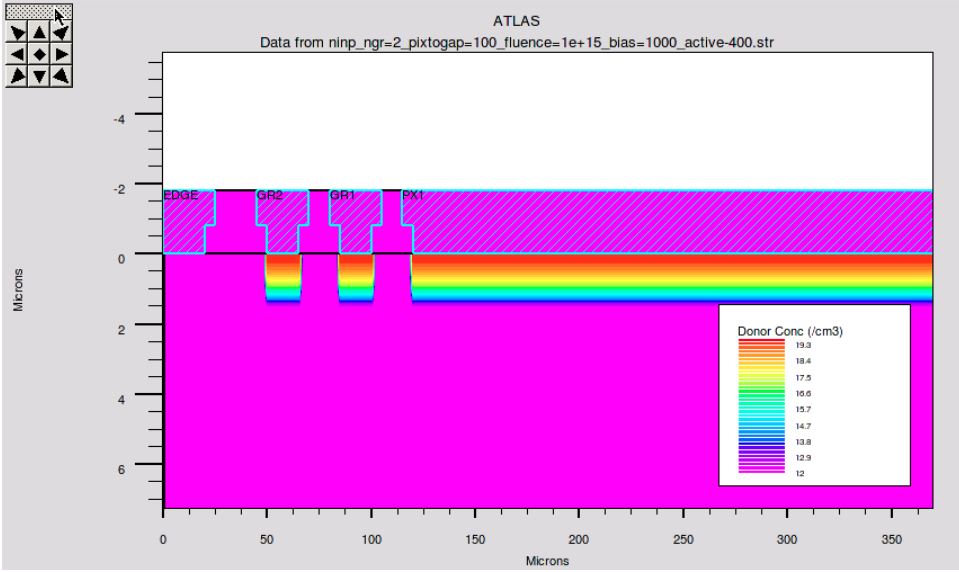
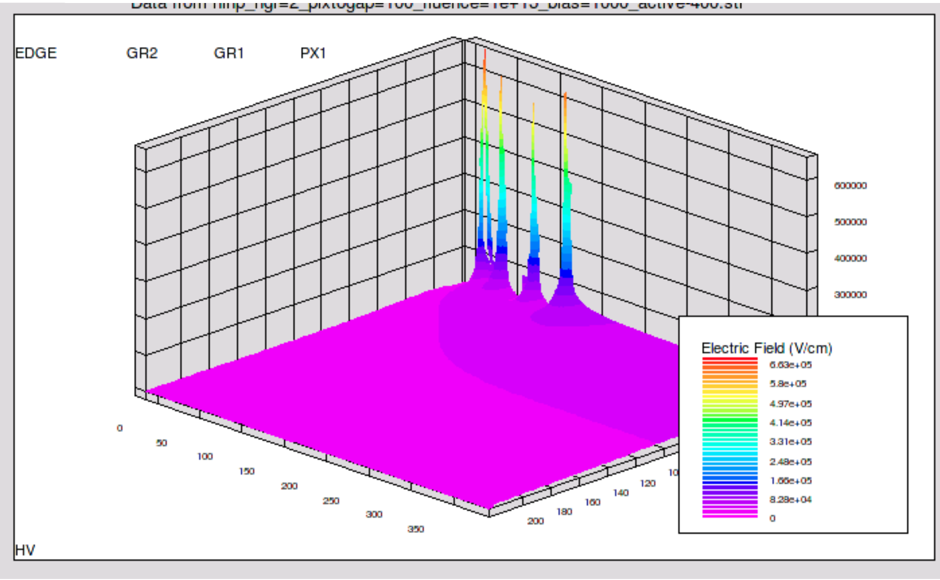
Introduction to TCAD Simulations

Marco Bomben – LPNHE (Paris)





Outline

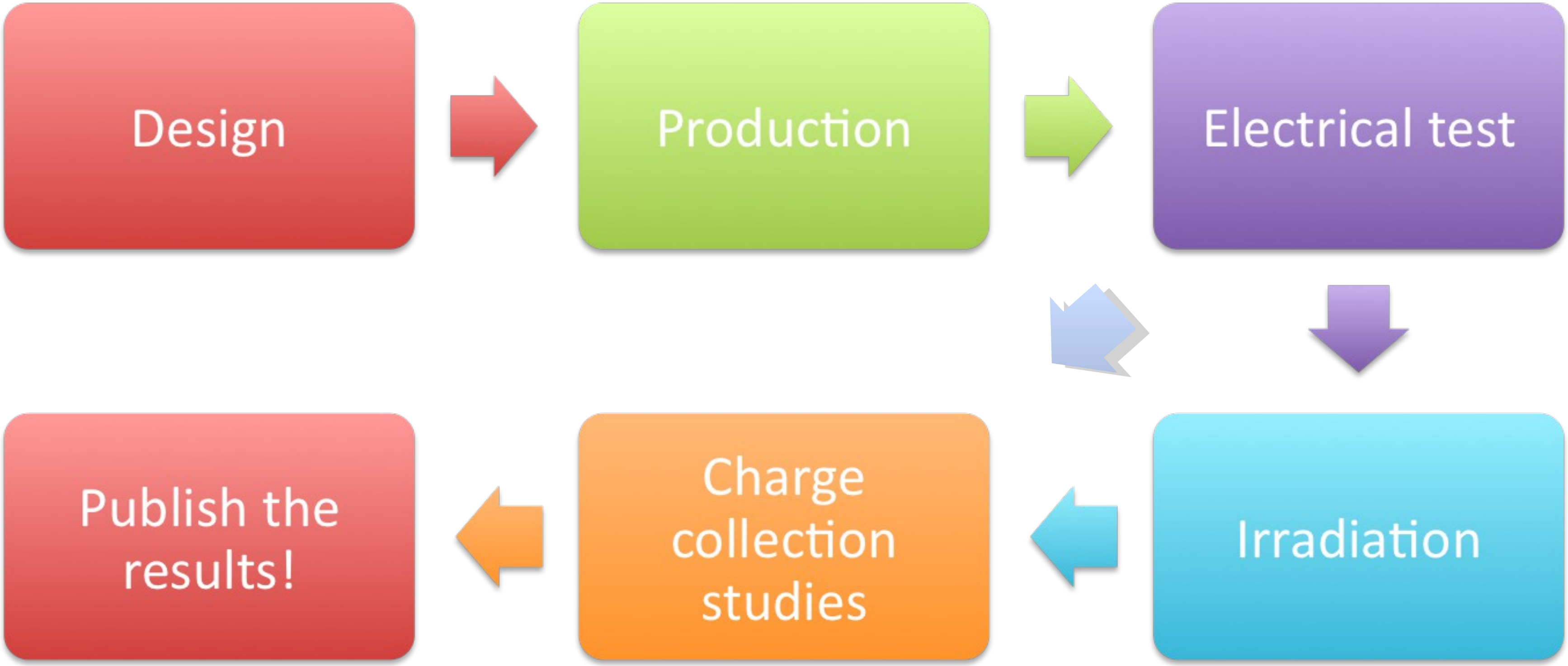
- Introduction
- Presentation of some of the packages
- Selected results
- Comments and conclusions

INTRODUCTION

Introduction

- Technology Computer Aided Design - TCAD

Normal work flow for a HEP silicon sensors



Design

Production

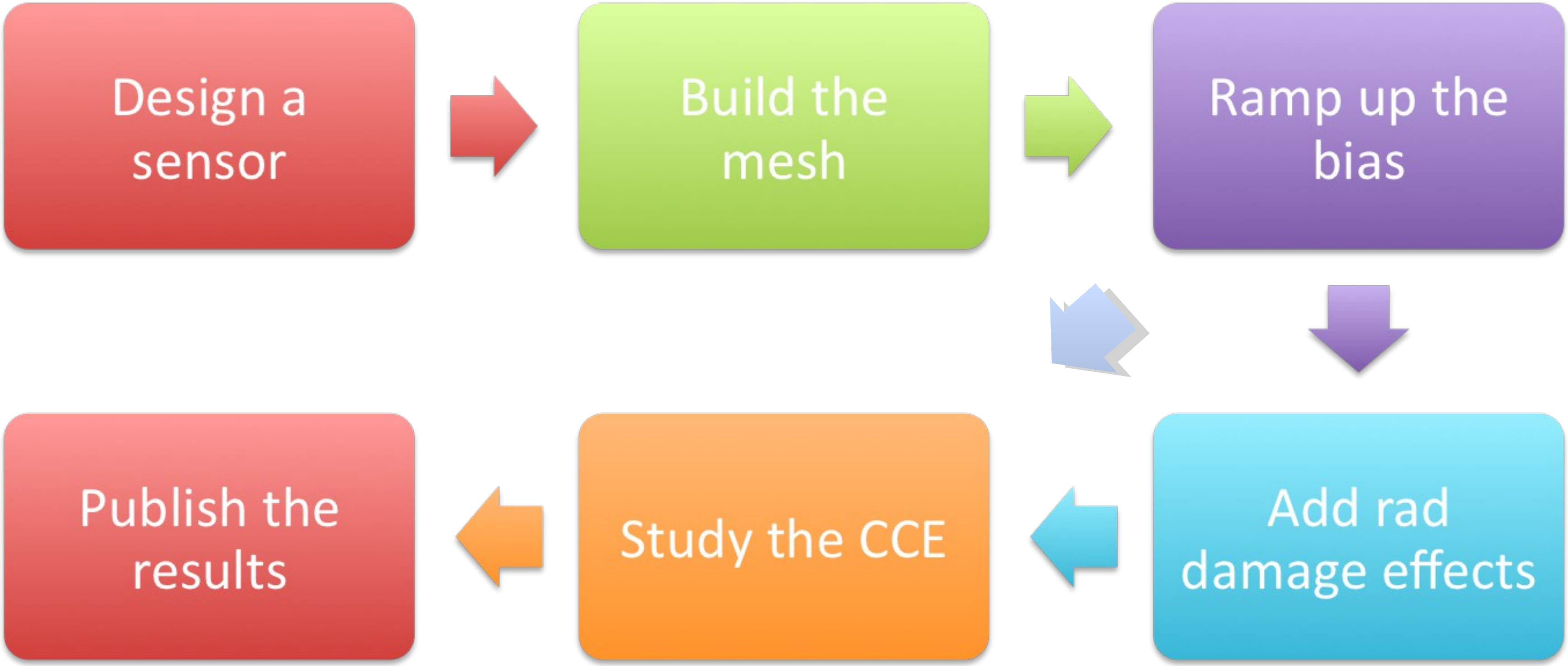
Electrical test

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

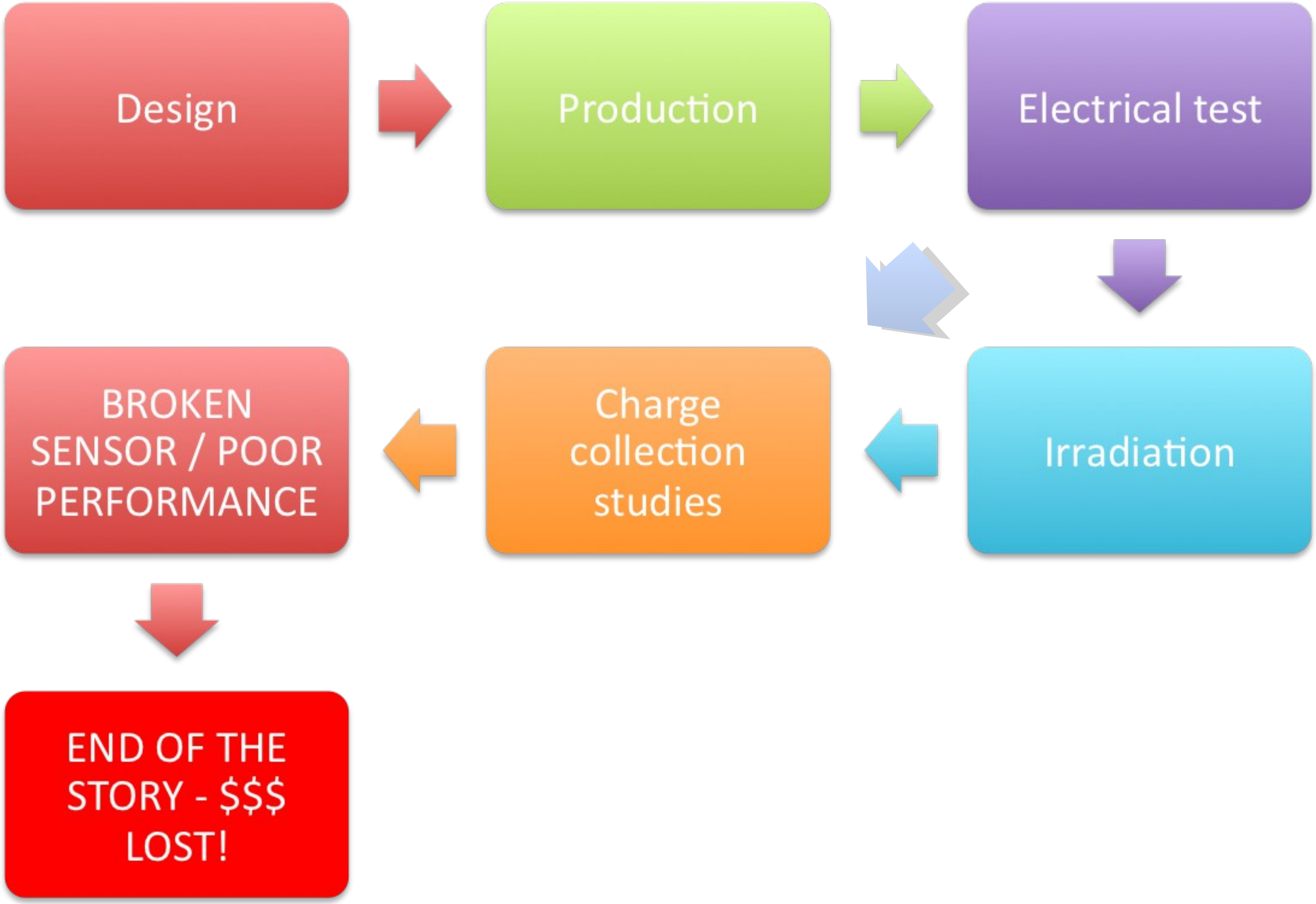
So why bother with simulations?

- 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

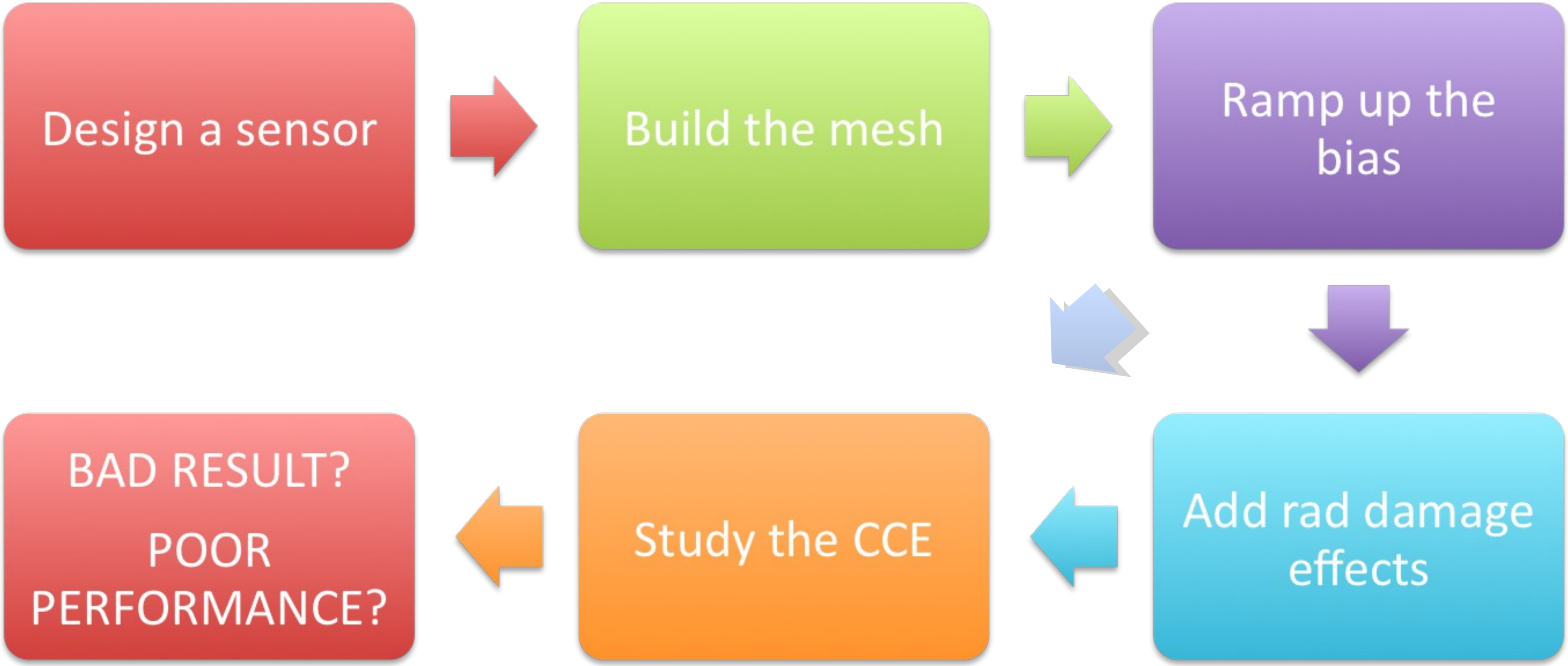
Irradiation

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

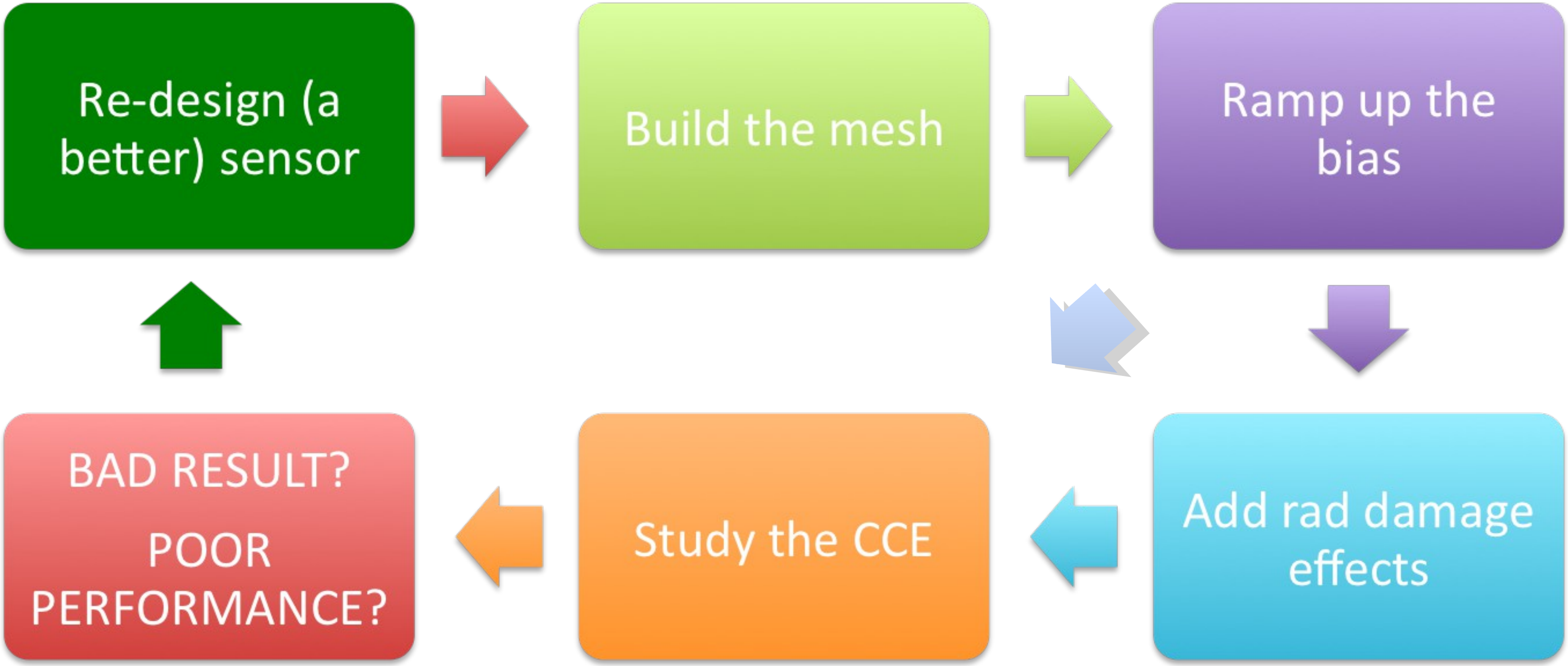
Add rad damage effects

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!

