry="${x_entry_point},${y_entry_point},0" exit="${x_exit_point},${y_exit_point},100" pcunits b.density=2.18e-5 \
                 radialgauss radius=5  t0=2.e-11 tc=0
# Log file for transient
assign name = log_file_name c.val="$'log_file_name'-SEU"
log outf="$'log_file_name'.log"
assign name = file_name c.val="$'file_name'-SEU"
```

Declare entry/exit point of charge deposition and the charge density

Save transient signals

Victorydevice – Transient signal simulation



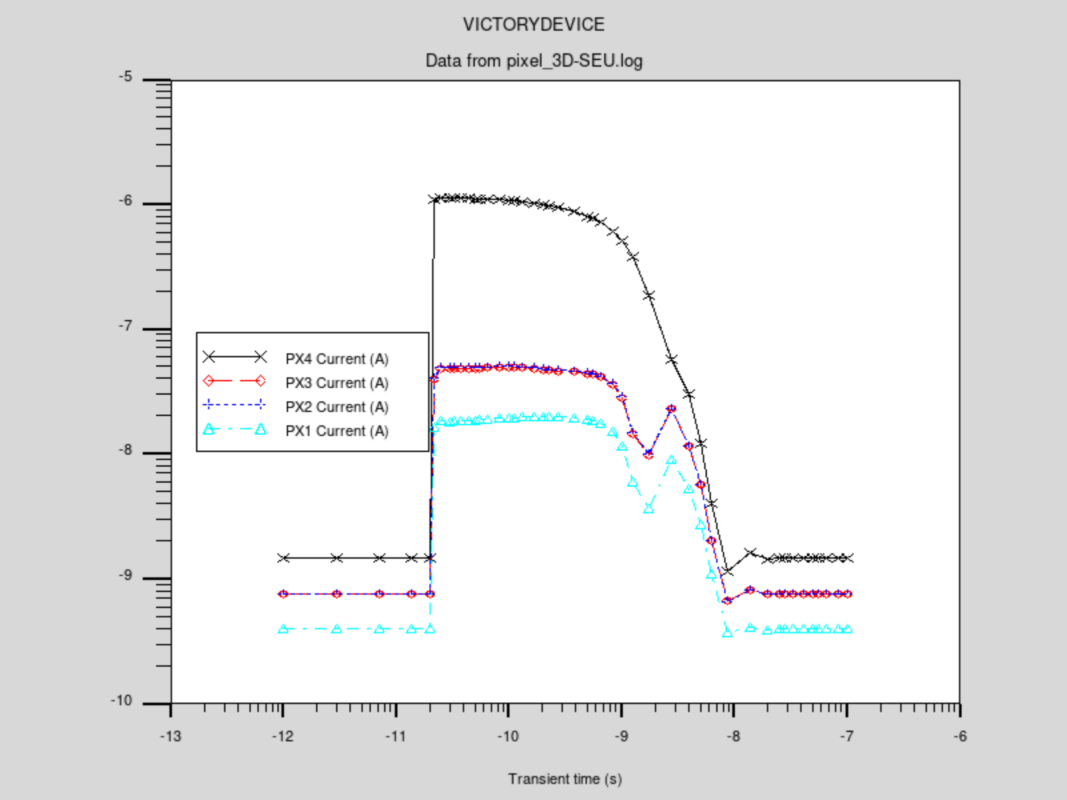
```
## seu peak
#method constant.timestep
solve tfinal=2.0e-11 tstep=1.0e-12
save outf="$'file_name'-before-seu.str"
#
## Response to particle strike
#method lte.timestep tstep.incr=1.25 dt.max=2.5e-11
solve tfinal=3e-11 tstep=1.5e-12 prev
save outf="$'file_name'-during-seu.str"
#
## after 50 ps
#method lte.timestep tstep.incr=1.25 dt.max=2.5e-11
solve tfinal=5e-11 tstep=2.5e-12 prev
save outf="$'file_name'-after-50ps.str"
#
#
## after 100 ps
#method lte.timestep tstep.incr=1.25 dt.max=2.5e-11
solve tfinal=1e-10 tstep=5.0e-12 prev
save outf="$'file_name'-after-100ps.str"
#
#
## after 200 ps
#method lte.timestep tstep.incr=1.25 dt.max=2.5e-11
solve tfinal=2.0e-10 tstep=1.0e-11 prev
save outf="$'file_name'-after-200ps.str"
#
## after 500 ps
solve tfinal=5.0e-10 tstep=2.5e-11 prev
save outf="$'file_name'-after-500ps.str"
#
## after 1 ns
solve tfinal=1e-9 tstep=5.0e-11 prev
save outf="$'file_name'-after-1ns.str"
#
```

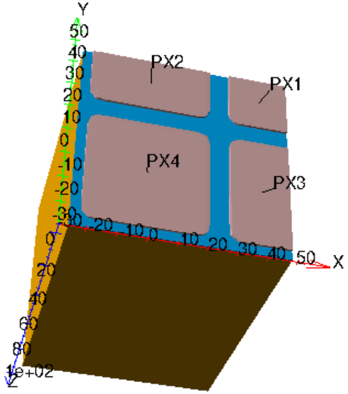
Solve as a function of time by defining the final and incremental time

Save the simulated structure

Repeat as many times as needed, to capture the evolution of many observables (concentrations, current densities, generation rates, etcetera)

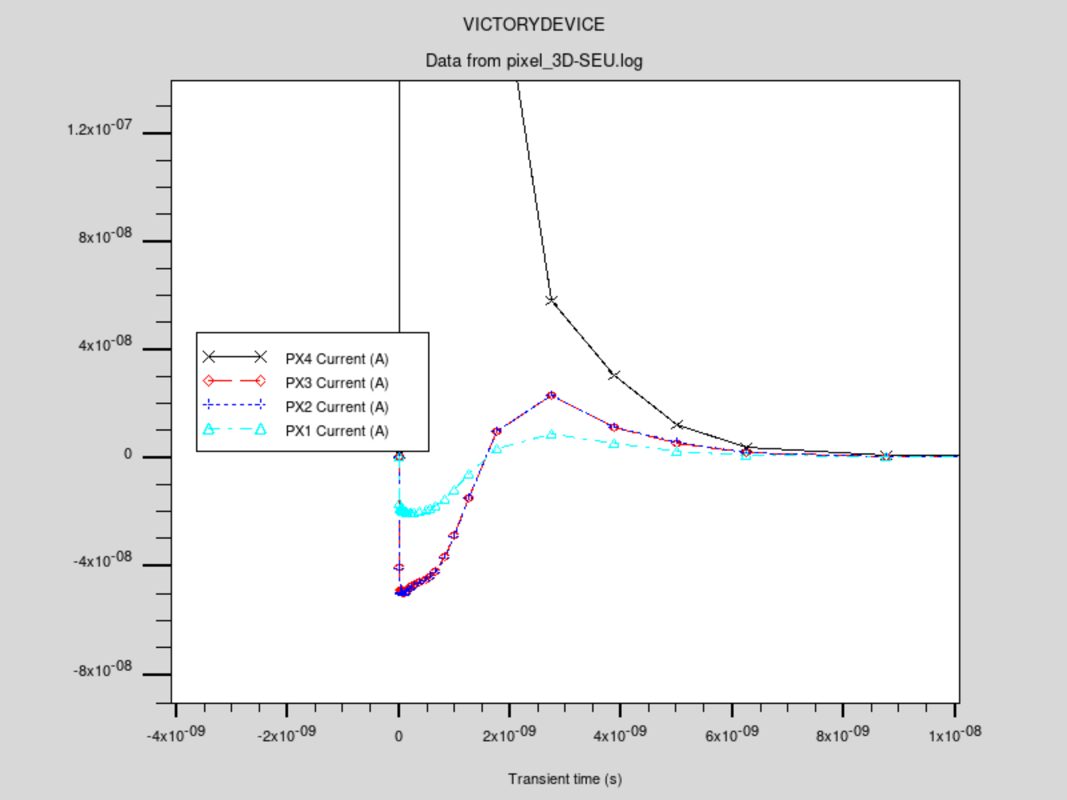
Tonyplot – Transient currents

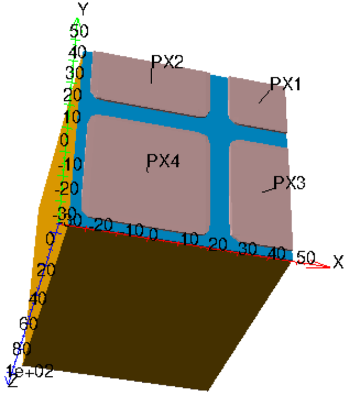




Particle striking in the middle of PX4