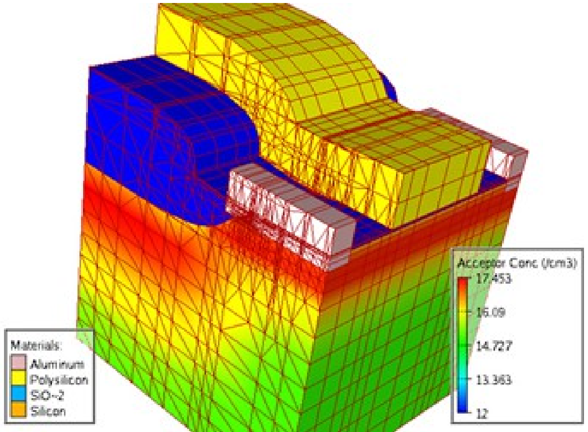
How simulation works

- Solve drift/diffusion & Poisson equations for electrons and holes:

$$J_n = qn\mu_n E + qD_n \frac{\partial n}{\partial x} \qquad J_p = qp\mu_p E - qD_p \frac{\partial p}{\partial x} \qquad \frac{\partial n}{\partial t} = \frac{1}{q}\frac{\partial J_n}{\partial x} + G_n - R_n$$

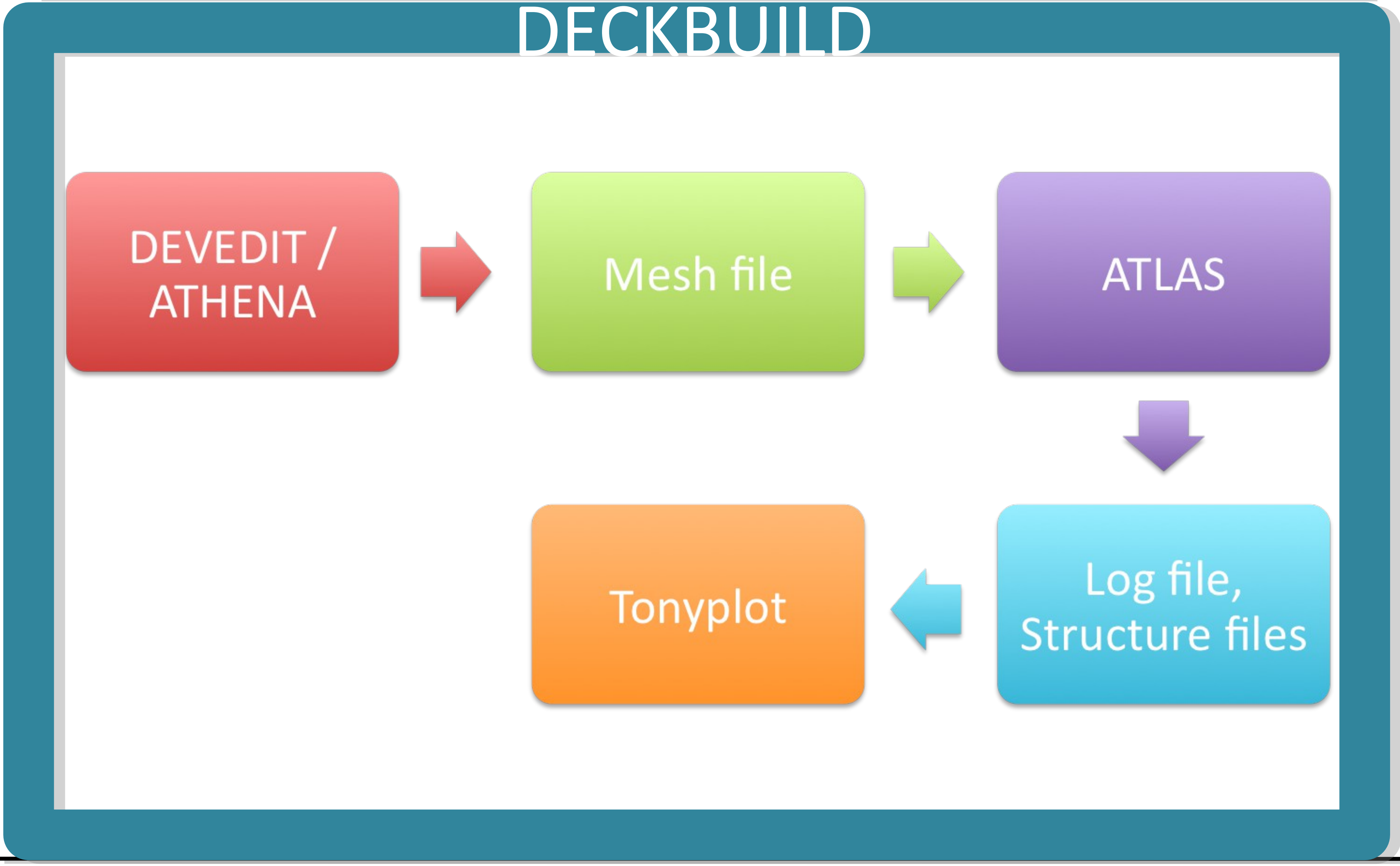
$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{q}{\epsilon_{Si}\epsilon_0}(N_D + p(x) - n(x) - N_A) \qquad \frac{\partial p}{\partial t} = -\frac{1}{q}\frac{\partial J_p}{\partial x} + G_p - R_p$$

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



SILVACO PACKAGES

TCAD packages & work flow



DECKBUILD

DEVEDIT / ATHENA

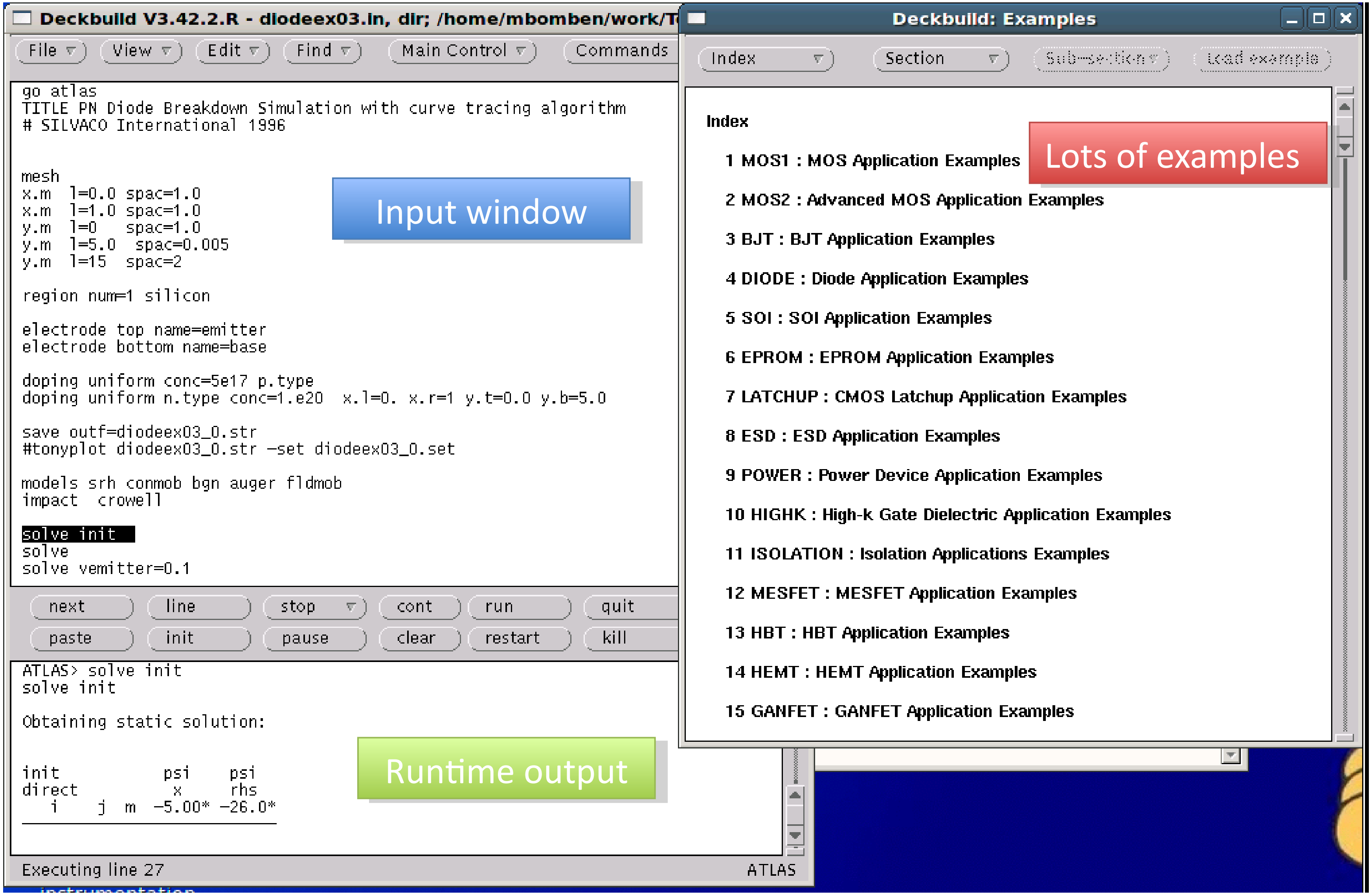
Mesh file

ATLAS

Log file, Structure files

Tonyplot

A Deckbuild session



Input window

```
go atlas
TITLE PN Diode Breakdown Simulation with curve tracing algorithm
# SILVACO International 1996


mesh
x.m  l=0.0 spac=1.0
x.m  l=1.0 spac=1.0
y.m  l=0   spac=1.0
y.m  l=5.0  spac=0.005
y.m  l=15  spac=2

region num=1 silicon

electrode top name=emitter
electrode bottom name=base

doping uniform conc=5e17 p.type
doping uniform n.type conc=1.e20  x.l=0. x.r=1 y.t=0.0 y.b=5.0

save outf=diodeex03_0.str
#tonyplot diodeex03_0.str -set diodeex03_0.set

models srh conmob bgn auger fldmob
impact  crowell

solve init
solve
solve vemitter=0.1
```

Runtime output

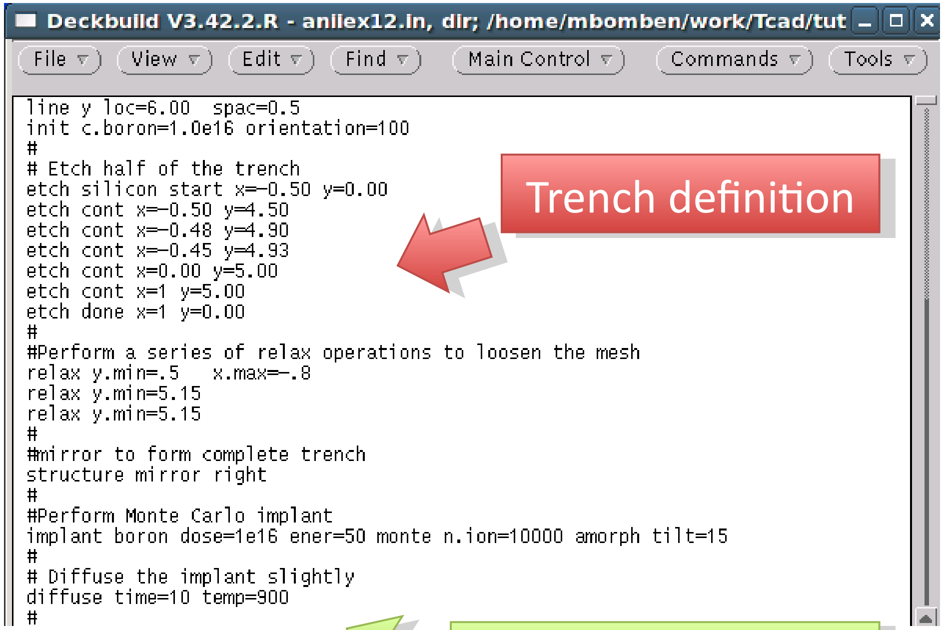
```
ATLAS> solve init
solve init

Obtaining static solution:


init            psi     psi
direct           x      rhs
  i     j  m  -5.00* -26.0*
```

Lots of examples

Index

1 MOS1 : MOS Application Examples
2 MOS2 : Advanced MOS Application Examples
3 BJT : BJT Application Examples
4 DIODE : Diode Application Examples
5 SOI : SOI Application Examples
6 EPROM : EPROM Application Examples
7 LATCHUP : CMOS Latchup Application Examples
8 ESD : ESD Application Examples
9 POWER : Power Device Application Examples
10 HIGHK : High-k Gate Dielectric Application Examples
11 ISOLATION : Isolation Applications Examples
12 MESFET : MESFET Application Examples
13 HBT : HBT Application Examples
14 HEMT : HEMT Application Examples
15 GANFET : GANFET Application Examples

Athena: semiconductor processing simulation

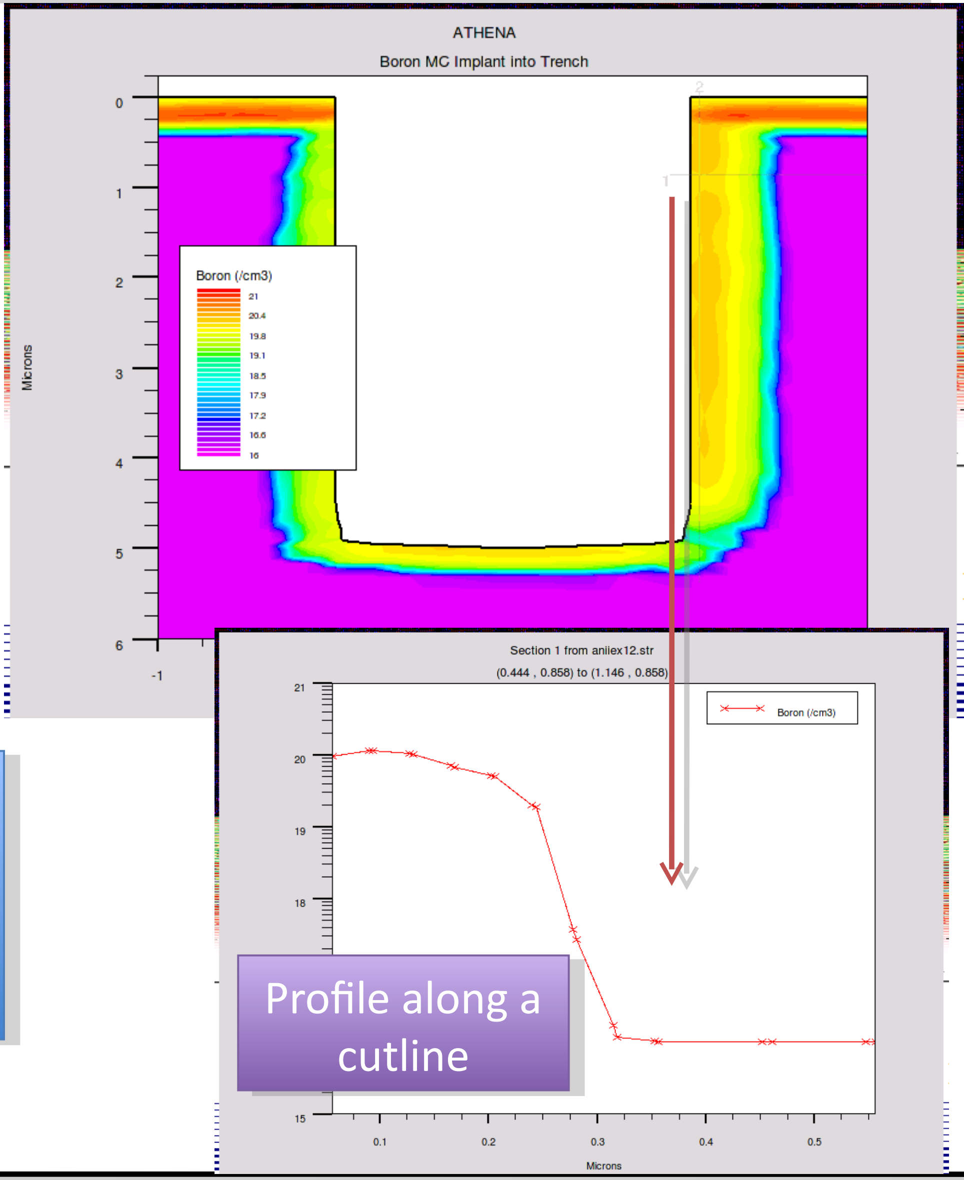


```
line y loc=6.00  spac=0.5
init c.boron=1.0e16 orientation=100
#
# Etch half of the trench
etch silicon start x=-0.50 y=0.00
etch cont x=-0.50 y=4.50
etch cont x=-0.48 y=4.90
etch cont x=-0.45 y=4.93
etch cont x=0.00 y=5.00
etch cont x=1 y=5.00
etch done x=1 y=0.00
#
#Perform a series of relax operations to loosen the mesh
relax y.min=.5   x.max=-.8
relax y.min=5.15
relax y.min=5.15
#
#mirror to form complete trench
structure mirror right
#
#Perform Monte Carlo implant
implant boron dose=1e16 ener=50 monte n.ion=10000 amorph tilt=15
#
# Diffuse the implant slightly
diffuse time=10 temp=900
#
```