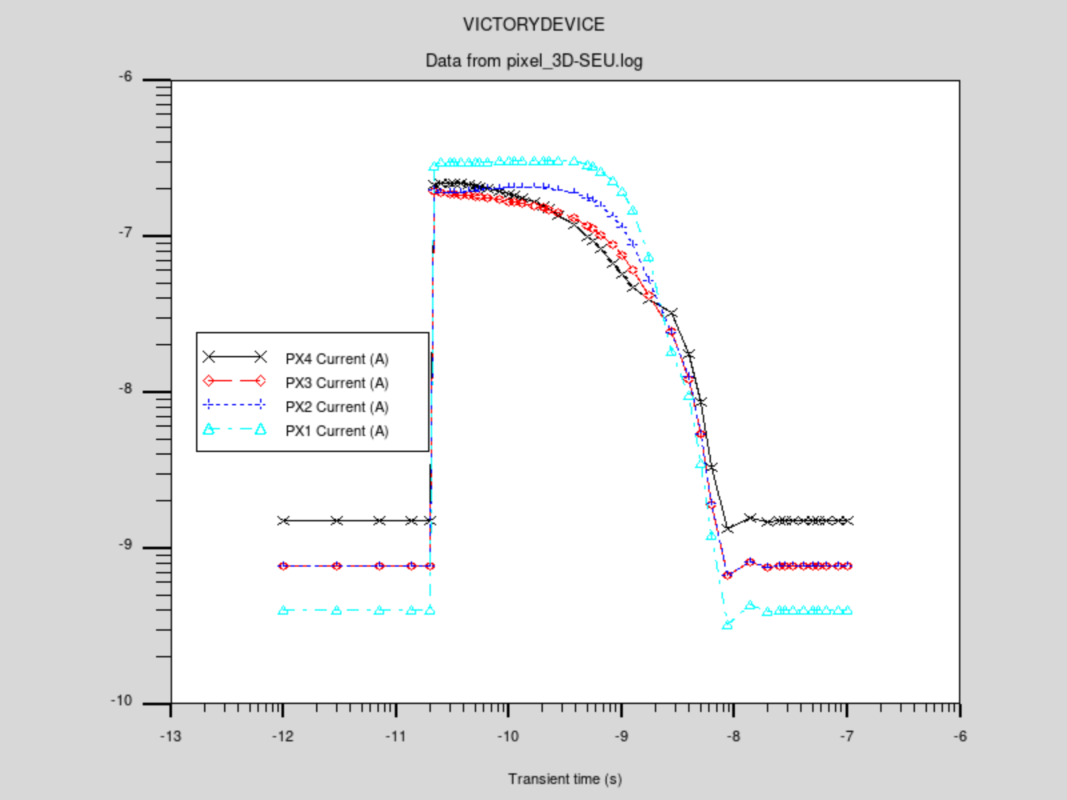
Tonyplot – Transient currents

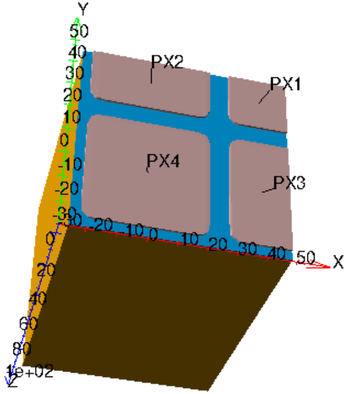




Opposite signal induced on neighbours

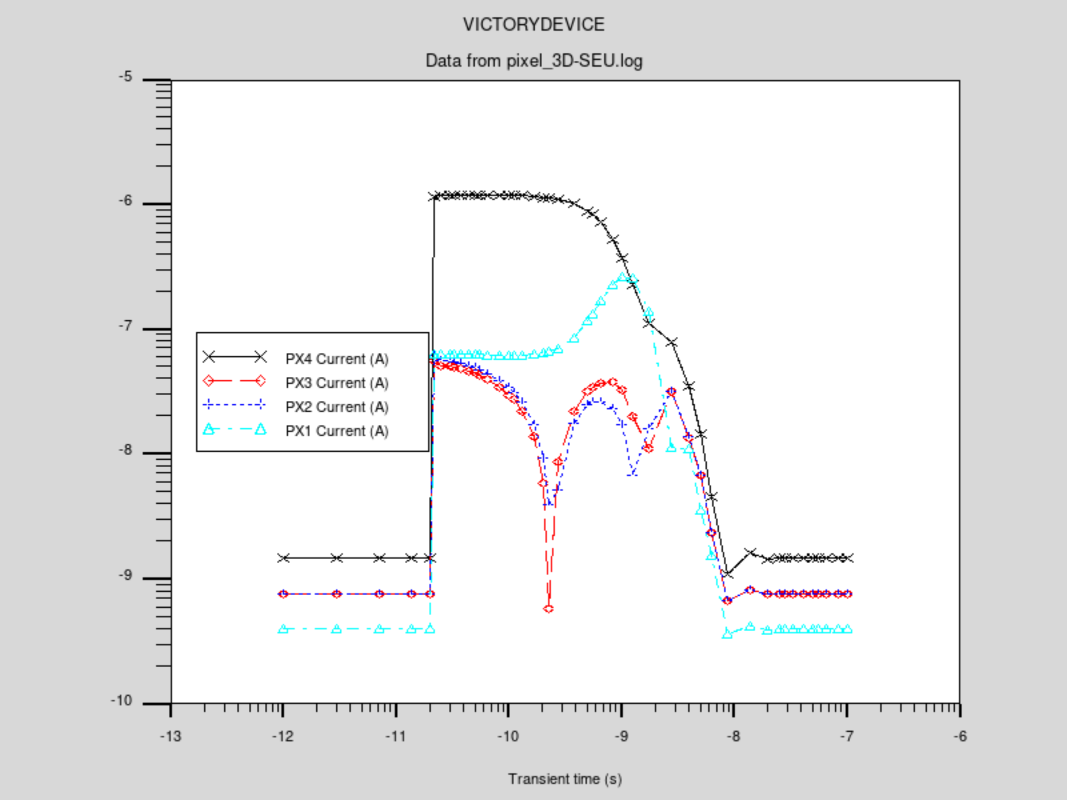
Tonyplot – Transient currents

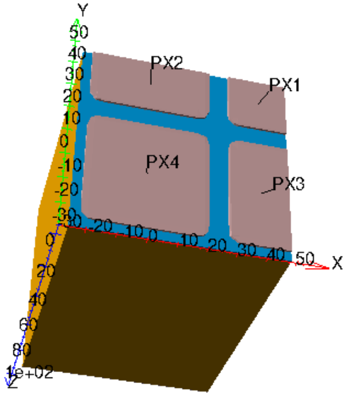




Particle striking in between pixels

Tonyplot – Transient currents





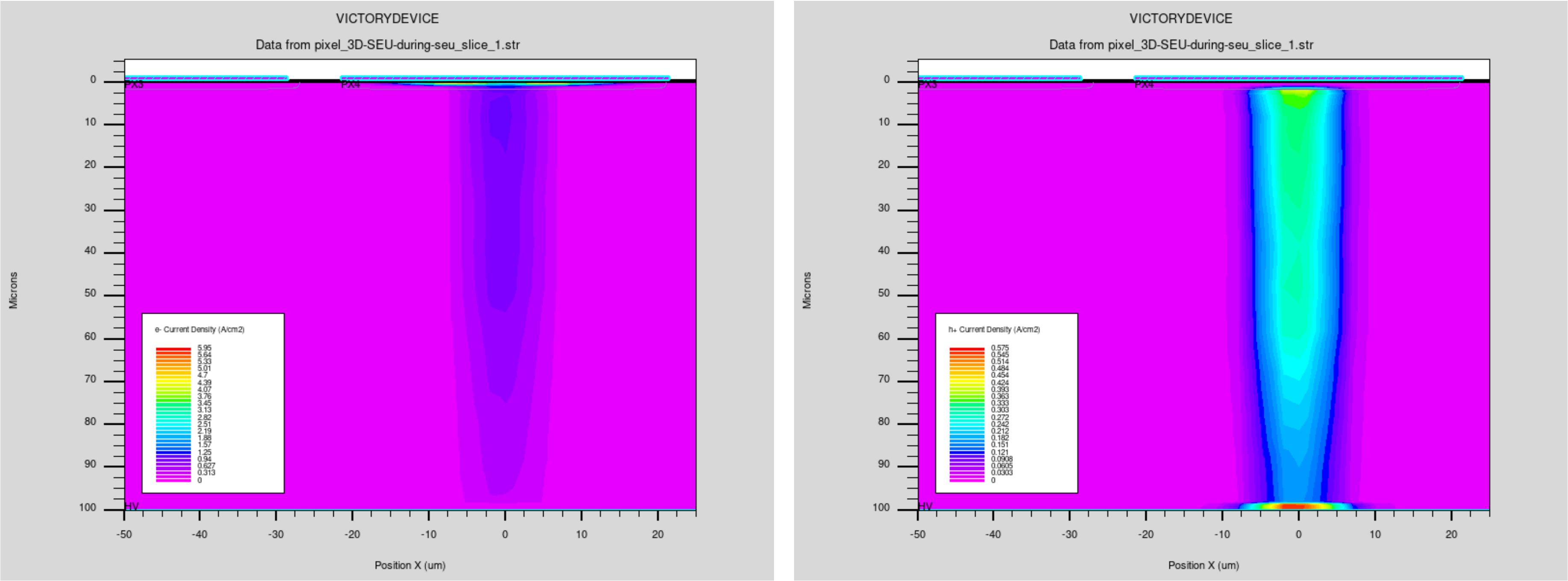
Particle striking diagonally

Tonyplot – Current densities

e-

1.5 ps after particle strike

h+

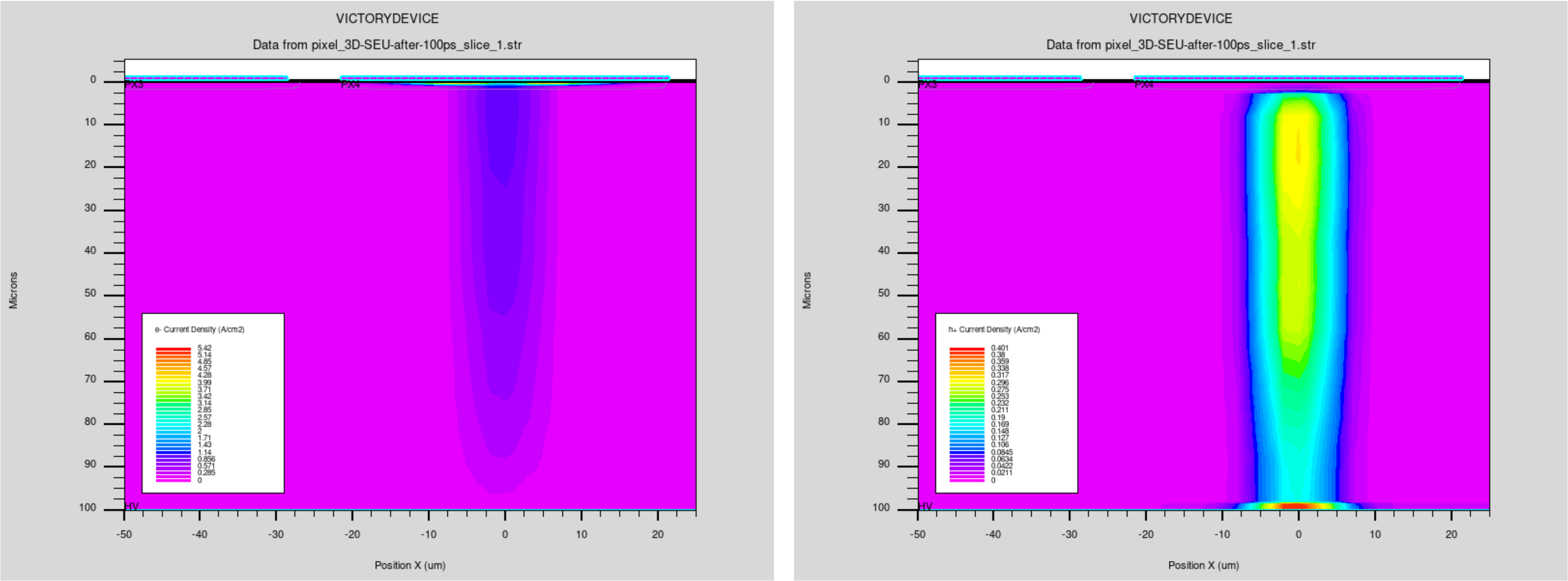


Tonyplot – Current densities

e-

100 ps after particle strike

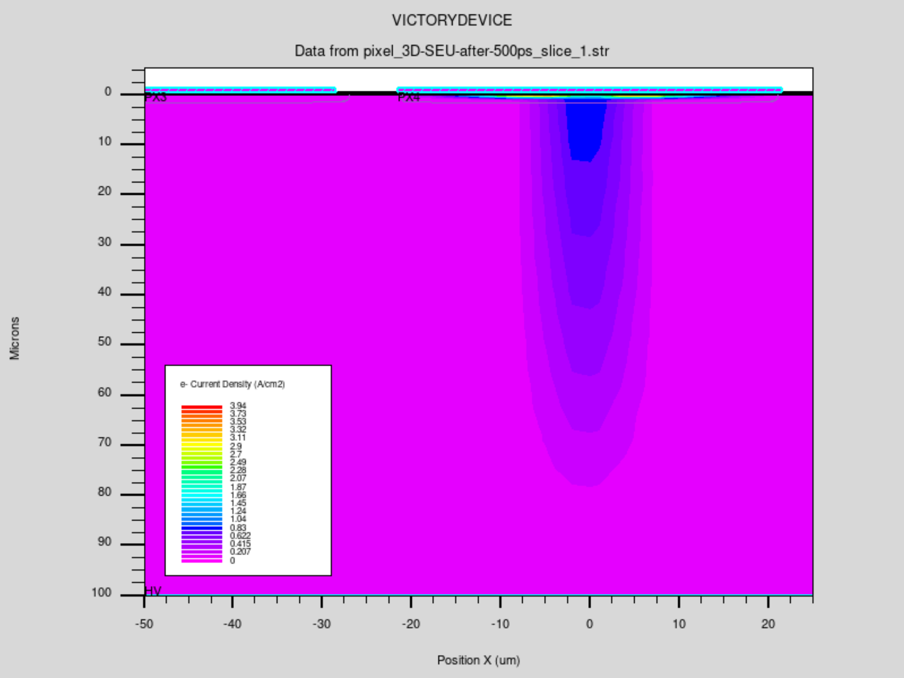
h+



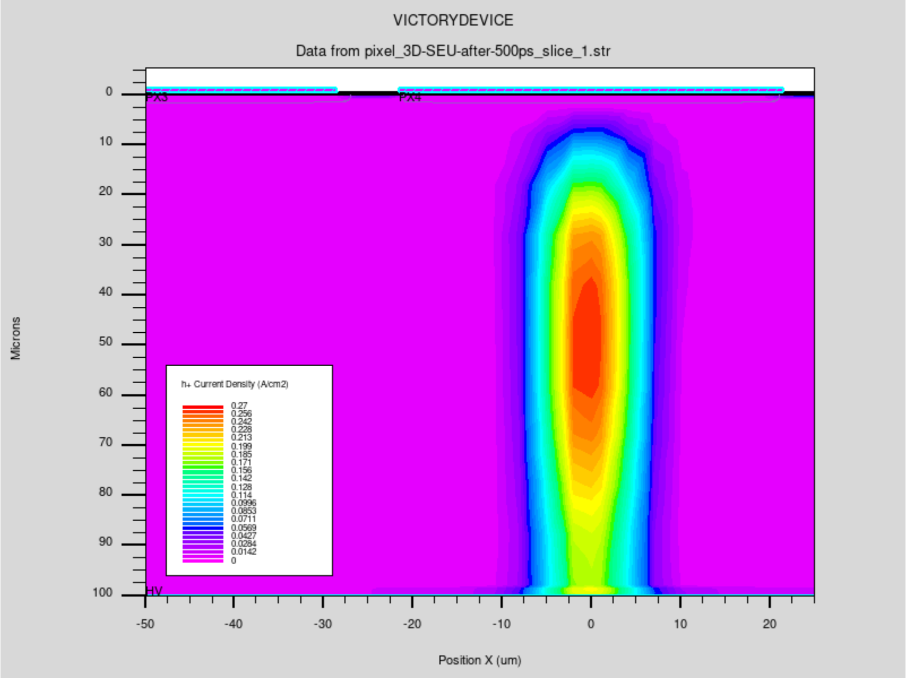
Tonyplot – Current densities

500 ps after particle strike

e-



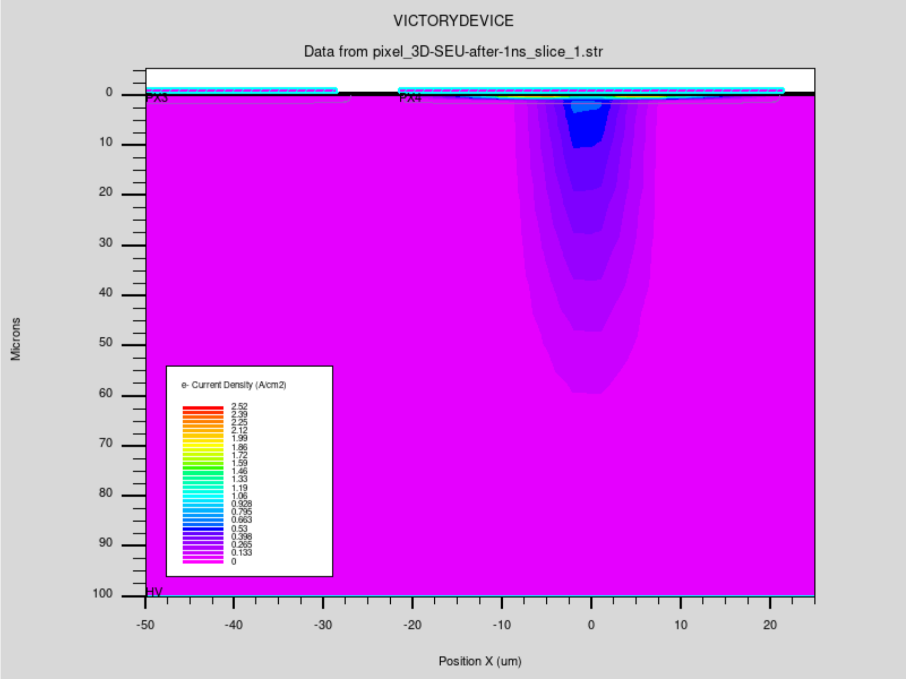
h+



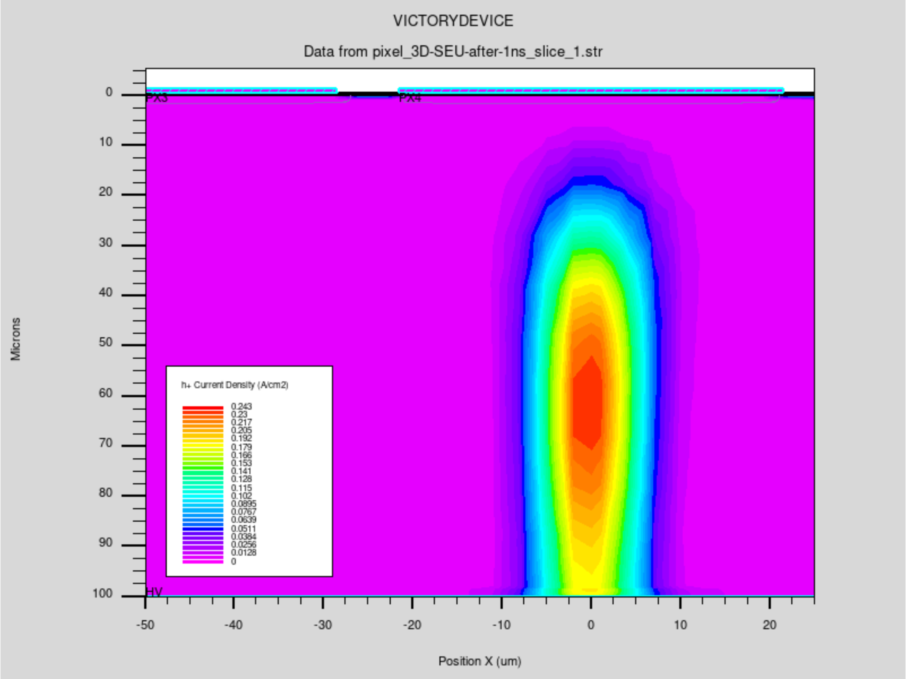
Tonyplot – Current densities

1 ns after particle strike

e-



h+

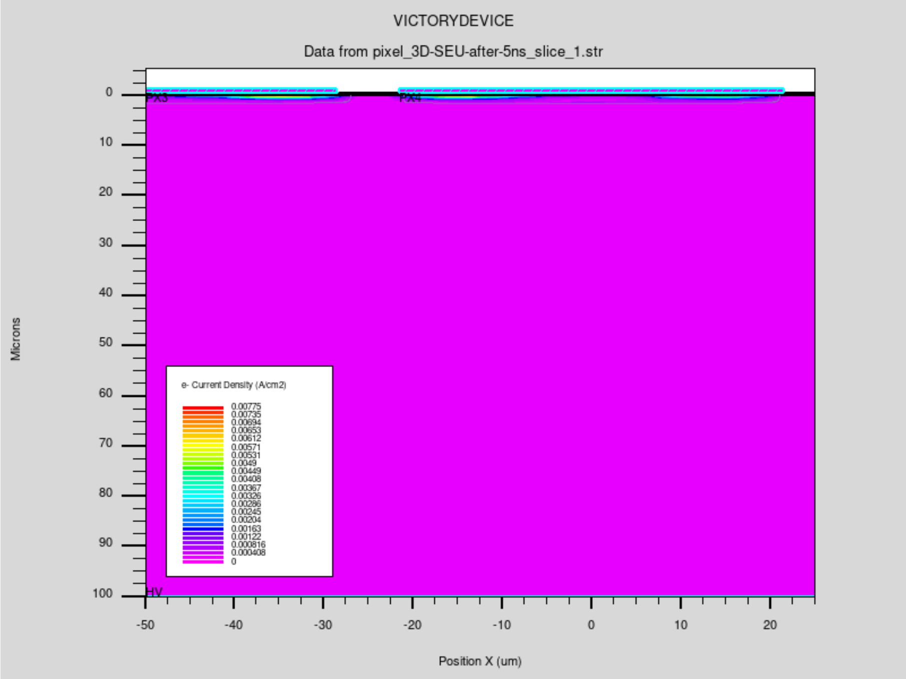