Trench definition

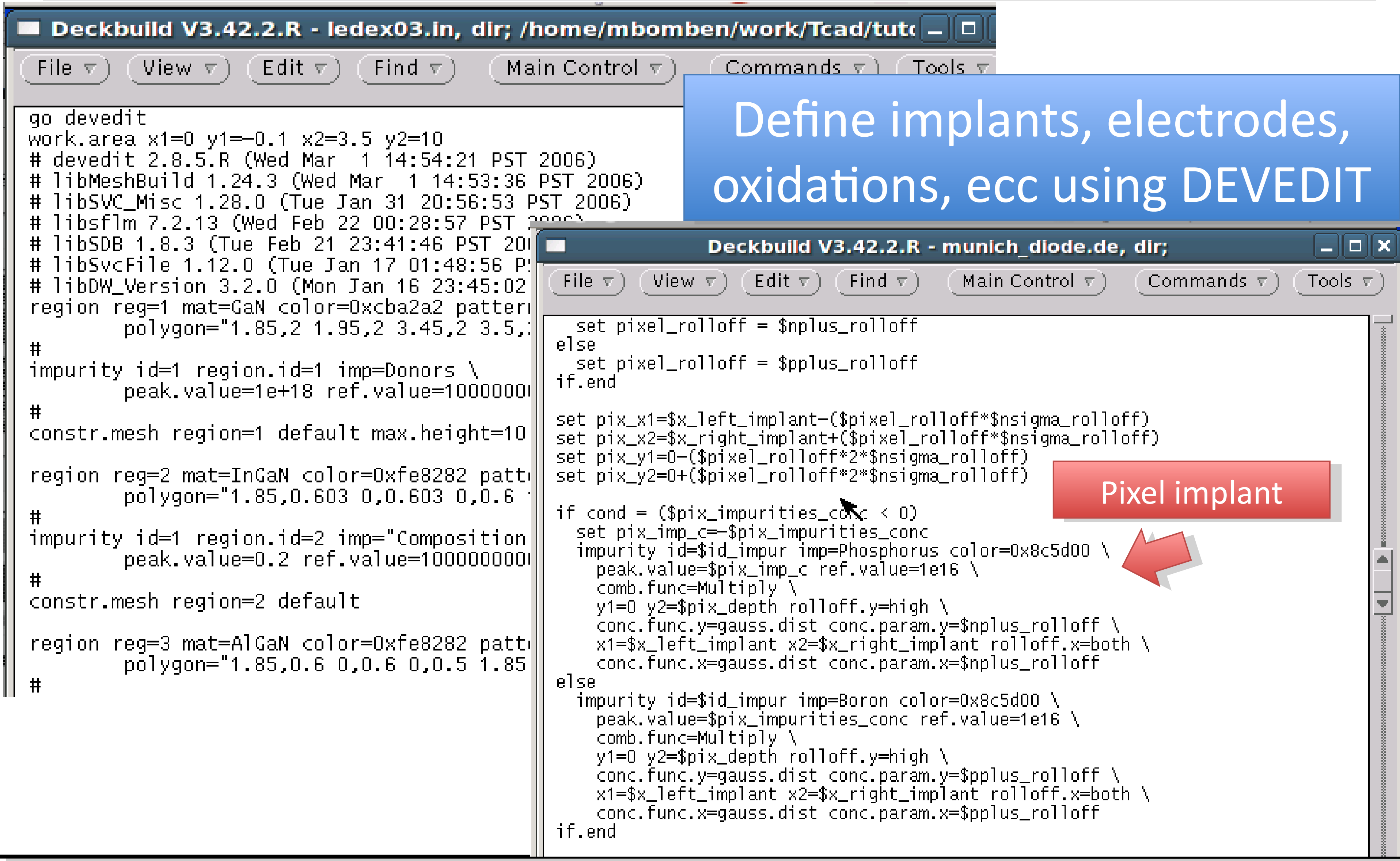
Implant definition

Define implants, trenches, oxidations, ecc using ATHENA



Profile along a cutline

Devedit: device structure editor



```
go devedit
work.area x1=0 y1=-0.1 x2=3.5 y2=10
# devedit 2.8.5.R (Wed Mar  1 14:54:21 PST 2006)
# libMeshBuild 1.24.3 (Wed Mar  1 14:53:36 PST 2006)
# libSVC_Misc 1.28.0 (Tue Jan 31 20:56:53 PST 2006)
# libsflm 7.2.13 (Wed Feb 22 00:28:57 PST
# libSDB 1.8.3 (Tue Feb 21 23:41:46 PST 20
# libSvcFile 1.12.0 (Tue Jan 17 01:48:56 P
# libDW_Version 3.2.0 (Mon Jan 16 23:45:02
region reg=1 mat=GaN color=0xcba2a2 patter
        polygon="1.85,2 1.95,2 3.45,2 3.5,
#
impurity id=1 region.id=1 imp=Donors \
        peak.value=1e+18 ref.value=1000000
#
constr.mesh region=1 default max.height=10

region reg=2 mat=InGaN color=0xfe8282 patt
        polygon="1.85,0.603 0,0.603 0,0.6 
#
impurity id=1 region.id=2 imp="Composition
        peak.value=0.2 ref.value=100000000
#
constr.mesh region=2 default

region reg=3 mat=AlGaN color=0xfe8282 patt
        polygon="1.85,0.6 0,0.6 0,0.5 1.85
#
```

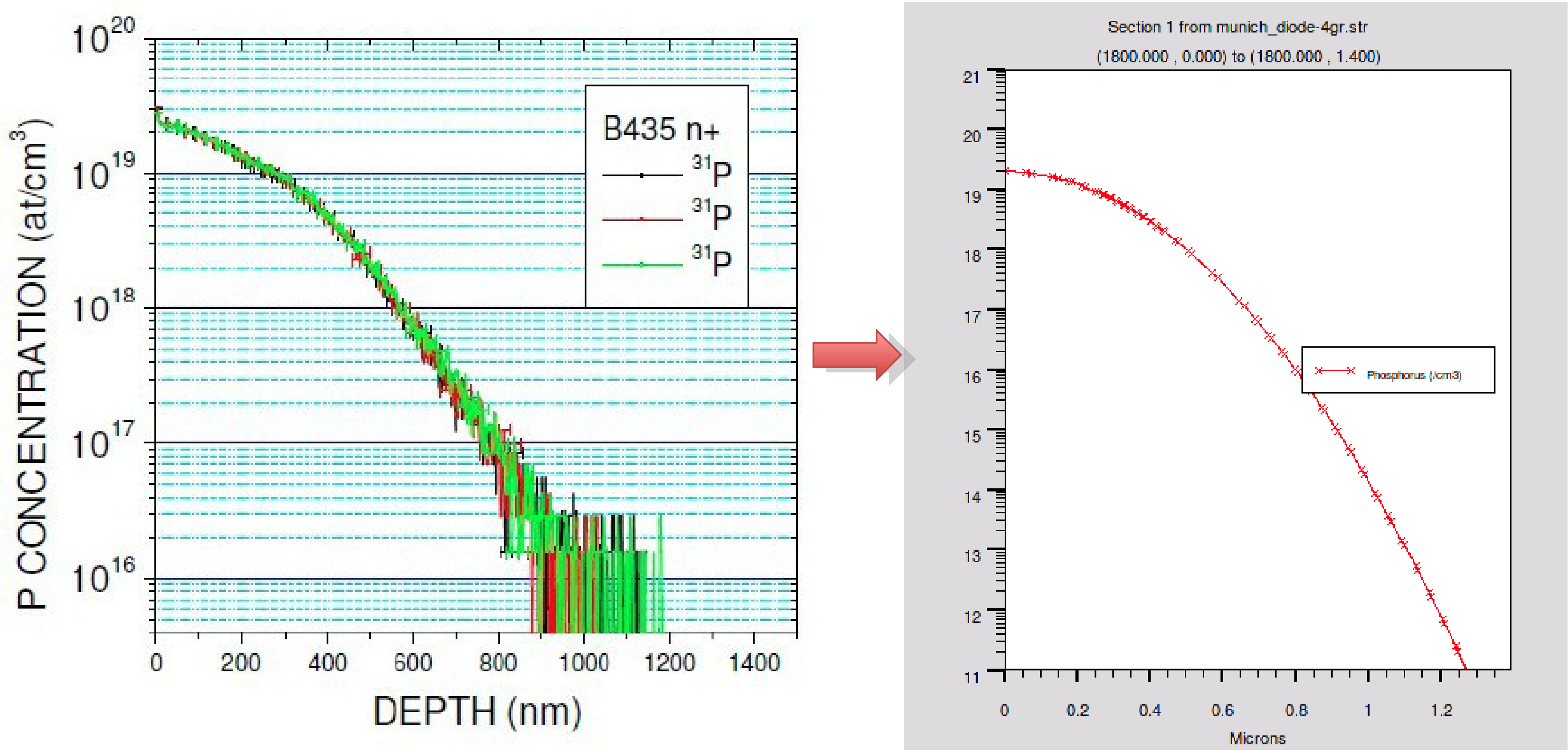
Define implants, electrodes, oxidations, ecc using DEVEDIT

```
  set pixel_rolloff = $nplus_rolloff
else
  set pixel_rolloff = $pplus_rolloff
if.end

set pix_x1=$x_left_implant-($pixel_rolloff*$nsigma_rolloff)
set pix_x2=$x_right_implant+($pixel_rolloff*$nsigma_rolloff)
set pix_y1=0-($pixel_rolloff*2*$nsigma_rolloff)
set pix_y2=0+($pixel_rolloff*2*$nsigma_rolloff)

if cond = ($pix_impurities_conc < 0)
  set pix_imp_c=-$pix_impurities_conc
  impurity id=$id_impur imp=Phosphorus color=0x8c5d00 \
    peak.value=$pix_imp_c ref.value=1e16 \
    comb.func=Multiply \
    y1=0 y2=$pix_depth rolloff.y=high \
    conc.func.y=gauss.dist conc.param.y=$nplus_rolloff \
    x1=$x_left_implant x2=$x_right_implant rolloff.x=both \
    conc.func.x=gauss.dist conc.param.x=$nplus_rolloff
else
  impurity id=$id_impur imp=Boron color=0x8c5d00 \
    peak.value=$pix_impurities_conc ref.value=1e16 \
    comb.func=Multiply \
    y1=0 y2=$pix_depth rolloff.y=high \
    conc.func.y=gauss.dist conc.param.y=$pplus_rolloff \
    x1=$x_left_implant x2=$x_right_implant rolloff.x=both \
    conc.func.x=gauss.dist conc.param.x=$pplus_rolloff
if.end
```

Pixel implant

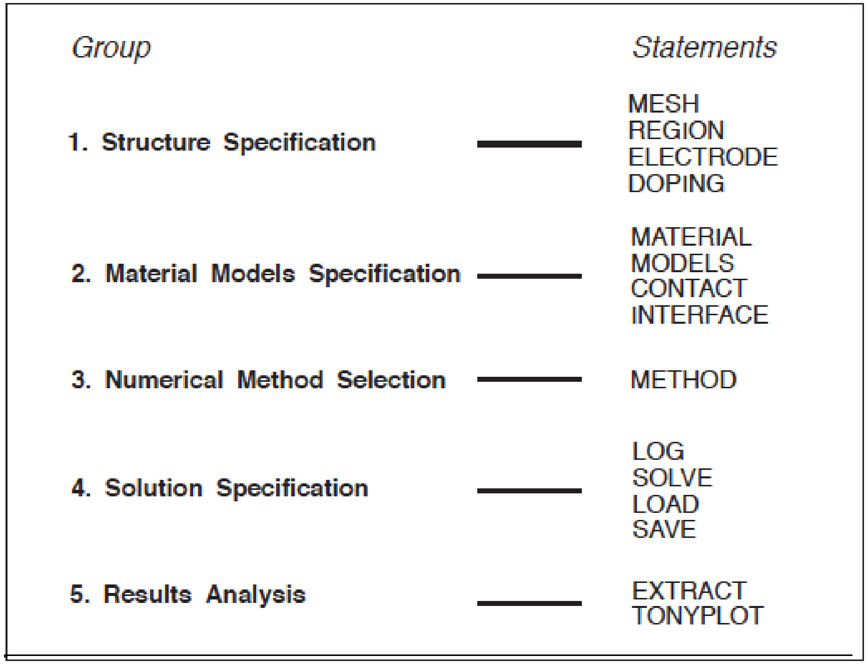
Intermezzo: TCAD inputs

- To get reliable predictions you need precise inputs; *e.g.* doping profiles via SIMS



ATLAS: device simulation

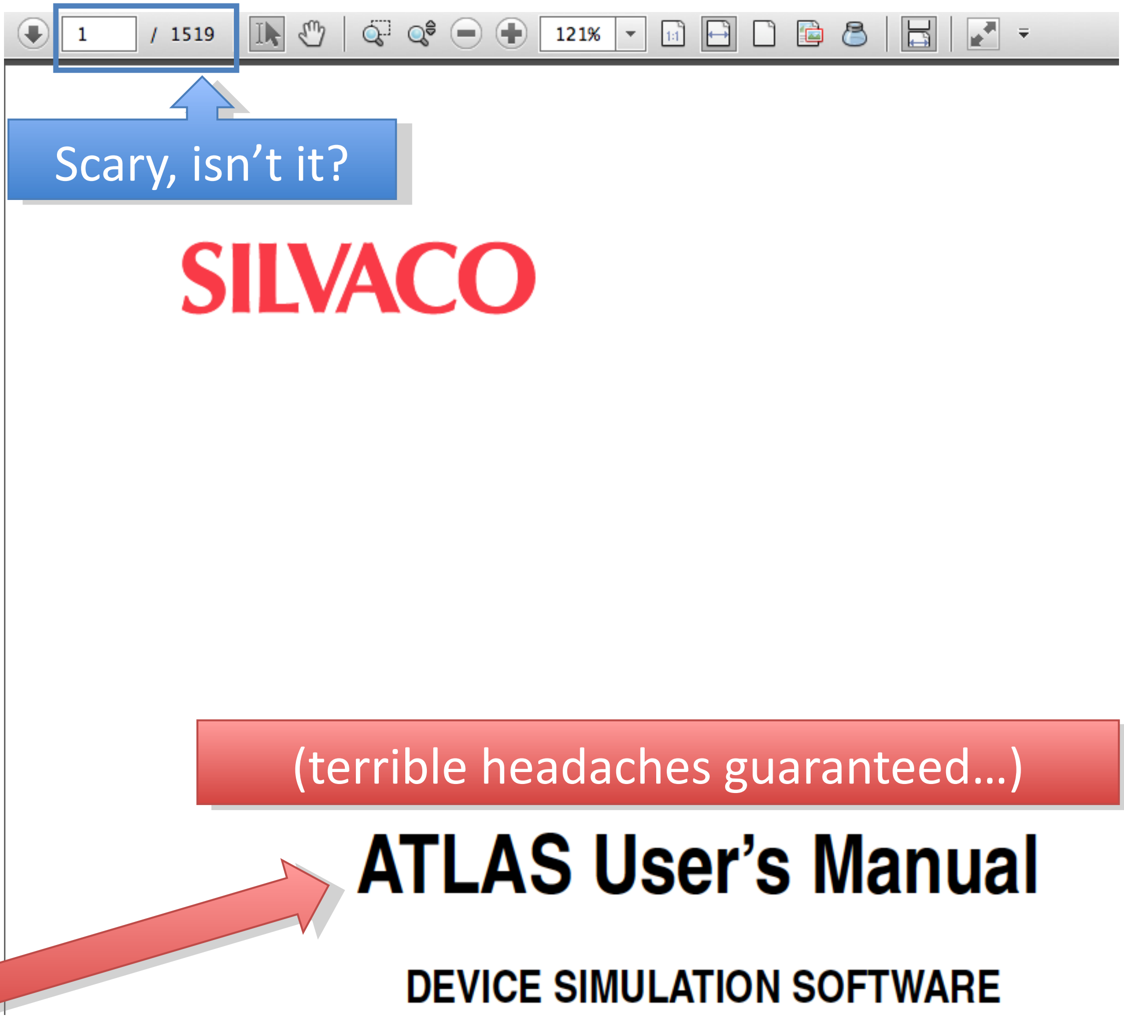
- ATLAS provides general capabilities for physically-based two (2D) and three-dimensional (3D) simulation of semiconductor devices.
- Typical simulation program structure →



Group	*Statements*
1. Structure Specification	MESH REGION ELECTRODE DOPING
2. Material Models Specification	MATERIAL MODELS CONTACT INTERFACE
3. Numerical Method Selection	METHOD
4. Solution Specification	LOG SOLVE LOAD SAVE
5. Results Analysis	EXTRACT TONYPLOT

ATLAS: main features

- TONS of models:
  - S-Pisces: Silicon Based 2D Simulator
  - 3D Device Simulator
  - Luminous: Optoelectronic Simulator
  - Single Event Upset
  - …
- LOT of options
- HUGE manual



Scary, isn't it?

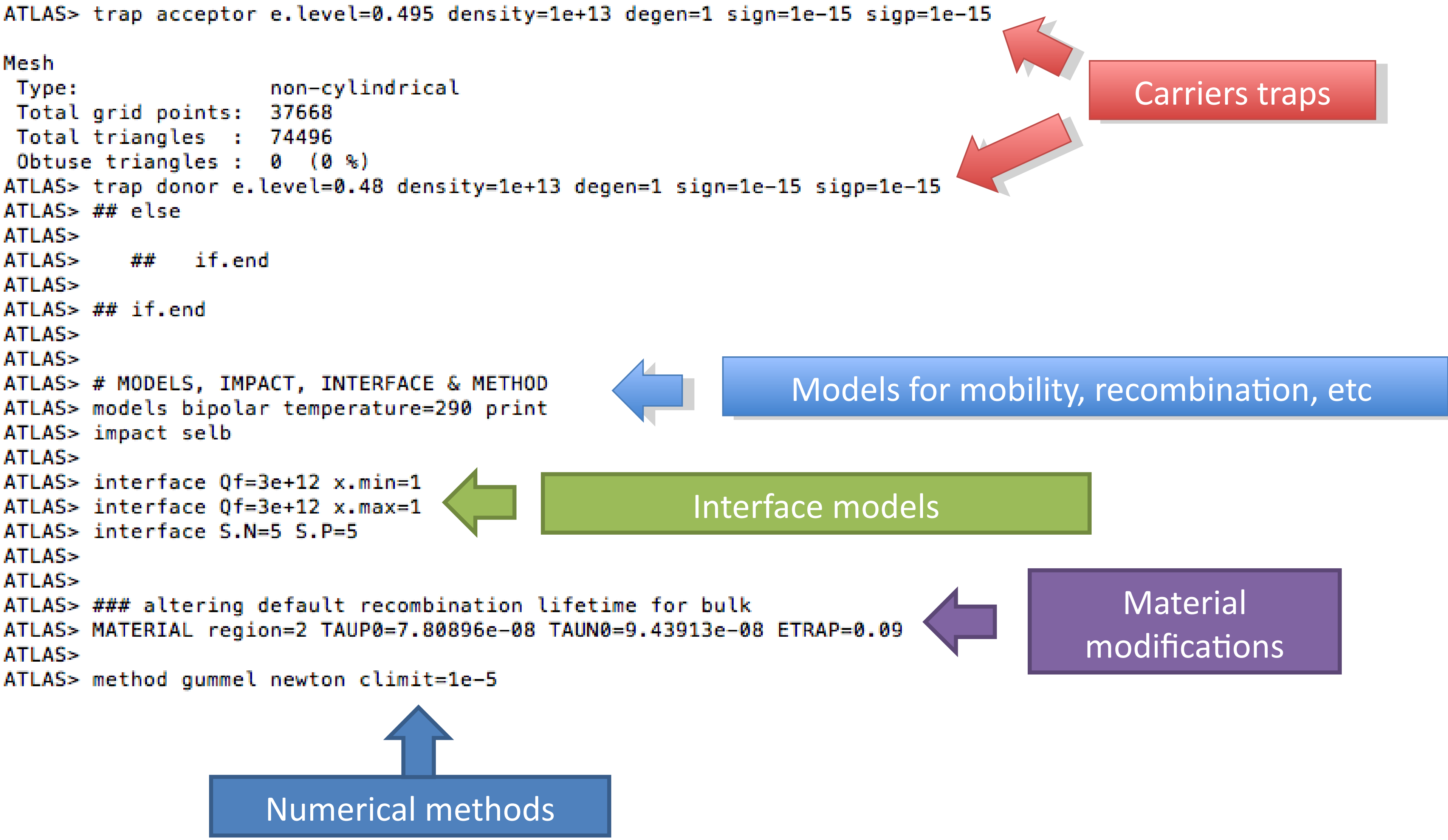
SILVACO

(terrible headaches guaranteed…)

ATLAS User's Manual

DEVICE SIMULATION SOFTWARE

ATLAS: an example



```
ATLAS> trap acceptor e.level=0.495 density=1e+13 degen=1 sign=1e-15 sigp=1e-15

Mesh
 Type:                  non-cylindrical
 Total grid points:   37668
 Total triangles   :  74496
 Obtuse triangles :   0  (0 %)
ATLAS> trap donor e.level=0.48 density=1e+13 degen=1 sign=1e-15 sigp=1e-15
ATLAS> ## else
ATLAS>
ATLAS>    ##    if.end
ATLAS>
ATLAS> ## if.end
ATLAS>
ATLAS>
ATLAS> # MODELS, IMPACT, INTERFACE & METHOD
ATLAS> models bipolar temperature=290 print
ATLAS> impact selb
ATLAS>
ATLAS> interface Qf=3e+12 x.min=1
ATLAS> interface Qf=3e+12 x.max=1
ATLAS> interface S.N=5 S.P=5
ATLAS>
ATLAS>
ATLAS> ### altering default recombination lifetime for bulk
ATLAS> MATERIAL region=2 TAUP0=7.80896e-08 TAUN0=9.43913e-08 ETRAP=0.09
ATLAS>
ATLAS> method gummel newton climit=1e-5
```