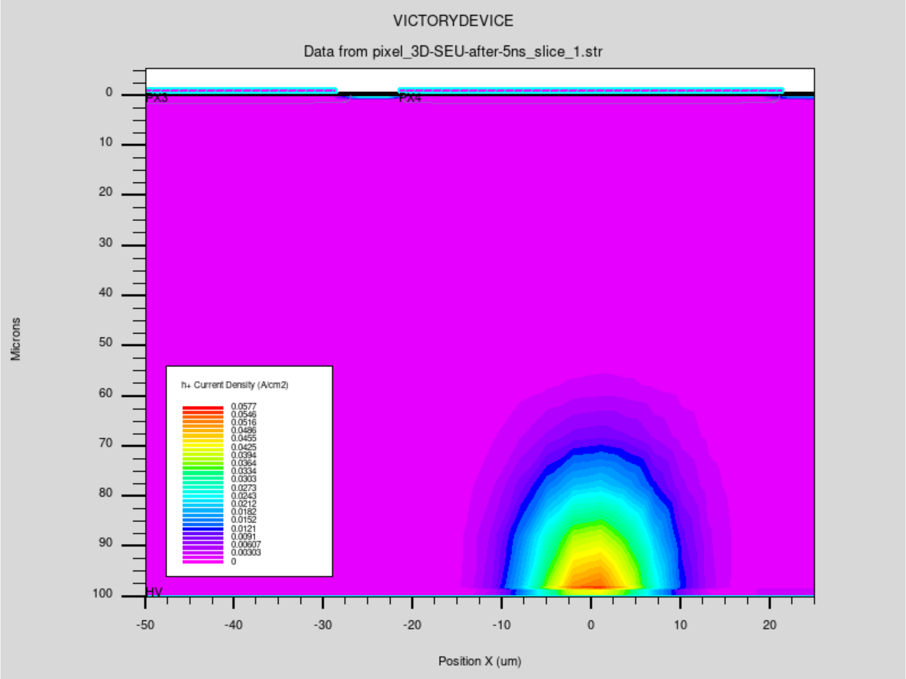
Tonyplot – Current densities

e-

5 ns after particle strike

h+

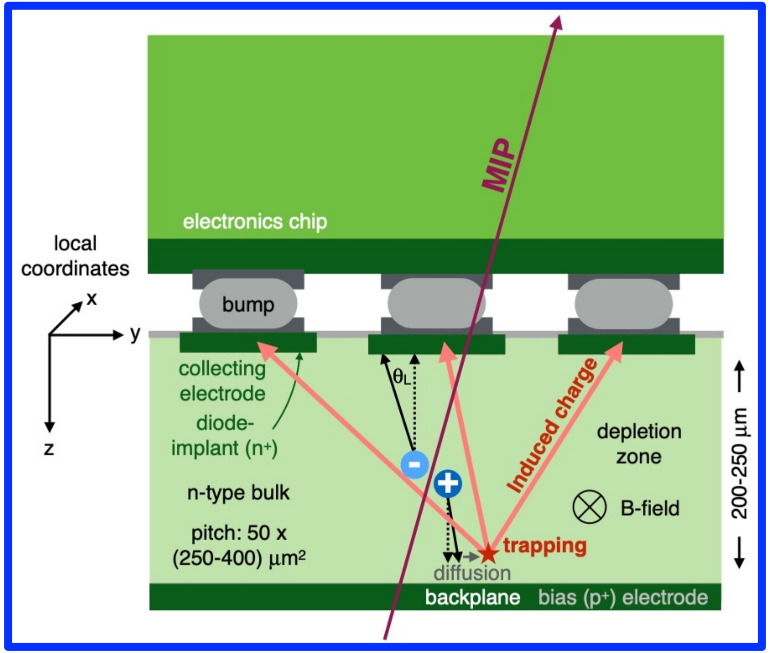




RADIATION DAMAGE SIMULATION FOR HL-LHC

Simulation radiation damage effects in ATLAS MC

Run 2 & 3



For each group of carriers the induced signal per pixel is evaluated

Modified pixel digitizer to include radiation damage effects is now the default for Run3

- ✓ Excellent agreement with data

- ➢ **But too slow for HL-LHC:**
- ➢ Increase in instantaneous and integrated luminosity from 4 to 8 with respect to the end of Run3
- ➢ Event, track and hit rate to increase similarly
- ➢ Innermost pixel layers in ATLAS to receive 1-2x10^{16} n_{eq}/cm^2 after 2000 fb^{-1} , x10 more fluence than end of Run2
- ➢ **Need for faster algorithm**

About ITk Pixel: see the overview talk

ATLAS strategy

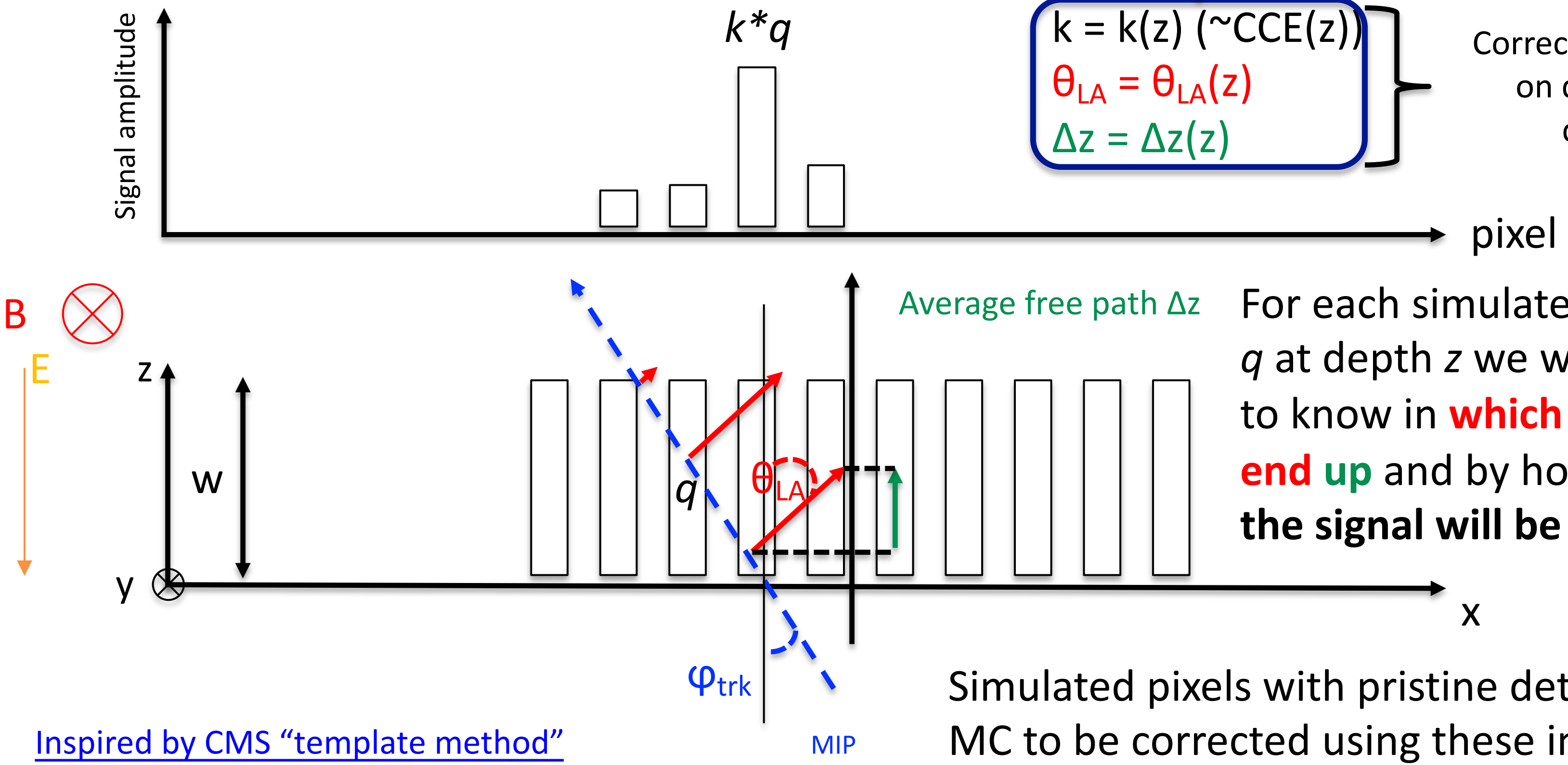
Lookup Tables (LUTs)

$k = k(z)$ (~CCE(z))

$\theta_{LA} = \theta_{LA}(z)$