Carriers traps

Models for mobility, recombination, etc

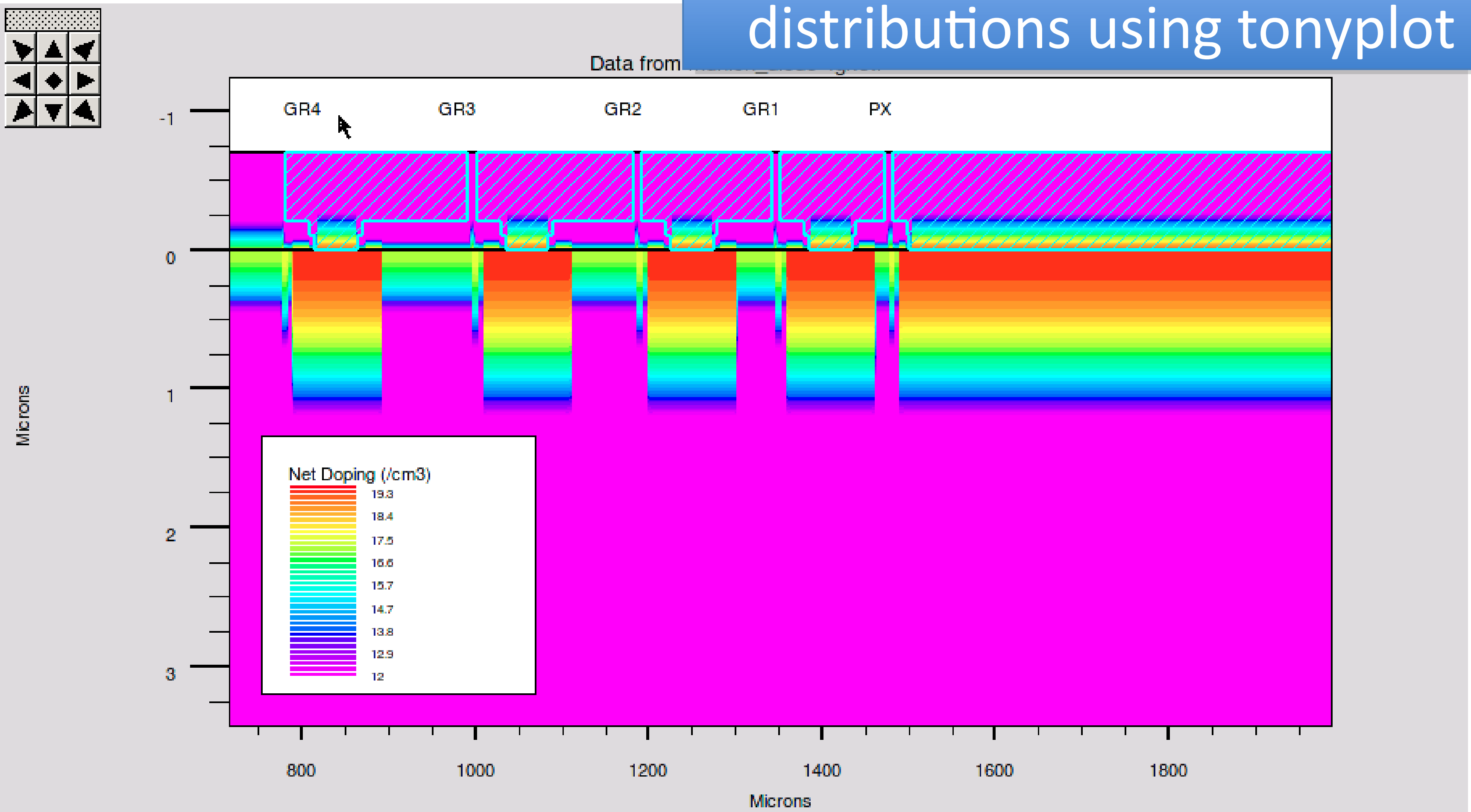
Interface models

Material modifications

Numerical methods

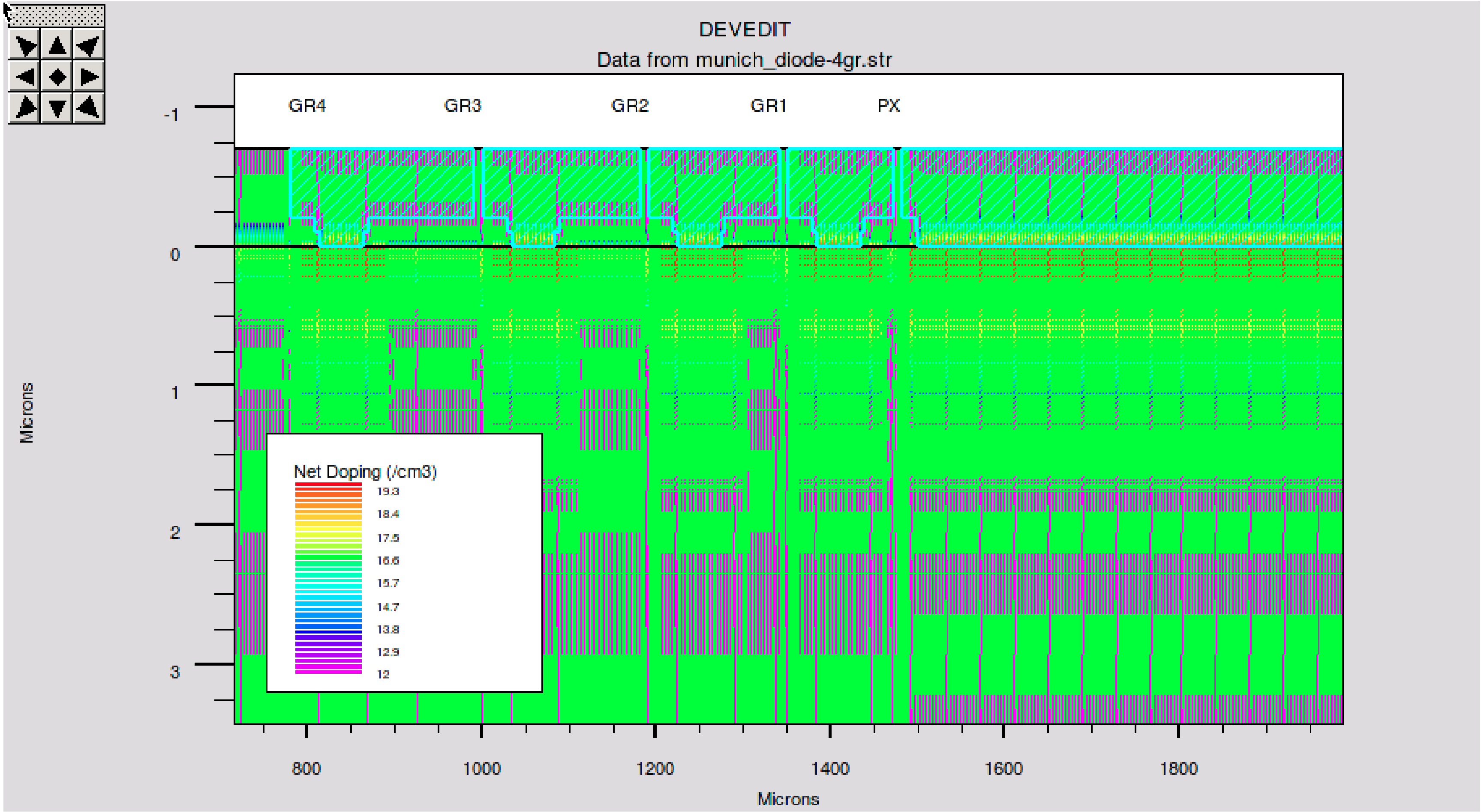
Tonyplot: plotting results

Check curves and 2D/3D distributions using tonyplot



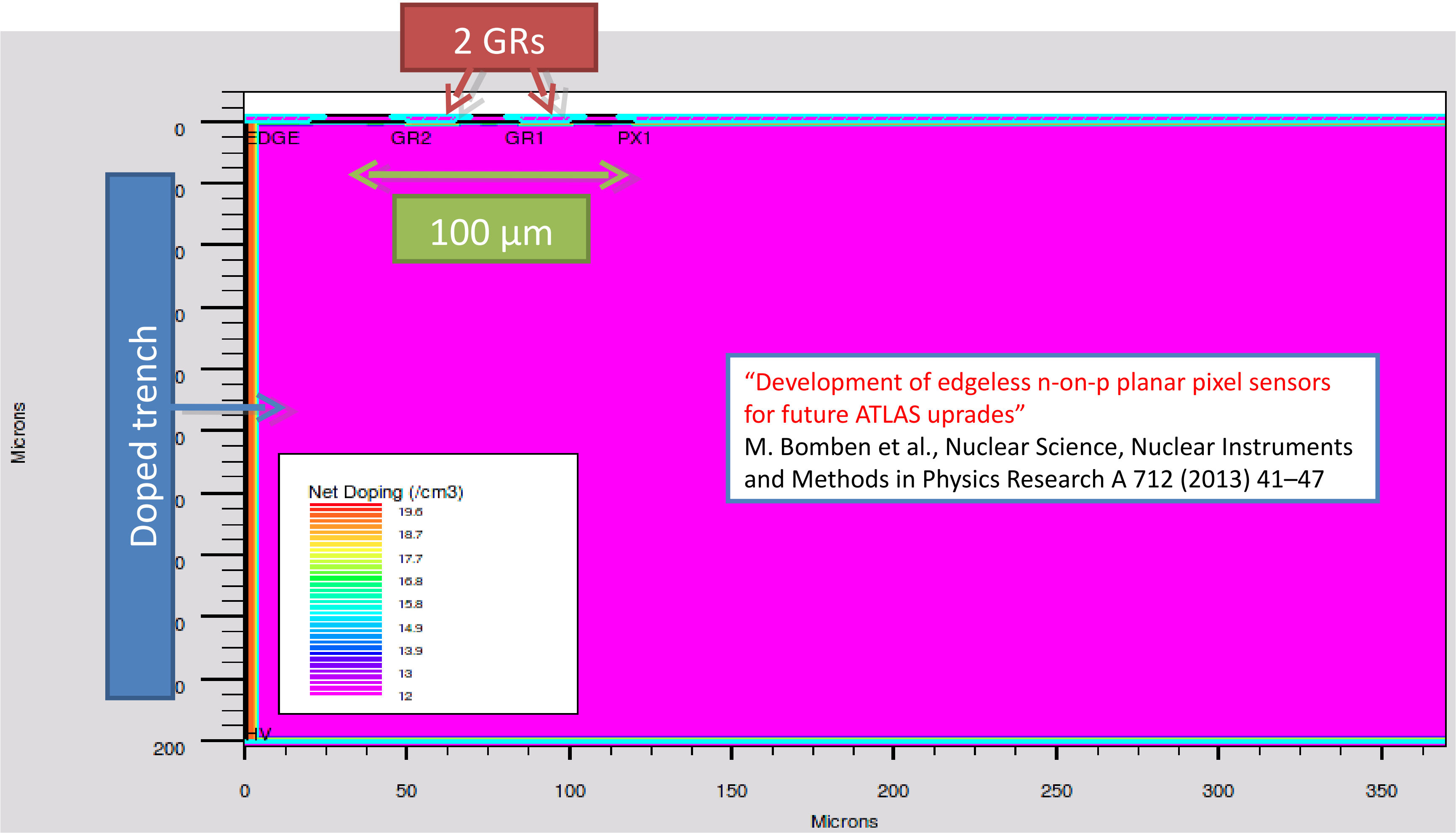
Tonyplot

Mesh structure



SELECTED RESULTS

A concrete example: Active Edge sensors



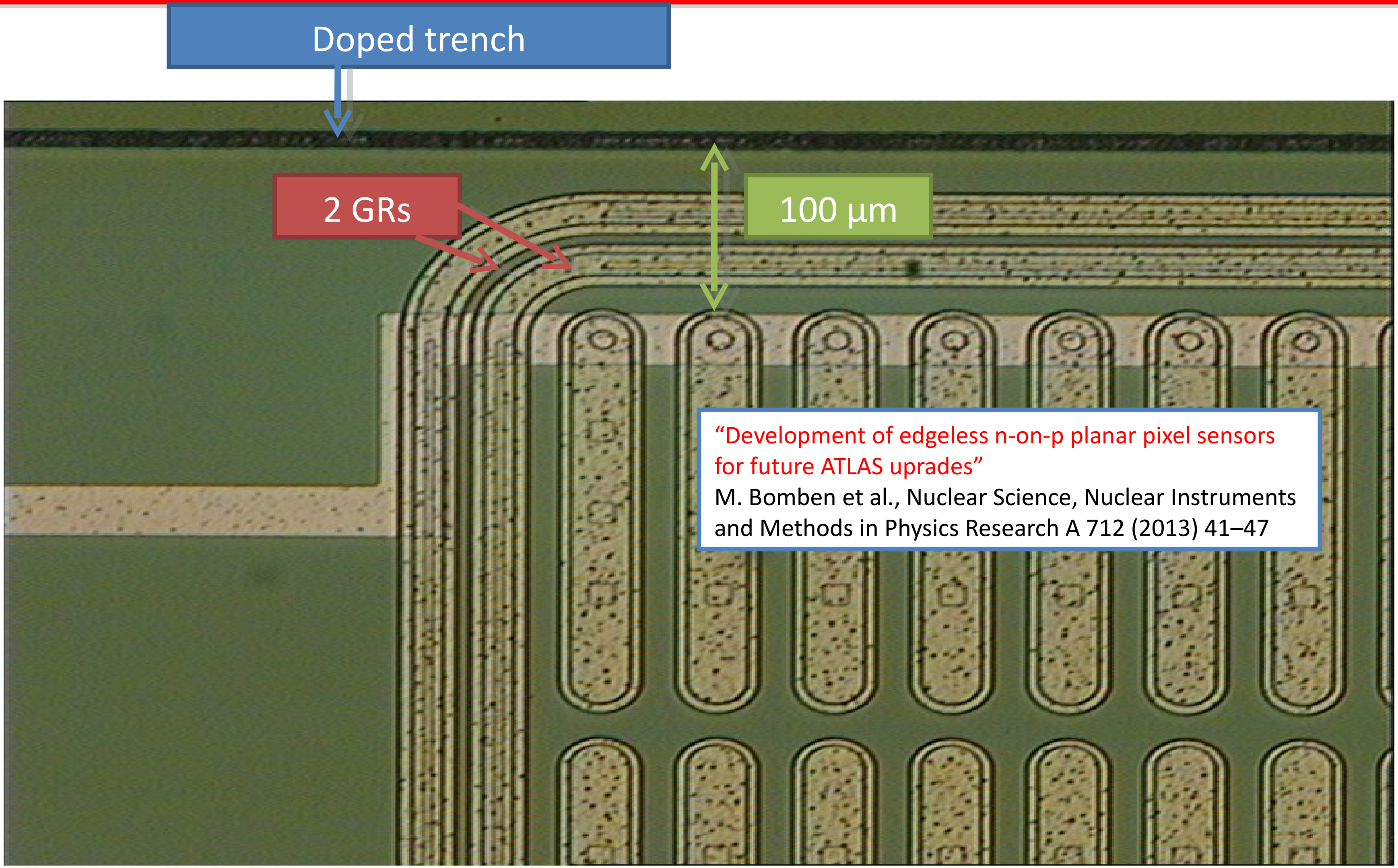
2 GRs

100 µm

Doped trench

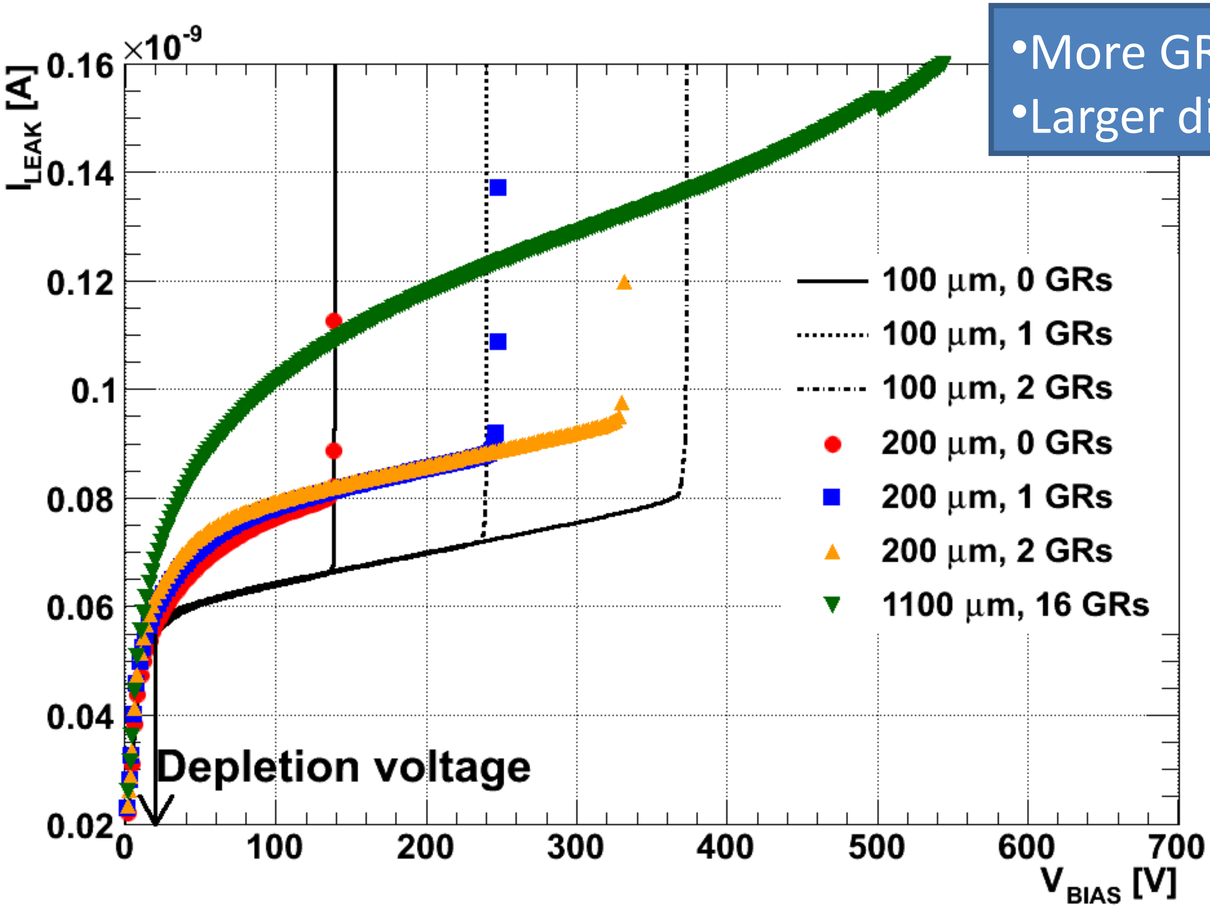
“Development of edgeless n-on-p planar pixel sensors for future ATLAS uprades”
M. Bomben et al., Nuclear Science, Nuclear Instruments and Methods in Physics Research A 712 (2013) 41–47

A concrete example: Active Edge sensors



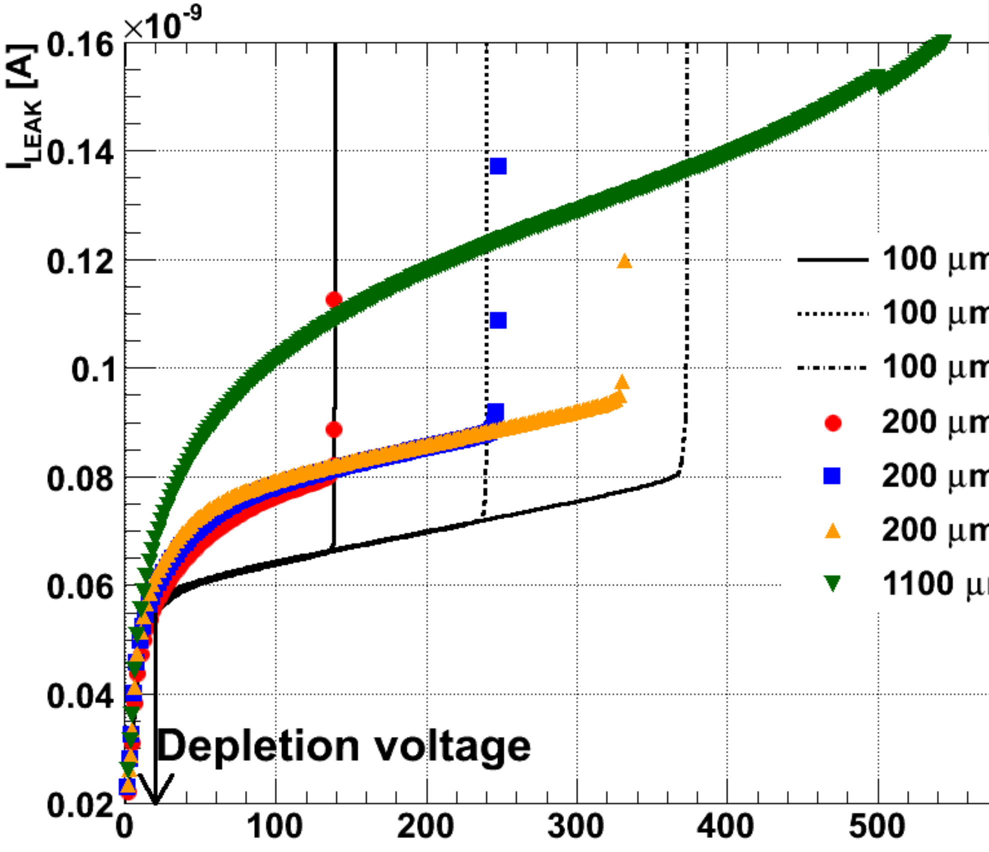
"Development of edgeless n-on-p planar pixel sensors for future ATLAS uprades"
M. Bomben et al., Nuclear Science, Nuclear Instruments and Methods in Physics Research A 712 (2013) 41–47

IV curves for different designs



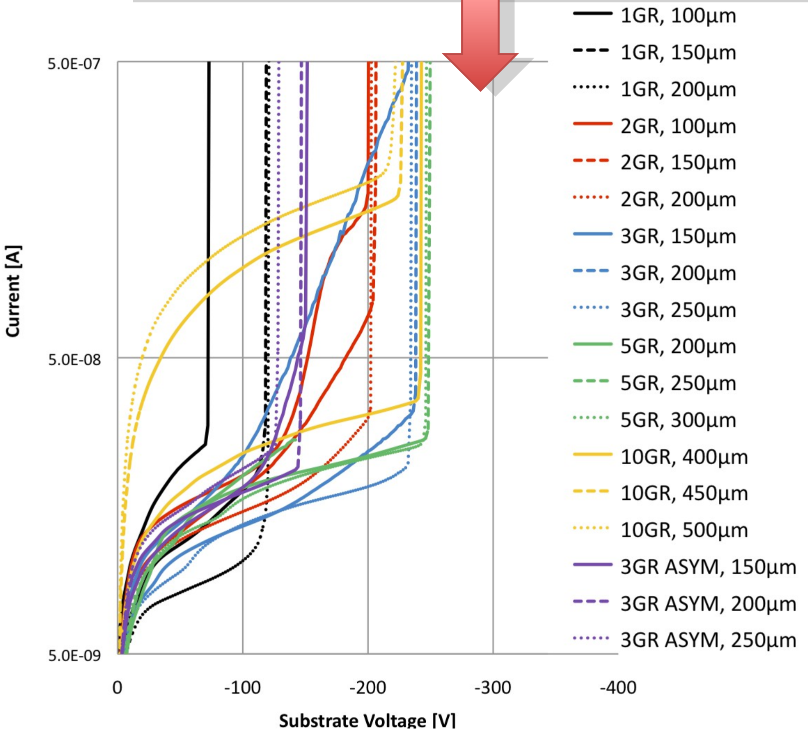
- More GRs, larger BD
- Larger distance, more current

IV curves for different designs



- More GRs, larger BD
- Larger distance, more current

As seen in data!!!



Radiation damage effects

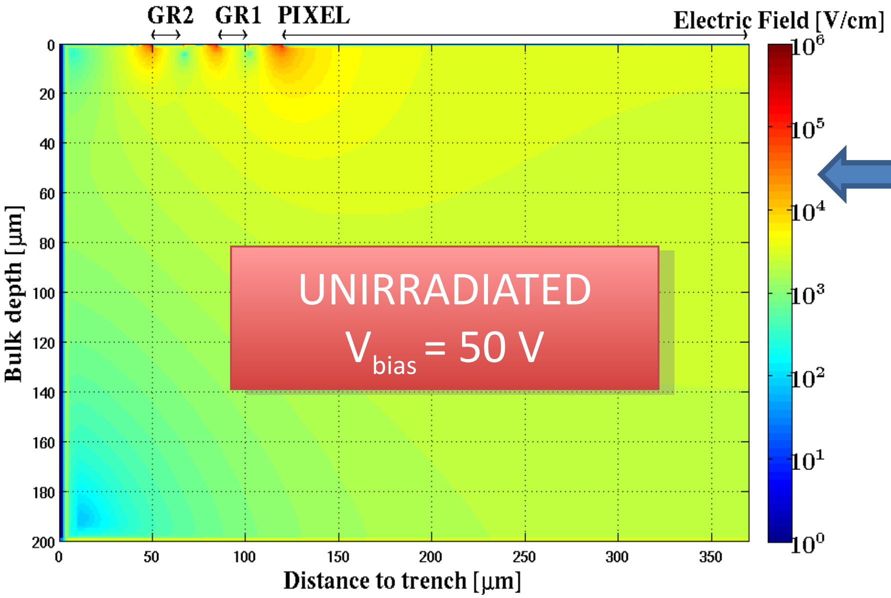
- Implement radiation damage effects via traps in the forbidden gap

$$N = \eta \times \phi$$

Type	Energy (eV)	$\sigma_e(\mathrm{cm}^2)$	$\sigma_h(\mathrm{cm}^2)$	$\eta(\mathrm{cm}^{-1})$
A	E_C -0.42	9.5×10^{-15}	9.5×10^{-14}	1.613
A	E_C -0.46	5.0×10^{-15}	5.0×10^{-14}	0.9
D	E_V +0.36	3.23×10^{-13}	3.23×10^{-14}	0.9 (1)

Radiation induced bulk damage mode by Pennicard et al.

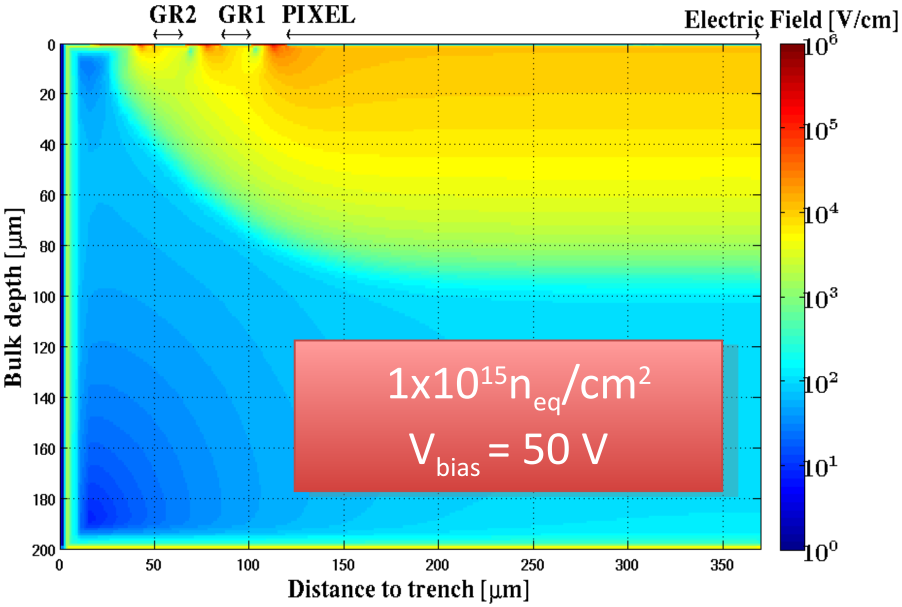
Electric field before and after irradiation



UNIRRADIATED

V_{bias} = 50 V

- For non irradiated device the bulk is completely depleted

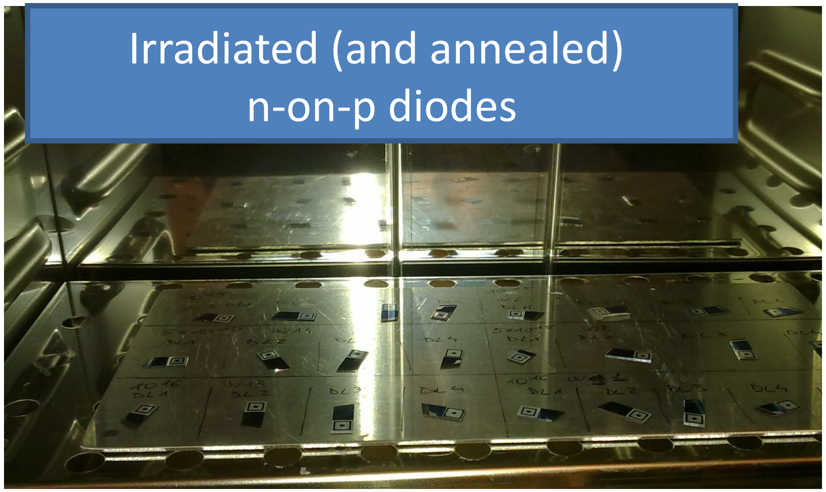


$1 \times 10^{15} n_{eq}/cm^2$

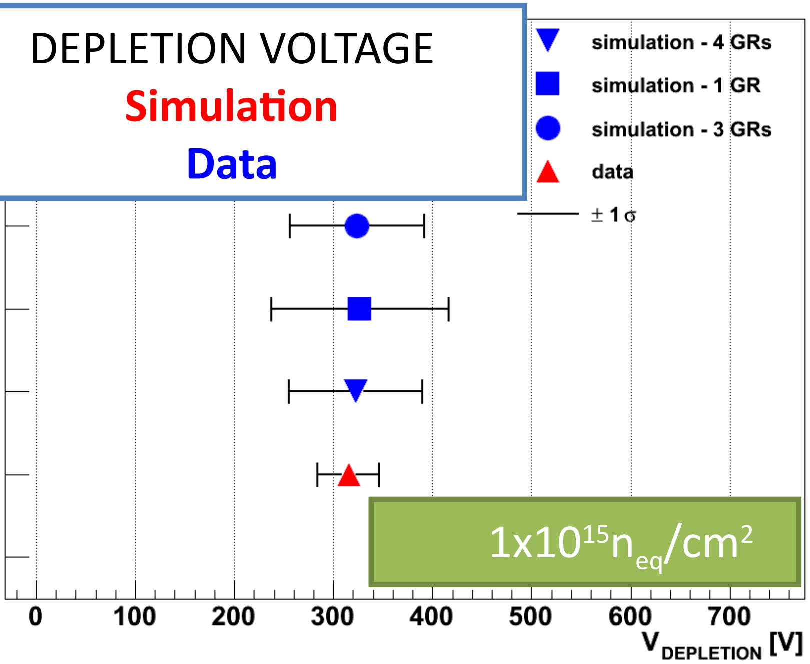
V_{bias} = 50 V

- Large fluences make effective doping concentrations higher
- Hence at low bias voltage a large portion of the bulk is undepleted