$\Delta z = \Delta z(z)$

Corrections depend on deposition depth z

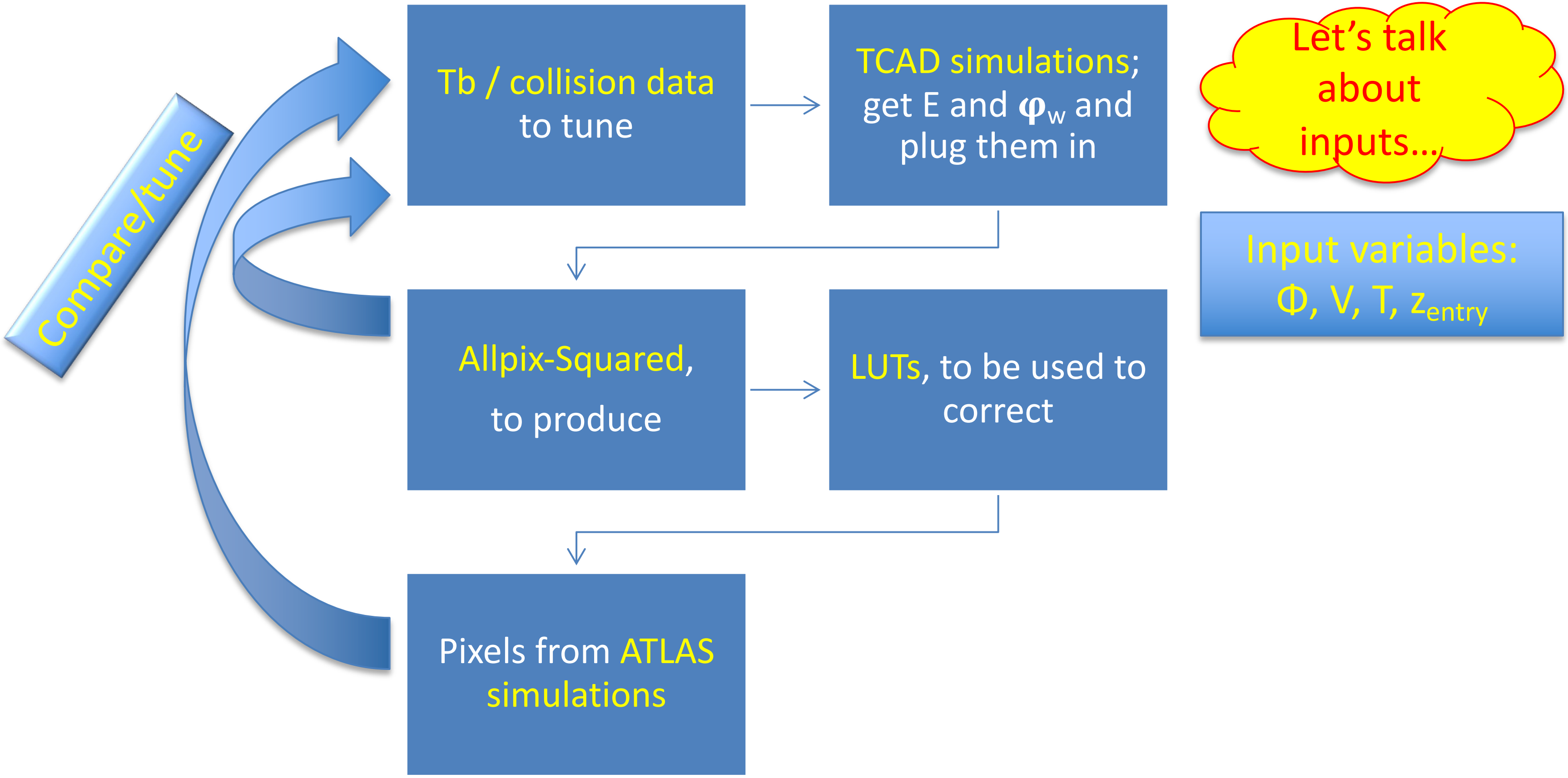


For each simulated charge *q* at depth *z* we want to know in **which pixel it will end up** and by how much (***k***) **the signal will be reduced**

Inspired by CMS "template method"

Simulated pixels with pristine detector in MC to be corrected using these information before digitization

Project workflow



Compare/tune

Tb / collision data to tune

TCAD simulations; get E and $\boldsymbol{\varphi}_w$ and plug them in

Let's talk about inputs…

Input variables: Φ, V, T, z_{entry}

Allpix-Squared, to produce

LUTs, to be used to correct

Pixels from ATLAS simulations

LHCb TCAD radiation damage model

Development of a silicon bulk radiation damage model for Sentaurus TCAD

Å. Folkestad[a,*,1], K. Akiba[b], M. van Beuzekom[c], E. Buchanan[e], P. Collins[a], E. Dall'Occo[c], A. Di Canto[a], T. Evans[d], V. Franco Lima[f], J. García Pardiñas[g], H. Schindler[a], M. Vicente[b], M. Vieites Diaz[g], M. Williams[a]

10.1016/j.nima.2017.08.042

Table 2
Parameters of the proposed radiation damage model. The energy levels are given with respect to the valence band (E_V) or the conduction band (E_C). The model is intended to be used in conjunction with the Van Overstraeten–De Man avalanche model.

Defect number	Type	Energy level [eV]	σ_e [cm^{-2}]	σ_h [cm^{-2}]	η [cm^{-1}]
1	Donor	$E_V + 0.48$	2×10^{-14}	1×10^{-14}	4
2	Acceptor	$E_C - 0.525$	5×10^{-15}	1×10^{-14}	0.75
3	Acceptor	$E_V + 0.90$	1×10^{-16}	1×10^{-16}	36

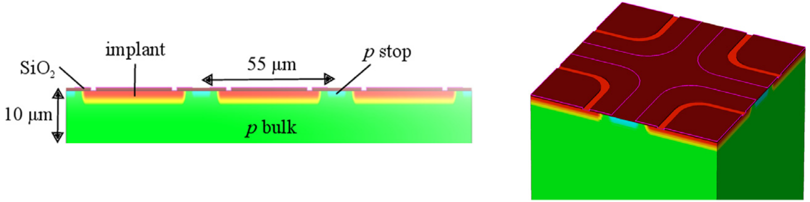


Fig. 1. Close-up of the pixel region of a (left) 2D geometry with three pixels and (right) a 3D geometry with four quarter pixels. The 2D mesh used in CCE simulations contains two additional pixels, i.e. a total of five.

Radiation damage model for n-on-p pixels

Tested up to 8x10^{15} n$_{eq}$/cm^2