Data vs TCAD simulations

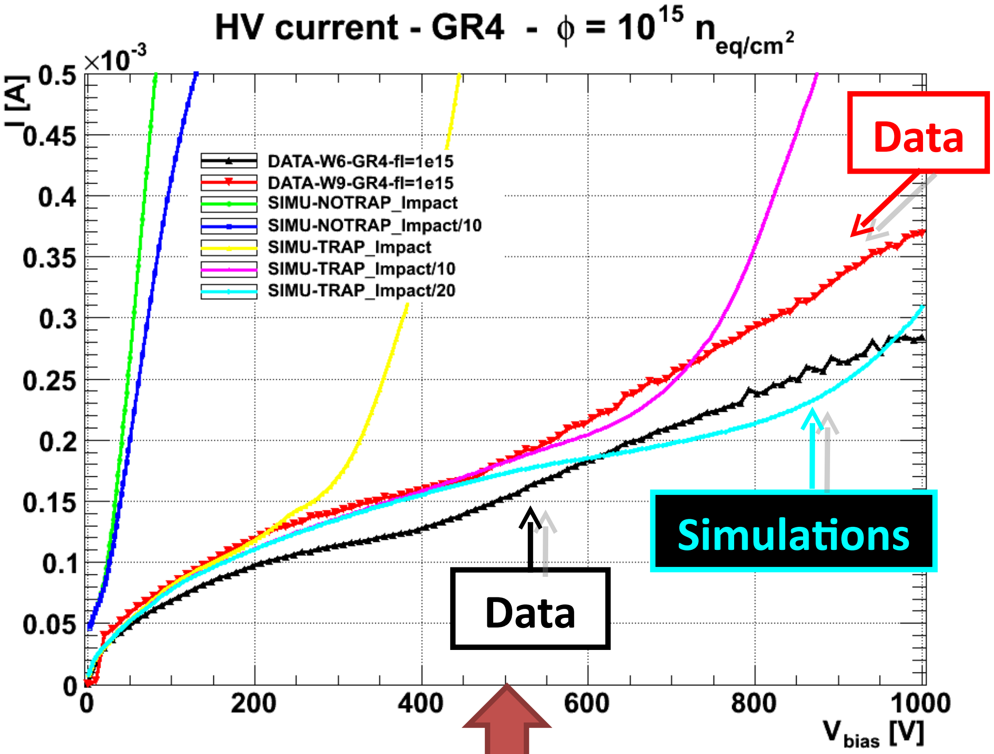


Irradiated (and annealed)
n-on-p diodes



DEPLETION VOLTAGE
Simulation
Data

$1x10^{15}n_{eq}/cm^2$



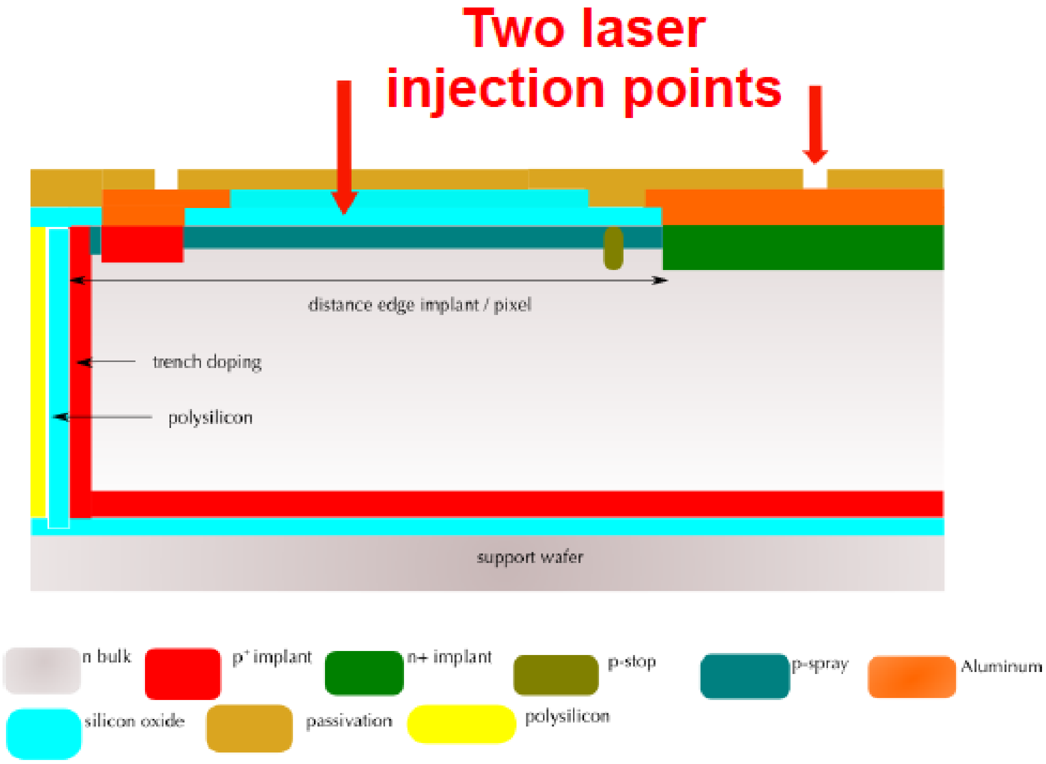
Data

Simulations

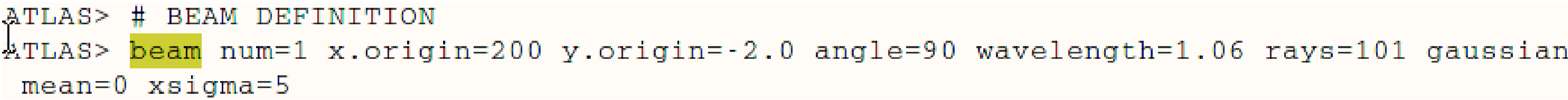
Data

A lot of work for impact ionization models and interface traps and charges

Simulation of CCE studies with laser



Two laser injection points



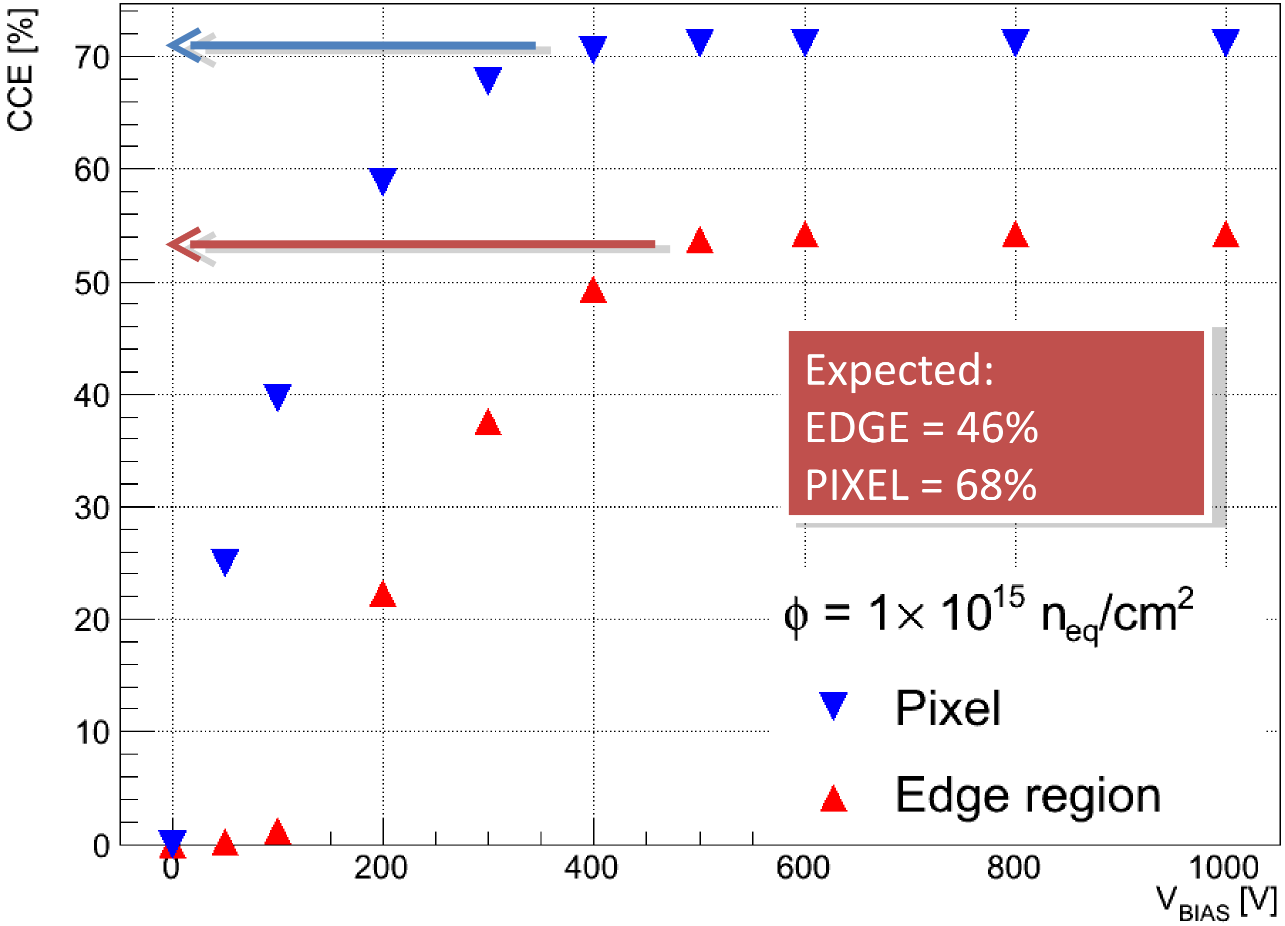
```
ATLAS> # BEAM DEFINITION
ATLAS> beam num=1 x.origin=200 y.origin=-2.0 angle=90 wavelength=1.06 rays=101 gaussian
 mean=0 xsigma=5
```

```
ATLAS> solve    b1=18 ramp.lit ramptime=1e-9 tstop=10e-9 tstep=2e-10
```

```
ATLAS> solve    b1=0 ramp.lit ramptime=1e-9 tstop=50e-9 tstep=5e-10
```

Results for irradiated edgeless device

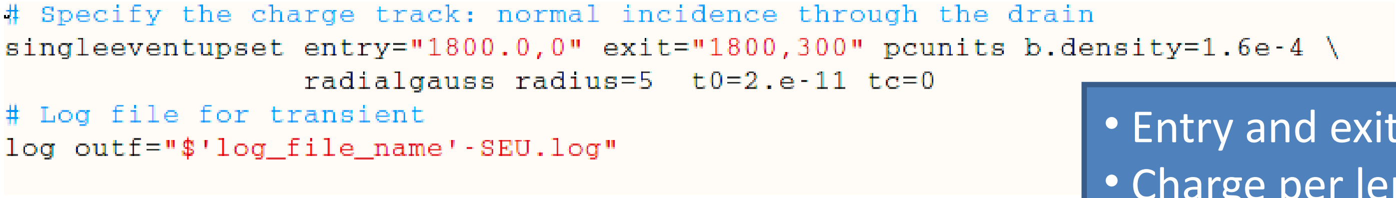
"Development of edgeless n-on-p planar pixel sensors for future ATLAS uprades"
M. Bomben et al., Nuclear Science, Nuclear Instruments and Methods in Physics Research A 712 (2013) 41–47



Expected:
EDGE = 46%
PIXEL = 68%

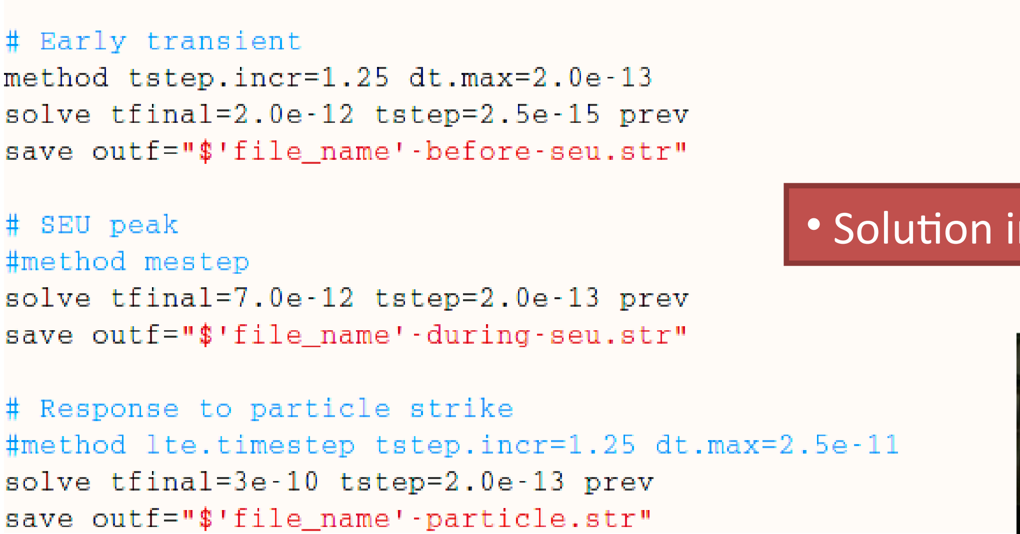
Charge collection efficiency with MIP

- We can profit of SEU module to study the drift of charge released along a track



```
# Specify the charge track: normal incidence through the drain
singleeventupset entry="1800.0,0" exit="1800,300" pcunits b.density=1.6e-4 \
                 radialgauss radius=5  t0=2.e-11 tc=0
# Log file for transient
log outf="$'log_file_name'-SEU.log"
```

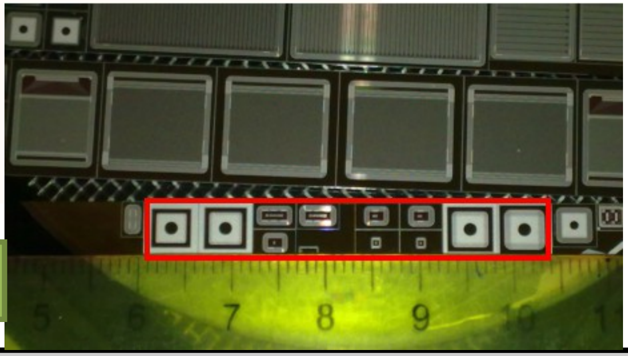
- Entry and exit point
- Charge per length unit
- Track time of arrival



```
# Early transient
method tstep.incr=1.25 dt.max=2.0e-13
solve tfinal=2.0e-12 tstep=2.5e-15 prev
save outf="$'file_name'-before-seu.str"

# SEU peak
#method mestep
solve tfinal=7.0e-12 tstep=2.0e-13 prev
save outf="$'file_name'-during-seu.str"

# Response to particle strike
#method lte.timestep tstep.incr=1.25 dt.max=2.5e-11
solve tfinal=3e-10 tstep=2.0e-13 prev
save outf="$'file_name'-particle.str"
```

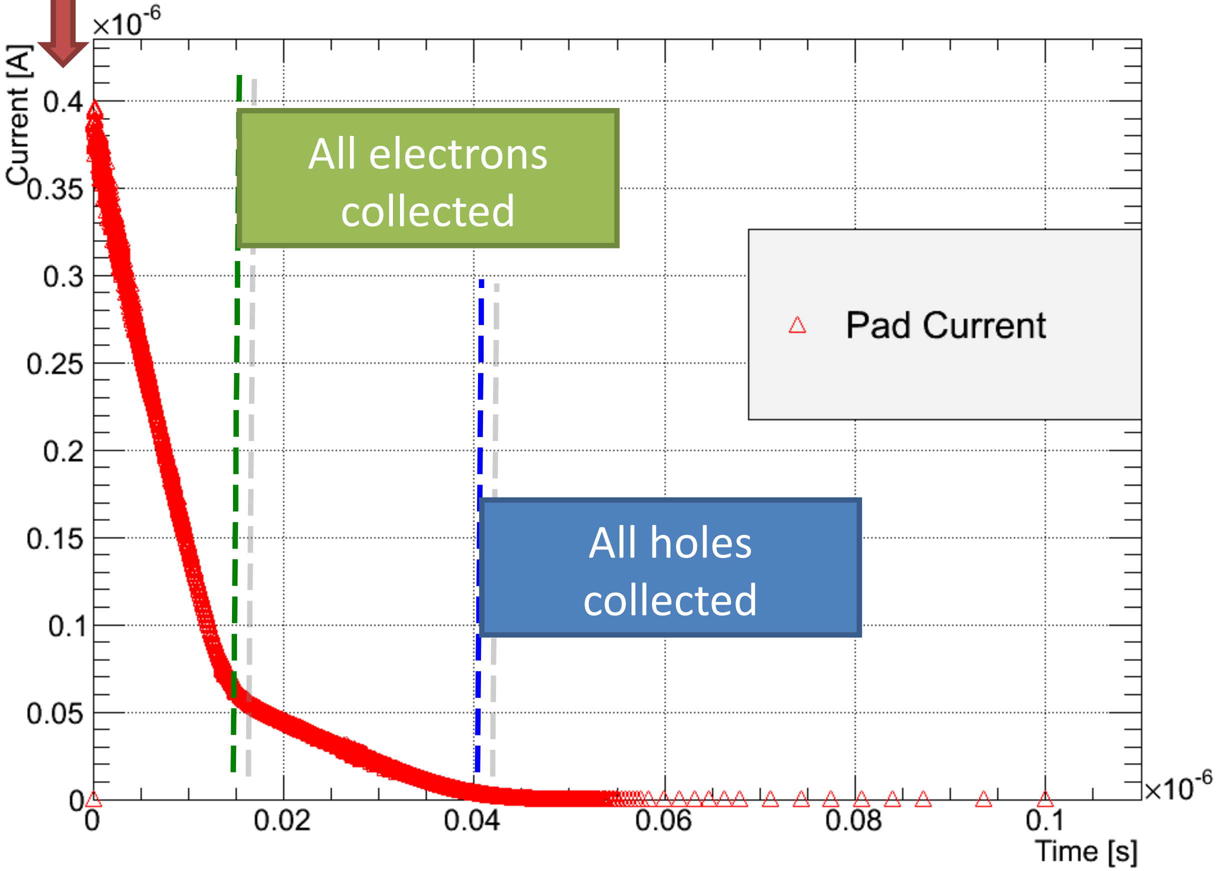
- Solution in the time-domain

In the following: results for n-on-p diodes



Response to a MIP

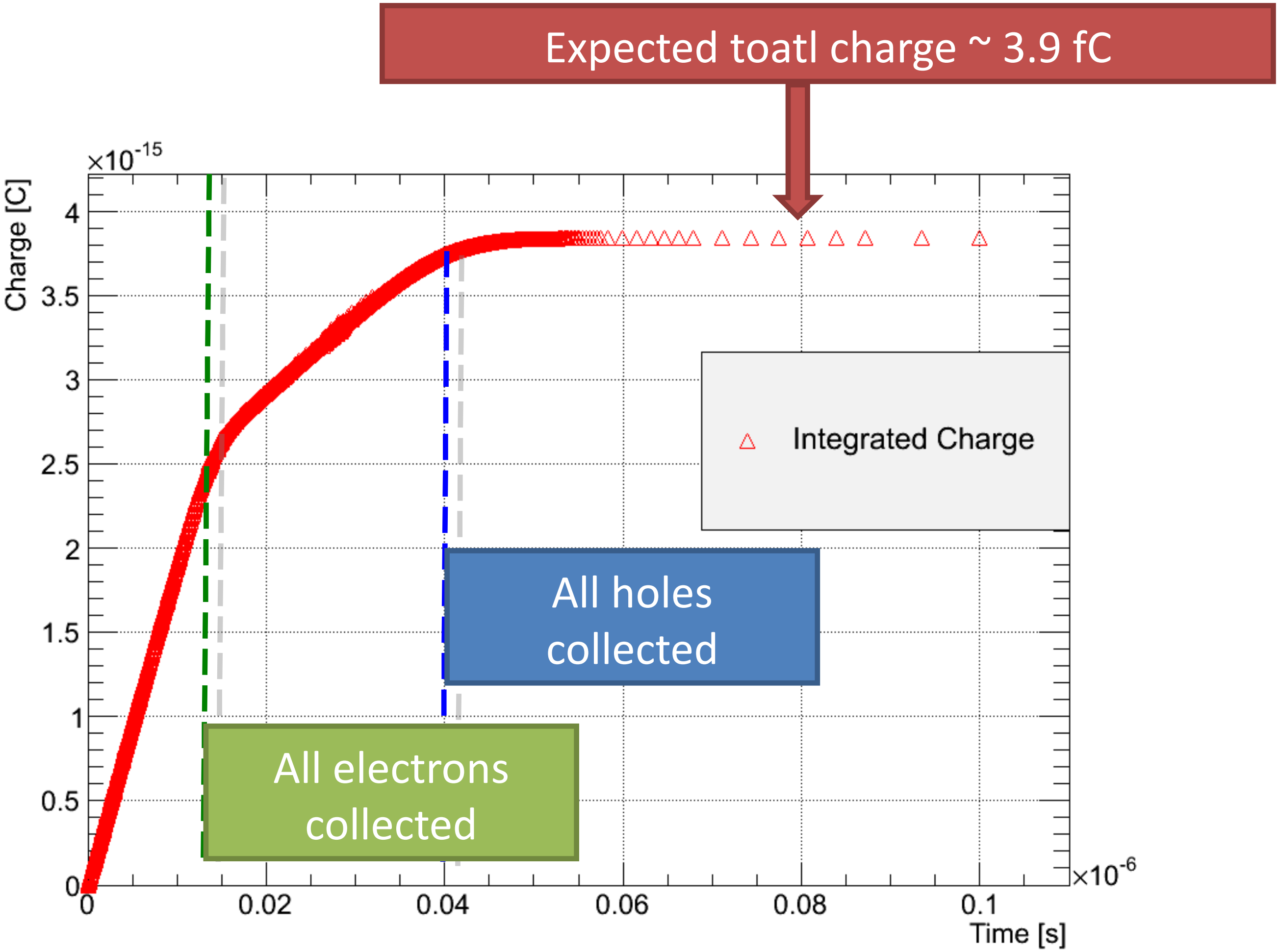
Expected Initial current ~ λ ($\langle v_e \rangle + \langle v_h \rangle$) = 3.9×10^{-7} A



All electrons collected

All holes collected

Response to a MIP

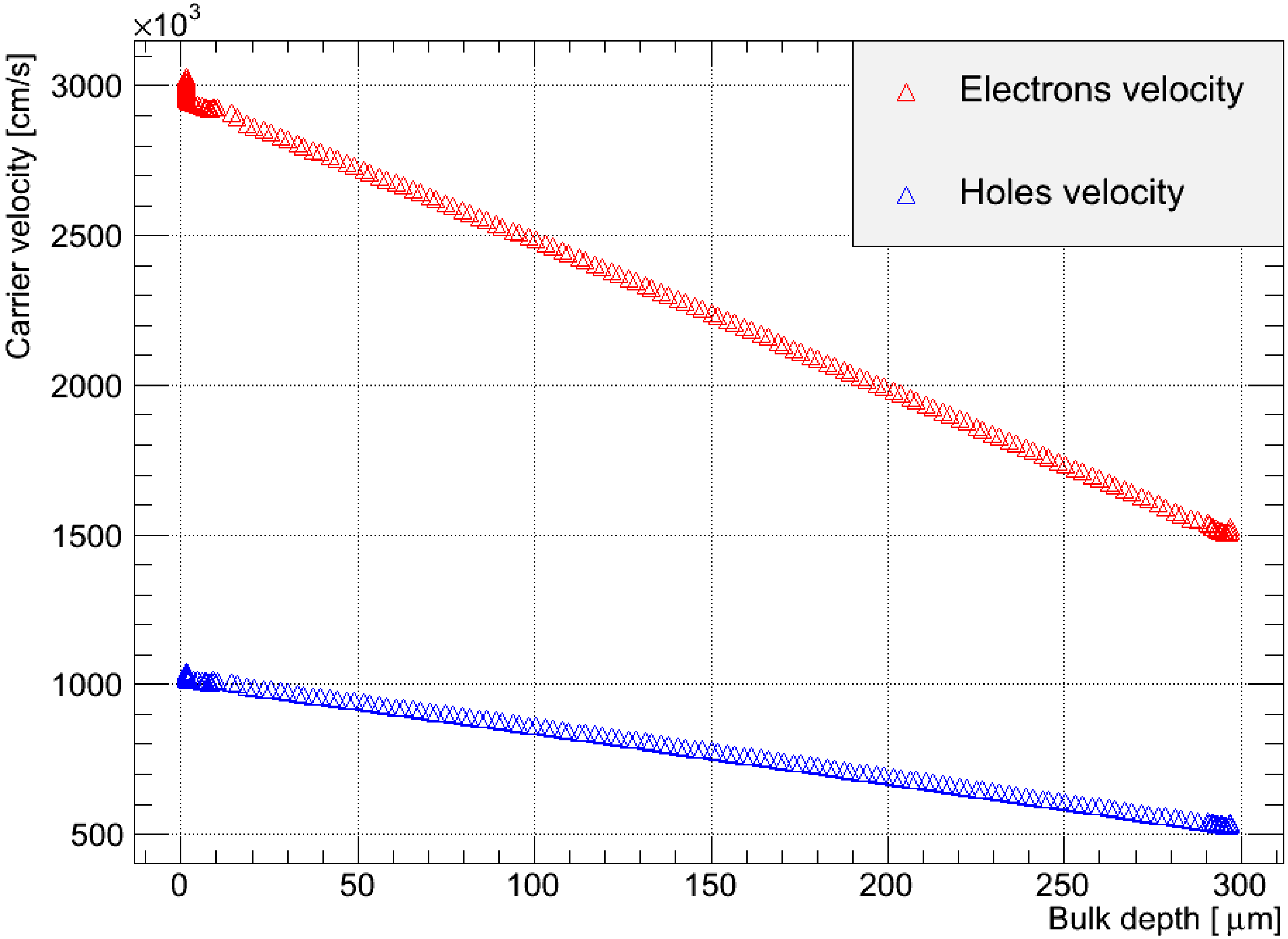


Expected toatl charge ~ 3.9 fC

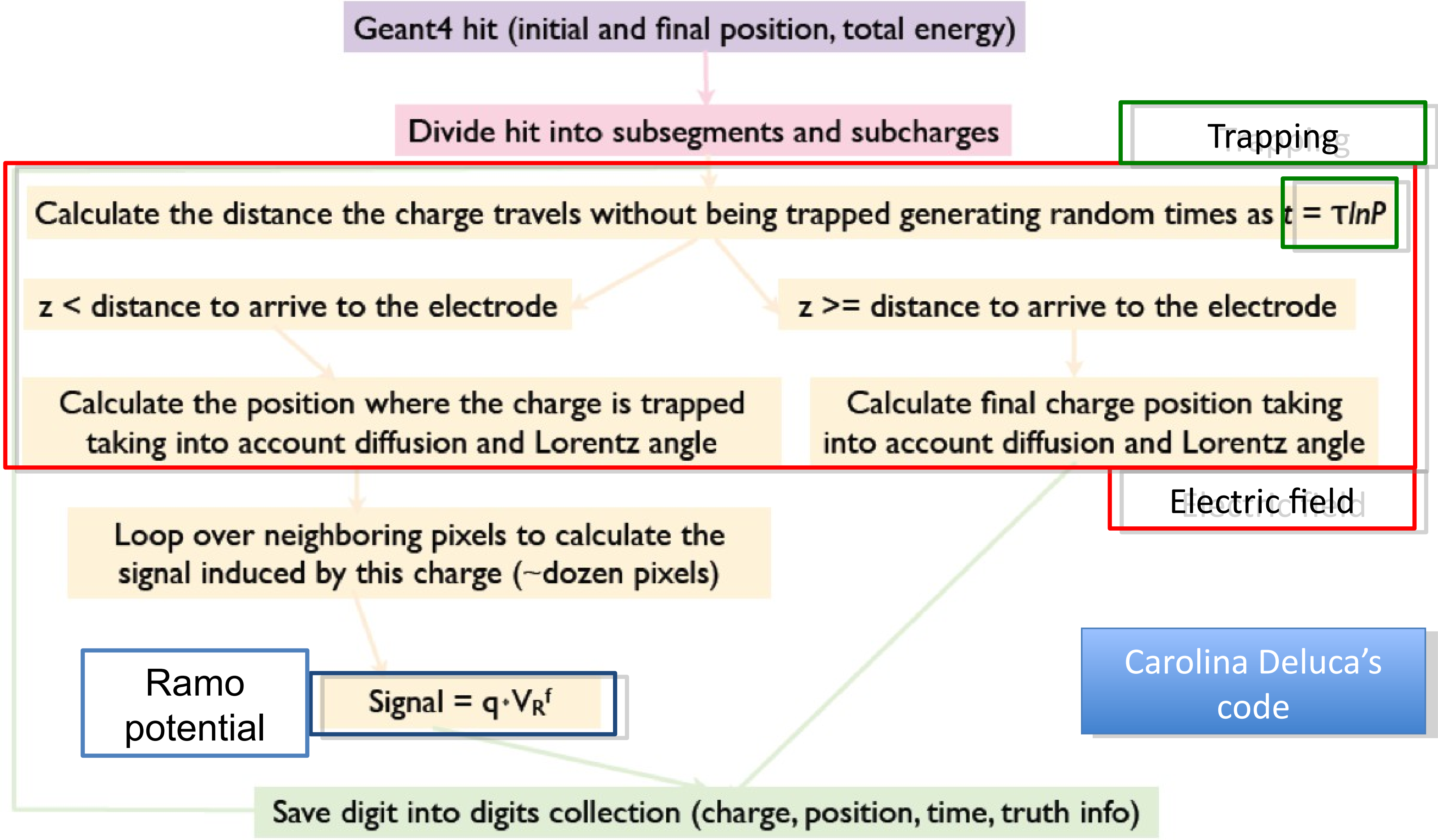
All holes collected

All electrons collected

Carrier velocities



New studies: pixel digitizer



Geant4 hit (initial and final position, total energy)

Divide hit into subsegments and subcharges

Trapping

Calculate the distance the charge travels without being trapped generating random times as $t = \tau \ln P$

z < distance to arrive to the electrode

z >= distance to arrive to the electrode

Calculate the position where the charge is trapped taking into account diffusion and Lorentz angle

Calculate final charge position taking into account diffusion and Lorentz angle

Electric field

Loop over neighboring pixels to calculate the signal induced by this charge (~dozen pixels)

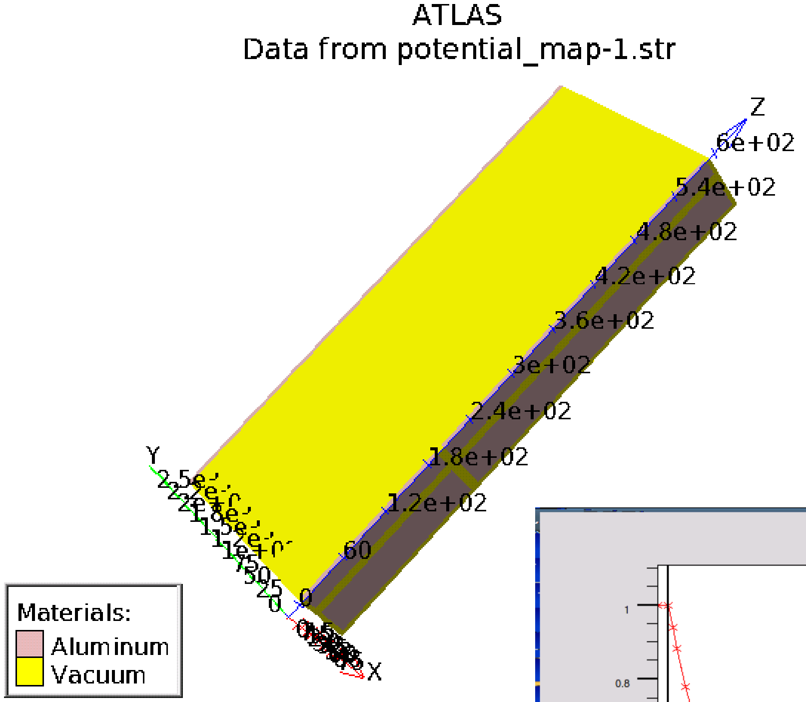
Ramo potential

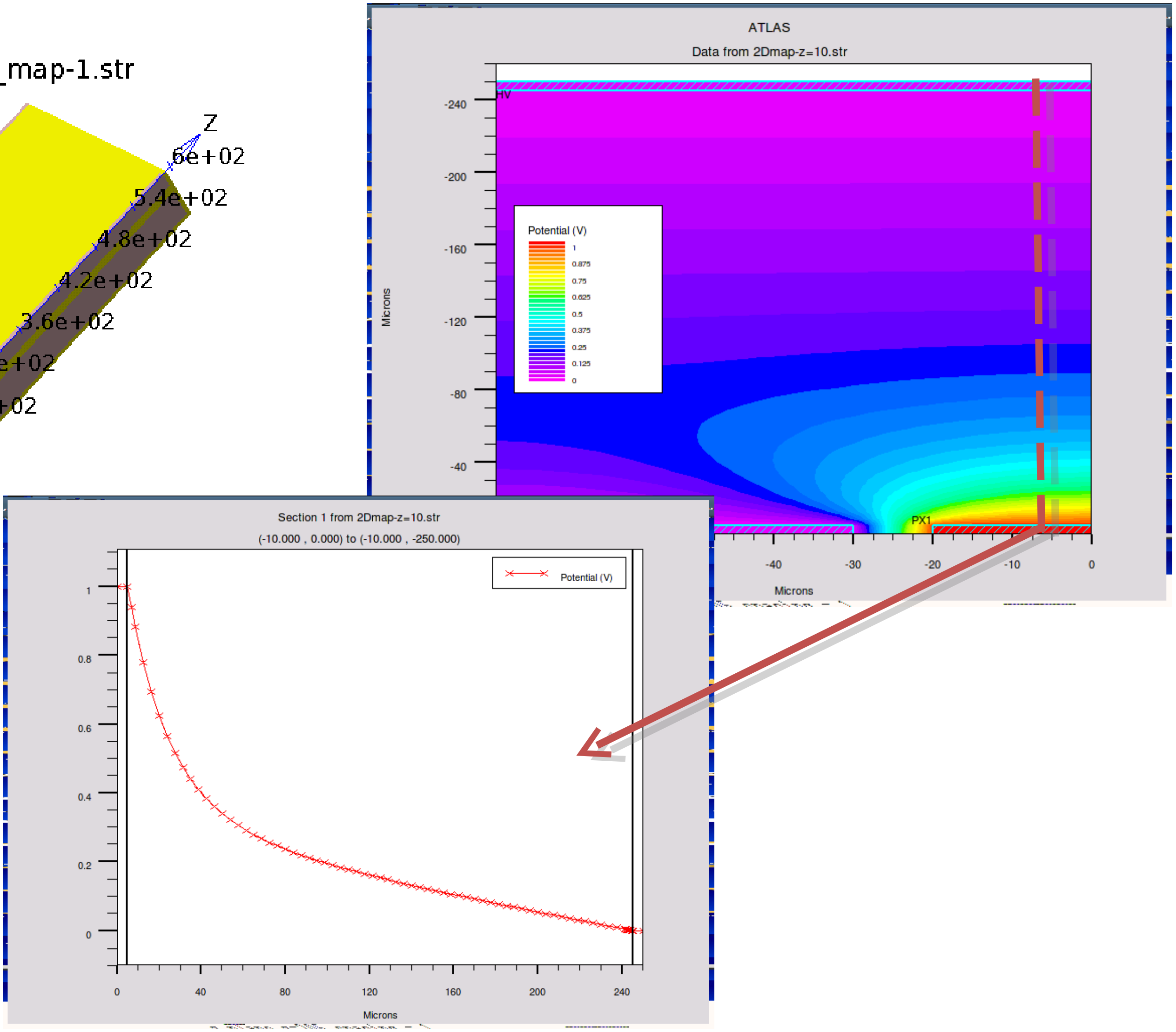
$\text{Signal} = q \cdot V_R^f$

Save digit into digits collection (charge, position, time, truth info)

Carolina Deluca's code

Digitizer inputs from TCAD: ramo potential





Digitizer inputs from TCAD: Electric field

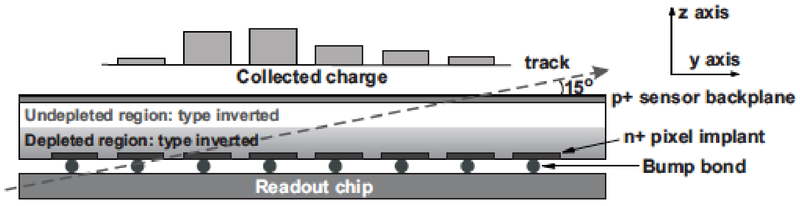
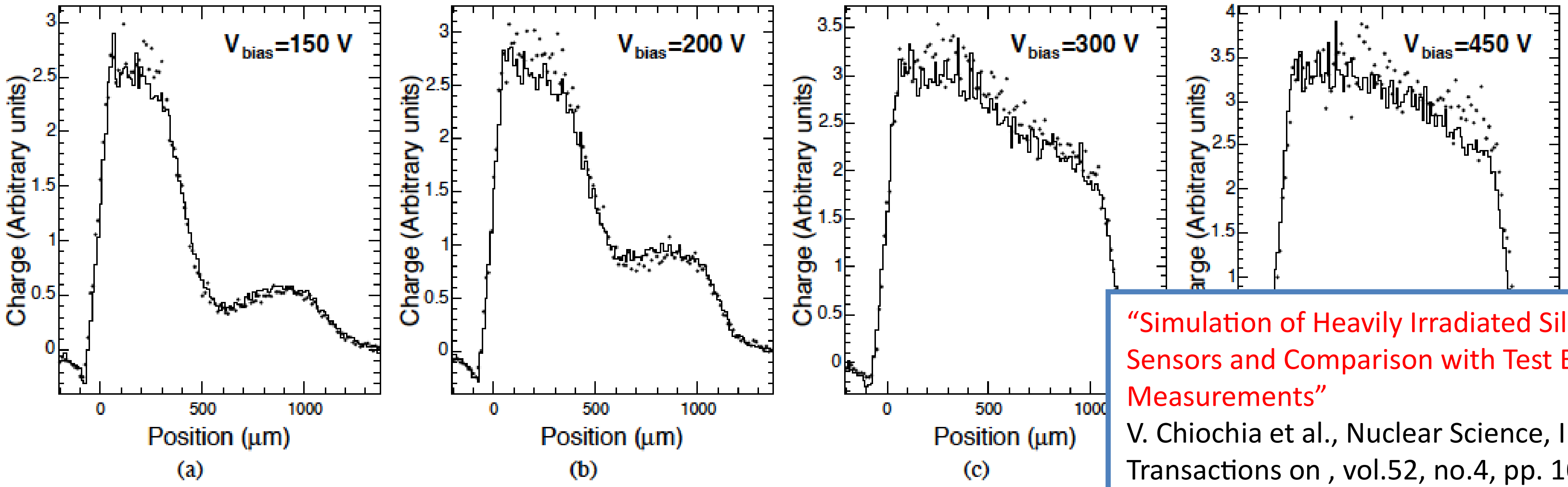


Fig. 2

THE GRAZING ANGLE TECHNIQUE FOR DETERMINING CHARGE COLLECTION PROFILES. THE CLUSTER LENGTH IS PROPORTIONAL TO THE DEPTH OVER WHICH CHARGE IS COLLECTED.