Already used for preliminary estimations for ITk

Developed on Synopsys

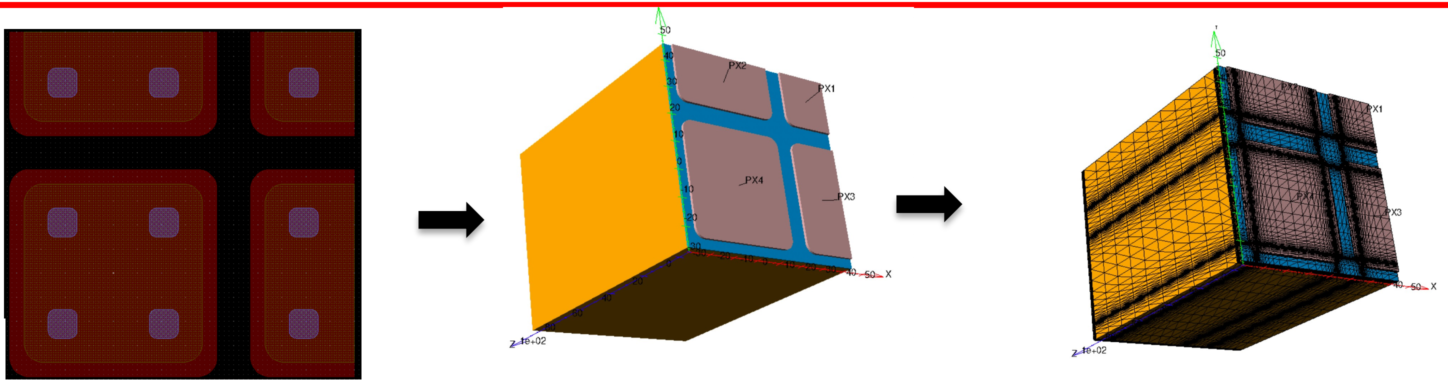
Trying to porting it in Silvaco

In the following: comparison of electric field simulations

ITk pixels simulations with TCAD

n-on-p
100 μm think
50 μm pitch

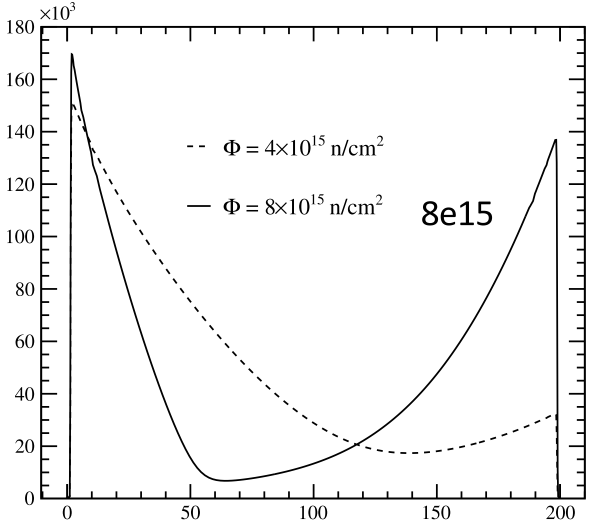
¼ of 3x3
pixels matrix

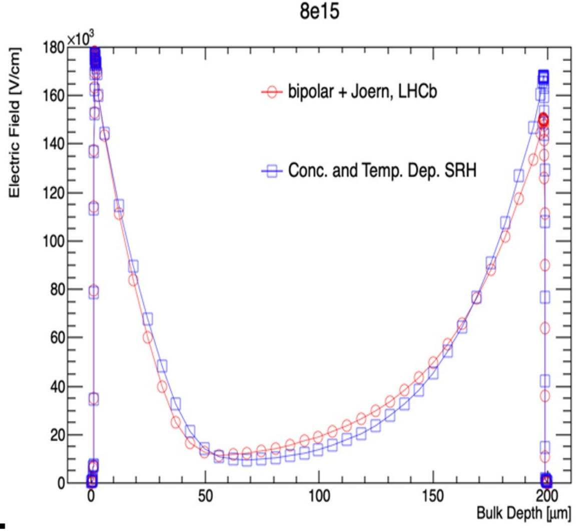


Full 3D simulation

Several models tested (mobility, recombination, bands…)

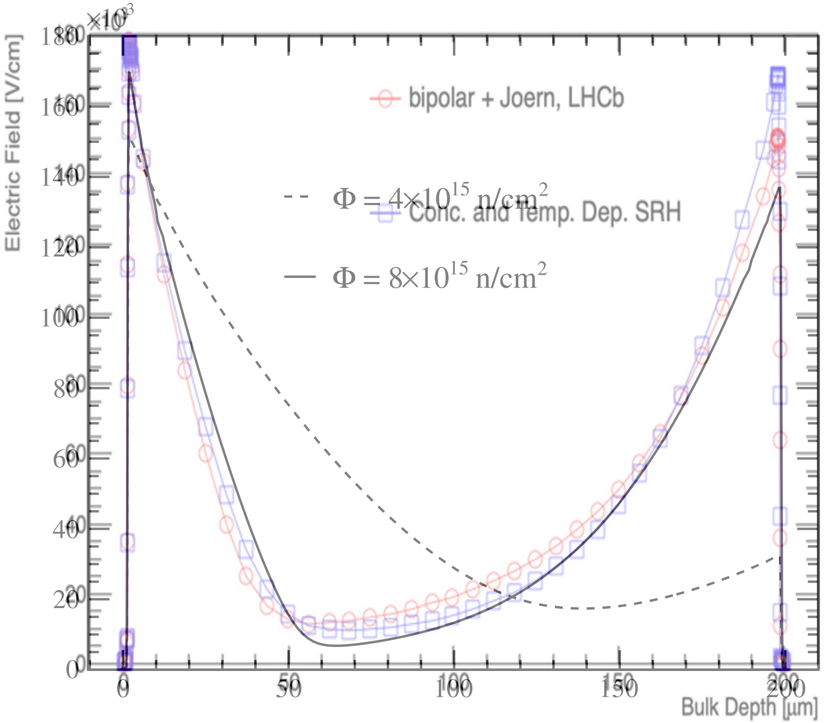
(validation done in 2D)





LHCb TCAD radiation damage model

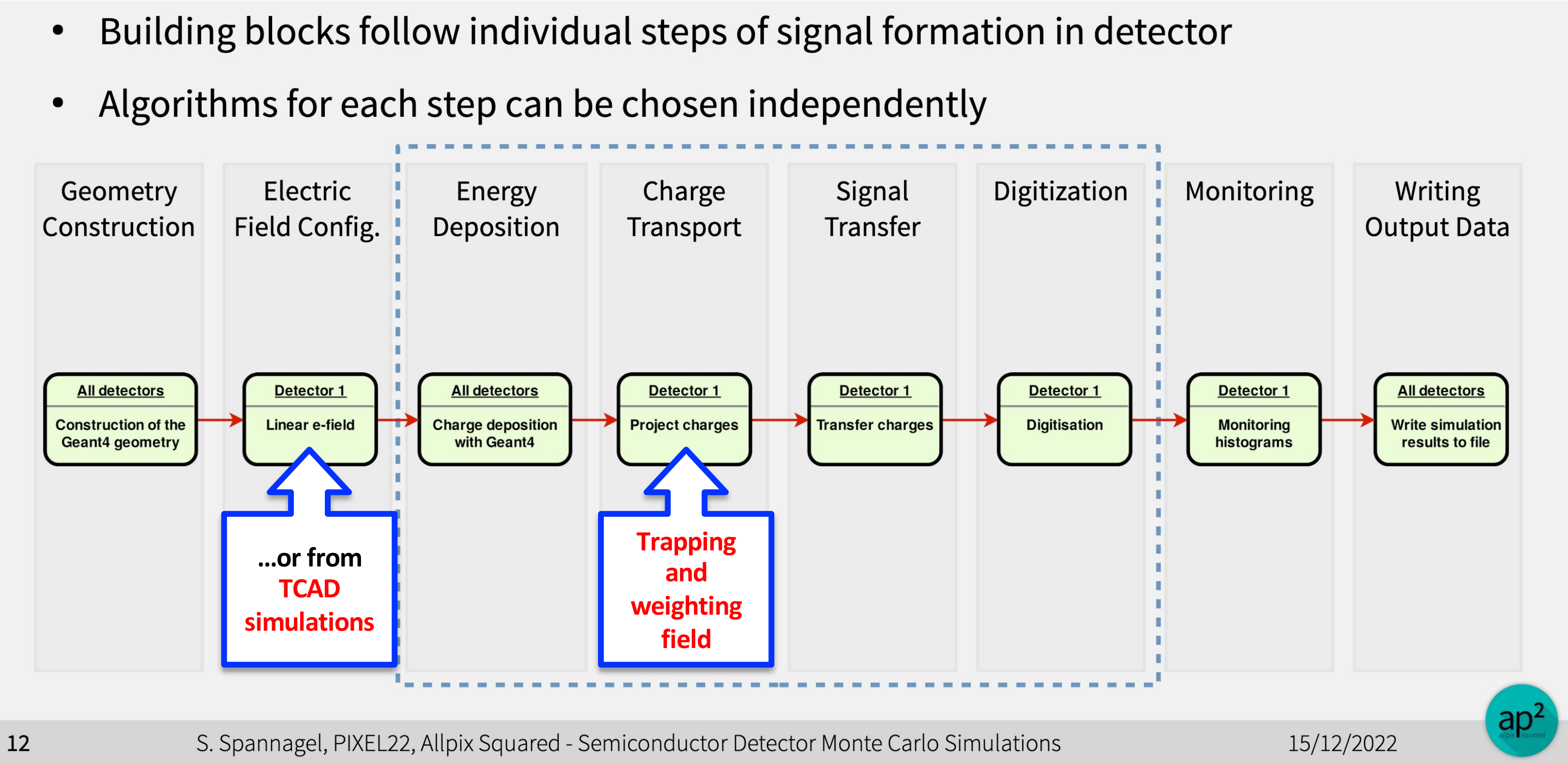
8e15



Good agreement!

LUTs calculated using Allpix2 together with TCAD

https://allpix-squared.docs.cern.ch/



- Building blocks follow individual steps of signal formation in detector
- Algorithms for each step can be chosen independently

Geometry Construction
All detectors
Construction of the Geant4 geometry

Electric Field Config.
Detector 1
Linear e-field

...or from **TCAD simulations**

Energy Deposition
All detectors
Charge deposition with Geant4

Charge Transport
Detector 1
Project charges

Trapping and weighting field

Signal Transfer
Detector 1
Transfer charges

Digitization
Detector 1
Digitisation

Monitoring
Detector 1
Monitoring histograms

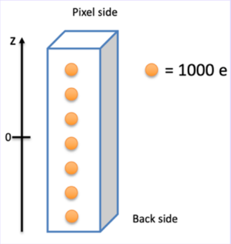
Writing Output Data
All detectors
Write simulation results to file

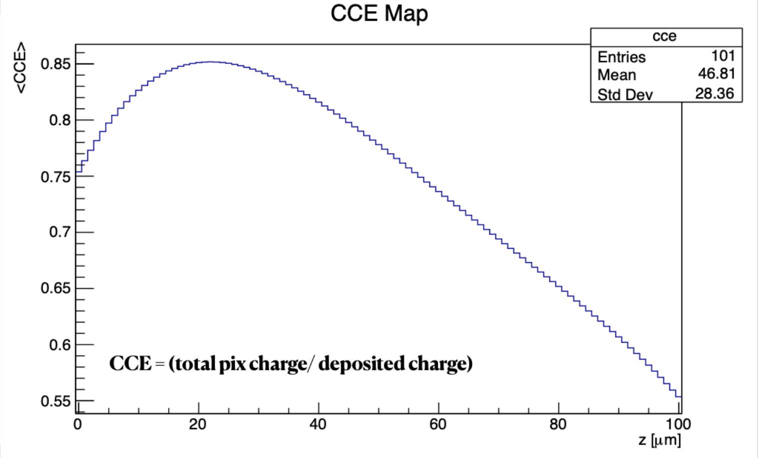
12 S. Spannagel, PIXEL22, Allpix Squared - Semiconductor Detector Monte Carlo Simulations 15/12/2022

LUTs example

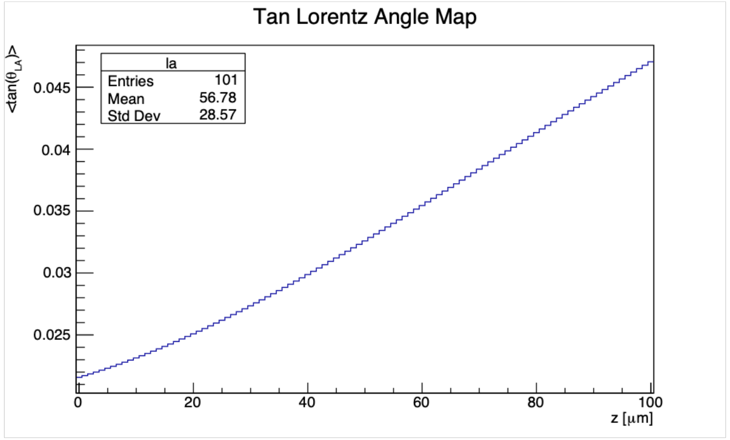
(Keerthi Nakkalil, APC)

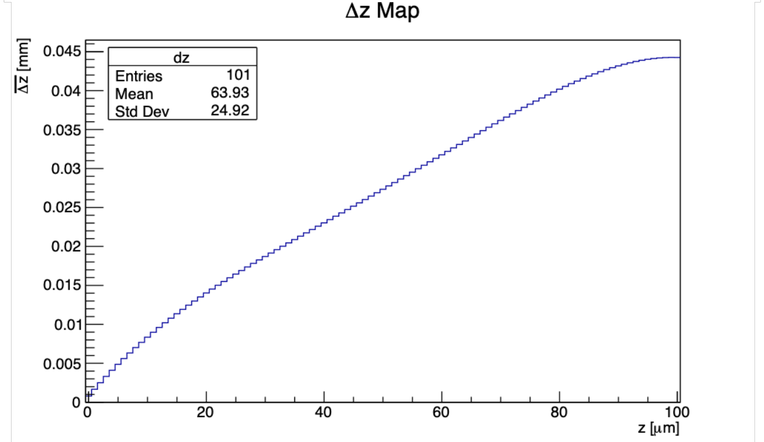
- Simulate point deposition ([DepositionPointCharge]) at different z position
  - 1 simulation per Z position
  - 100 events per Z position
  - 1000e deposited per event
  - Scan performed every 1 um
  - Simulation for 100 µm thick sensor at **4×10^{15} n_{eq}/cm^2** and **600 V**





CCE = (total pix charge/ deposited charge)

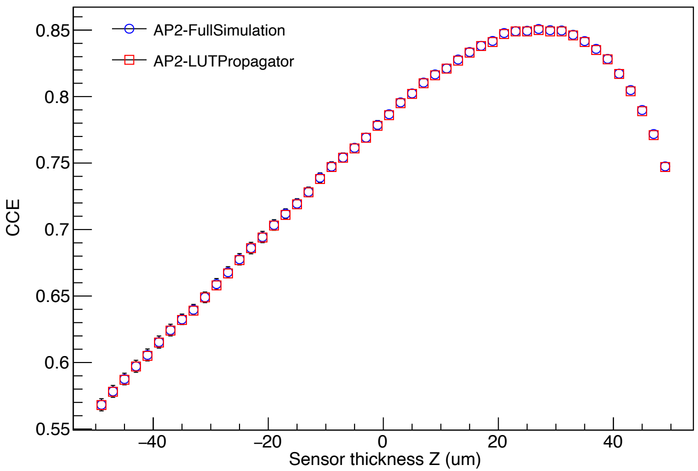


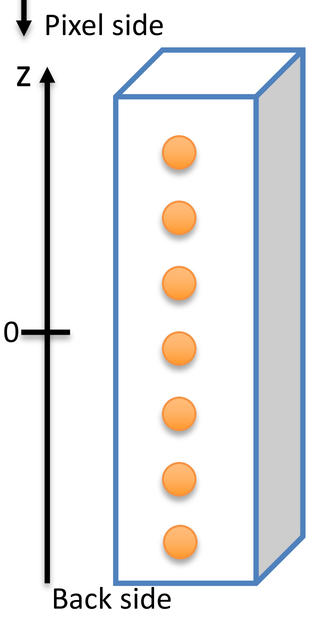


Closure test

(Keerthi Nakkalil, APC)

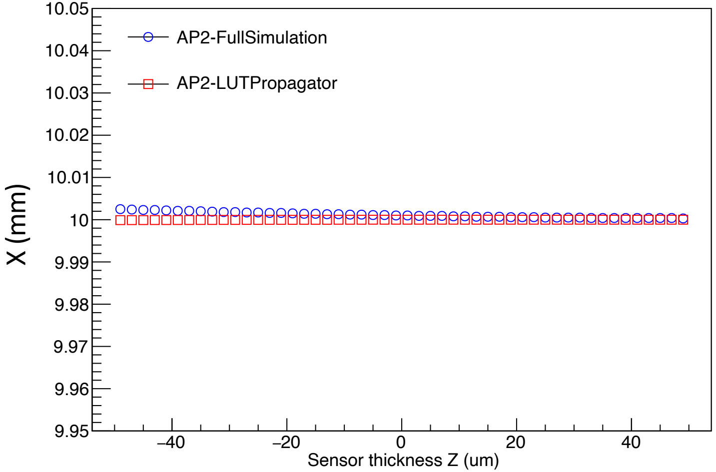
- Deposit 1000e every um along sensor bulk
- Scale the charges using **CCE** LUT
- Propagate the carriers using **tan(LA)** and **Δz** LUTs
- Compare the results with full AP2 simulation

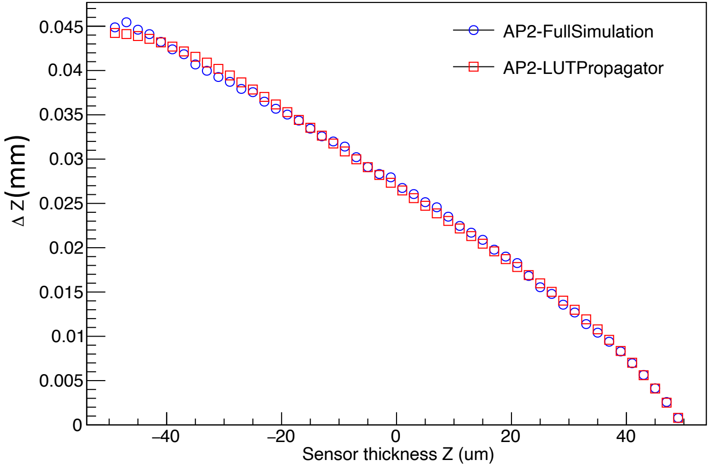




● = 1000 e

Excellent agreement!





CONCLUSIONS AND OUTLOOK

Conclusions and Outlook

- TCAD is a very powerful tool for HEP silicon sensors
- You can reduce the number of submission, and so cutting time and money to get results, and get insight into physics!
- Combining TCAD simulations, laboratory and testbeam data can probe fundamental quantities like electric field distribution, trapping, etc. and use them to making quantitative predictions, even after heavy irradiation
- A solid knowledge of semiconductor physics, and good data inputs are recommended to fully exploit TCAD simulations
- If you are interested in working with TCAD simulations, feel free to contact me: marco.bomben@cern.ch


https://indico.in2p3.fr/e/simdet2023
SIMDET
2023
5th school on silicon detectors simulation

THANK YOU!