- Study of Charge Collection as a function of charge deposition depth
- Parameterization of the Electric Filed in simulations
- Comparison data/simulation (next slides)



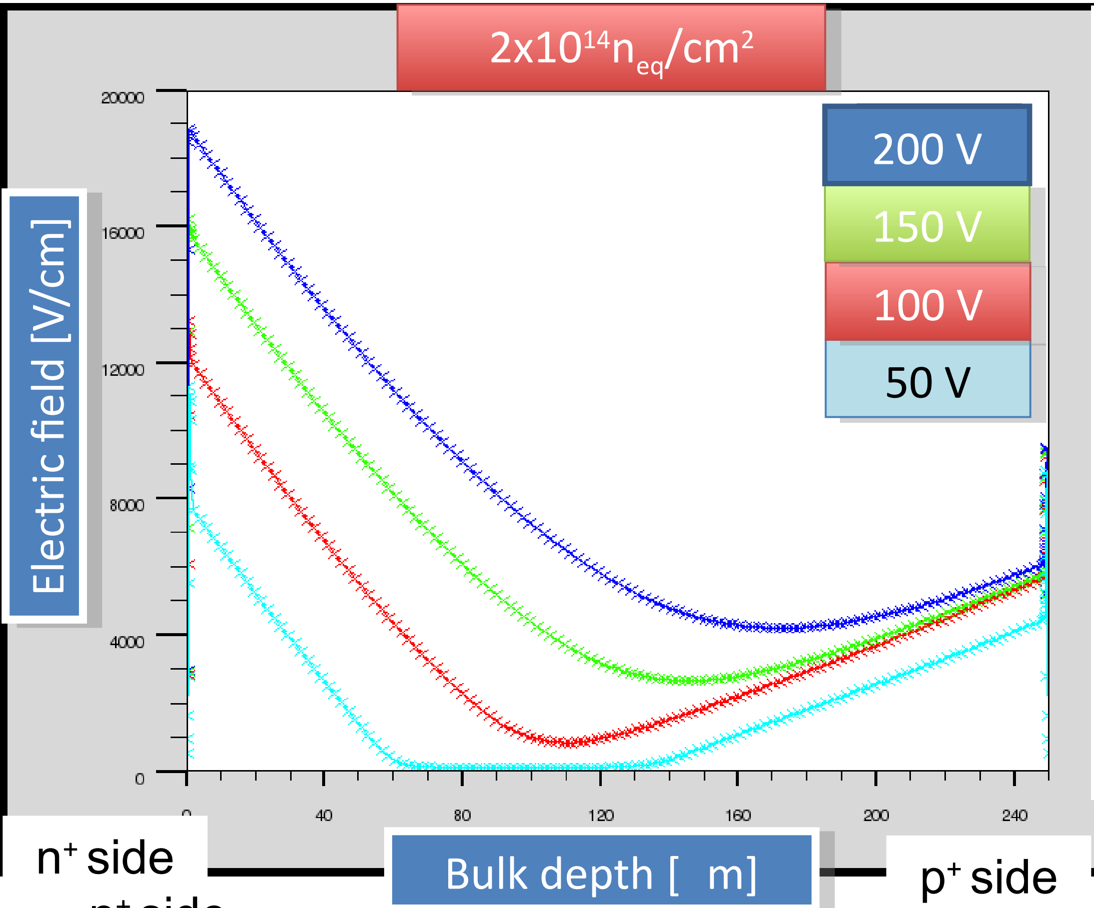
(a) (b) (c)

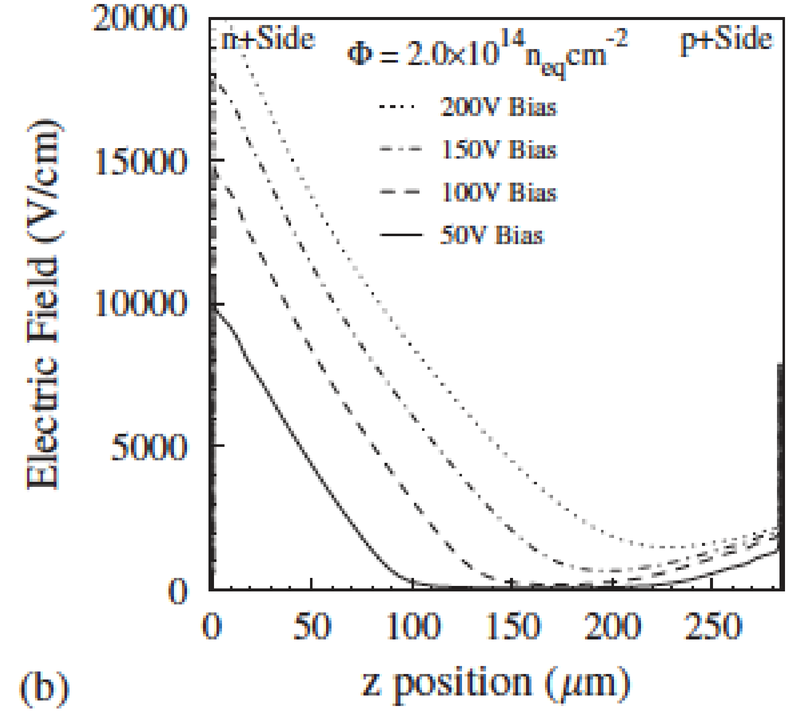
“Simulation of Heavily Irradiated Silicon Pixel Sensors and Comparison with Test Beam Measurements”
V. Chiochia et al., Nuclear Science, IEEE Transactions on , vol.52, no.4, pp. 1067- 1075, Aug. 2005

Fig. 10

THE MEASURED CHARGE COLLECTION PROFILES AT BIAS VOLTAGES OF 150 V, 200 V, 300 V, AND 450 V ARE SHOWN AS SOLID DOTS FOR FLUENCES OF $6 \times 10^{14}\ N_{eq}/\mathrm{CM}^2$. THE BF SIMULATION IS SHOWN AS THE SOLID HISTOGRAM IN EACH PLOT.

Digitizer inputs from TCAD: Electric field





n^+ side

p^+ side

- Goal: parameterize the electric field for different conditions (fluence, temperature, bias voltage, etc)

COMMENTS AND CONCLUSIONS

TCAD simulations for HEP sensors: my view

- Thanks to TCAD you can make powerful predictions on new sensors
- TCAD could save you money and time
- … but to learn it and produce reliable results takes time, a lot
- 1 year full time to be able to make useful predictions IMHO
- Better to have a good knowledge of semiconductor physics before using TCAD!

TCAD simulations: time needed

- The CPU time increases with number of meshing points
- Some analysis are not parallelized (*e.g.* AC)
- E.g. : 1 minute per bias point for ~ 100k nodes mesh on a 8 core 3GHz machine
- For irradiated sensors this translates into ~ 1 week to get full depletion
- Another example: time-domain solution. For the same structure above you need to solve for ~ 10 ns in time steps of ps, with ~ 1 minute per point ➔ 1 week needed

Conclusions

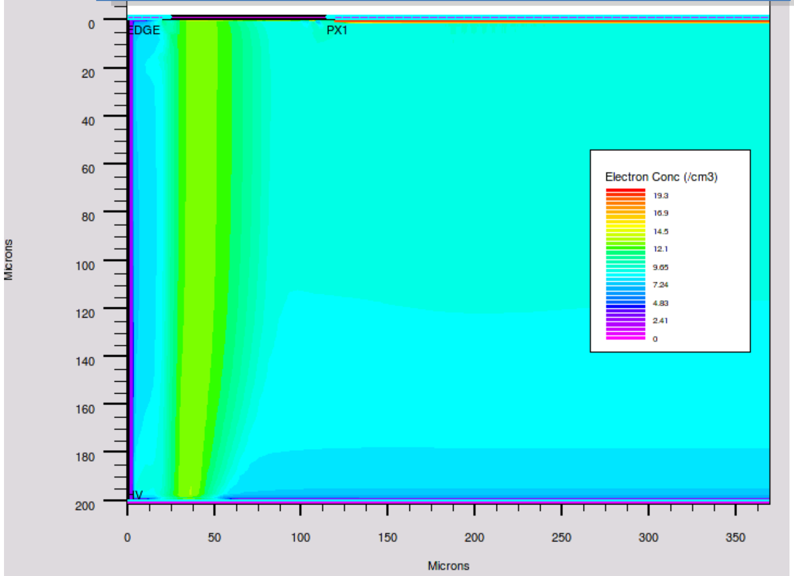
- TCAD is a very powerful tool for HEP silicon sensors
- You can reduce the number of submission, and so cutting time and money to get results
- But the program is very complex, and if you don’t know what you are doing is easy to get lost, for days
- In addition: SILVACO has no forums, tip-pages, etc
- So, if you want to use TCAD, it is recommended to have a solid knowledge of semiconductor physics, good data inputs and a big dose of patience ☺

One last thing

- It could be nice and funny after all to work with TCAD simulations ☺
- So if you are interested in working with TCAD simulations, feel free to contact me: marco.bomben@cern.ch

➢ Thank you!

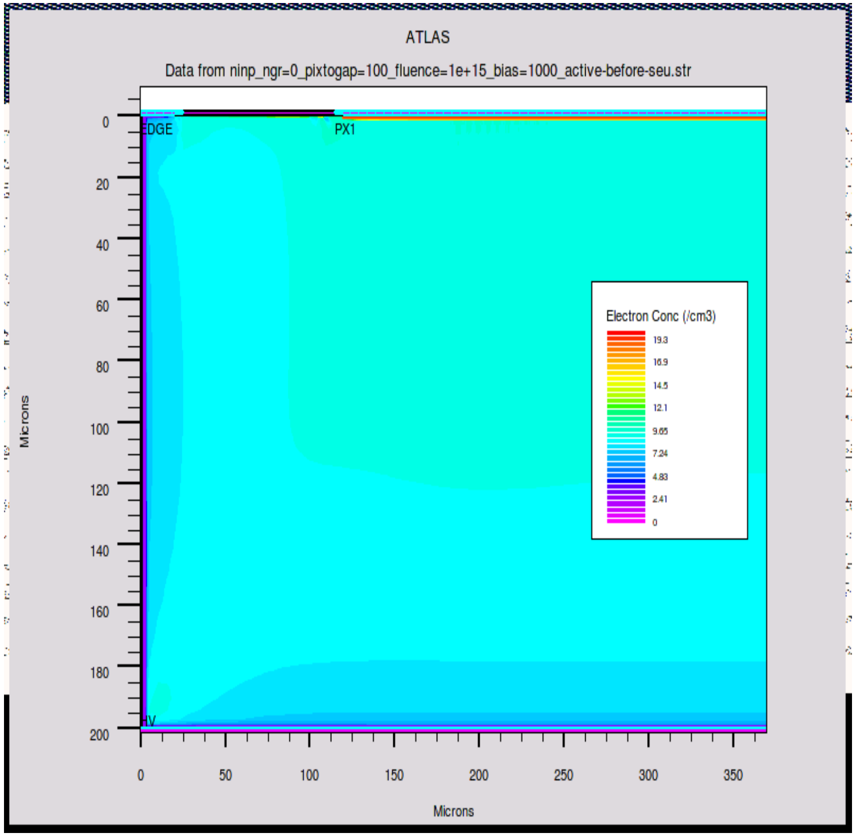
Electrons happily drifting after a particle hit the sensor



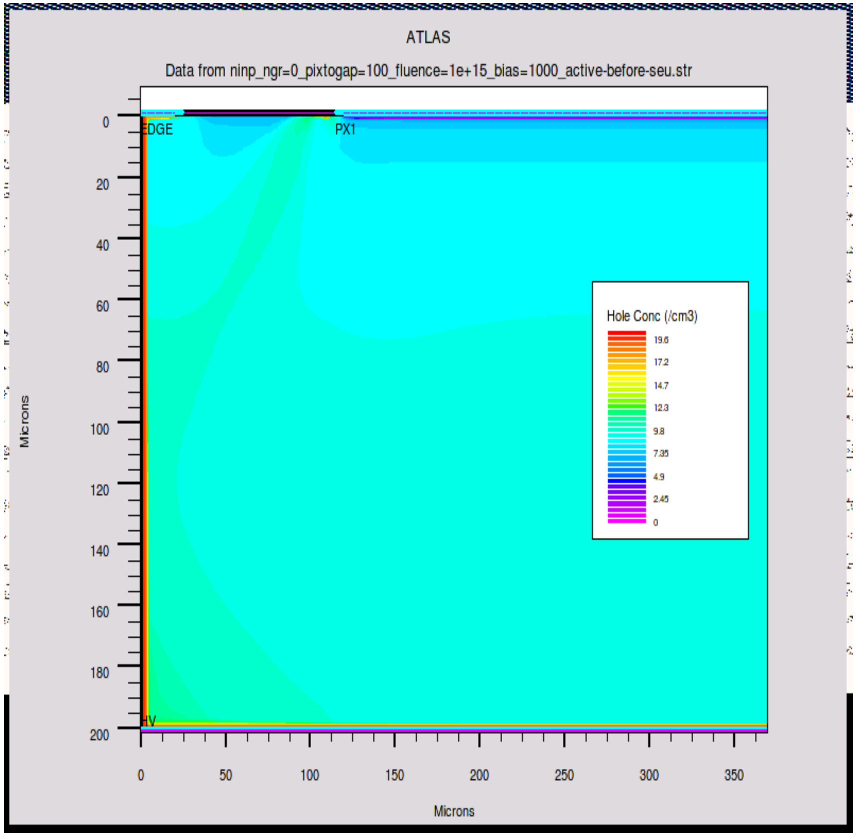
BACKUP MATERIAL

Before strike

Electrons

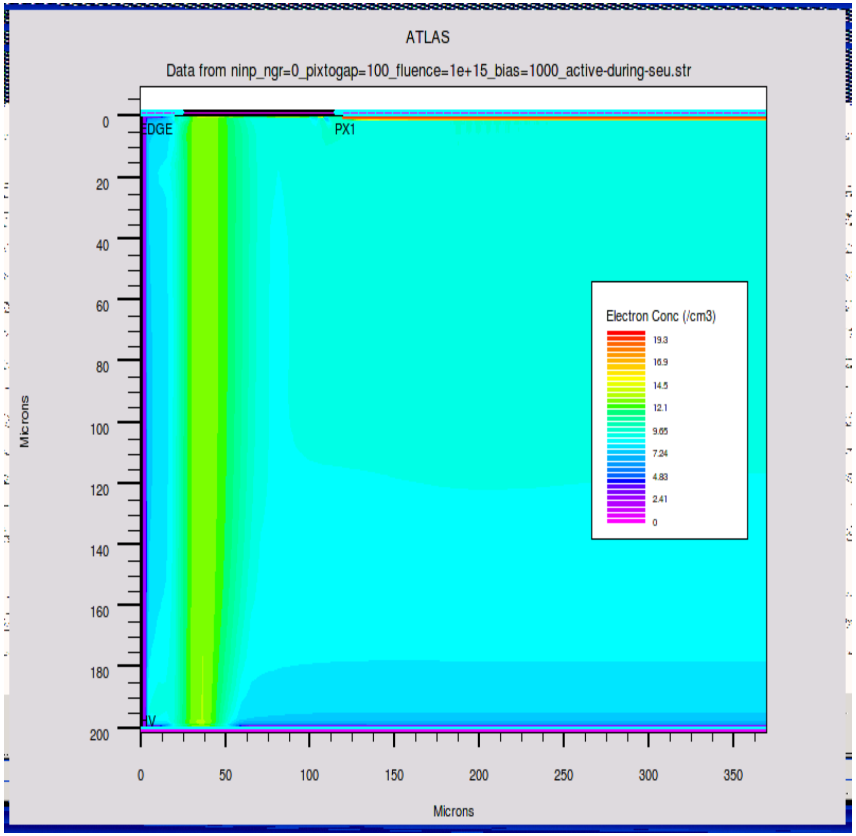


Holes

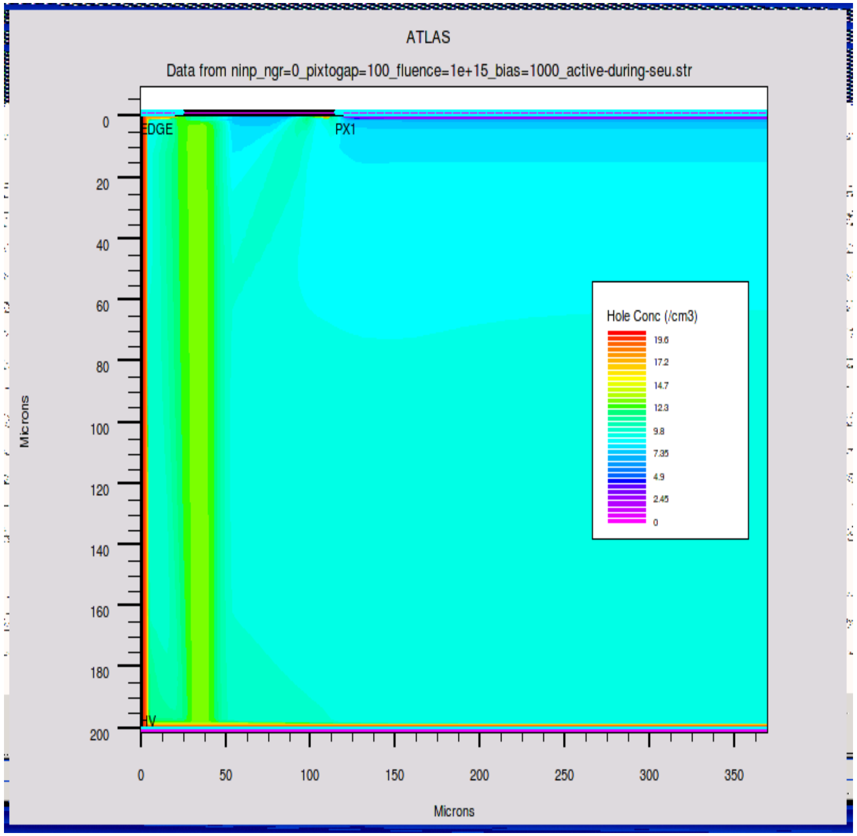


30 ps after particle hit

Electrons

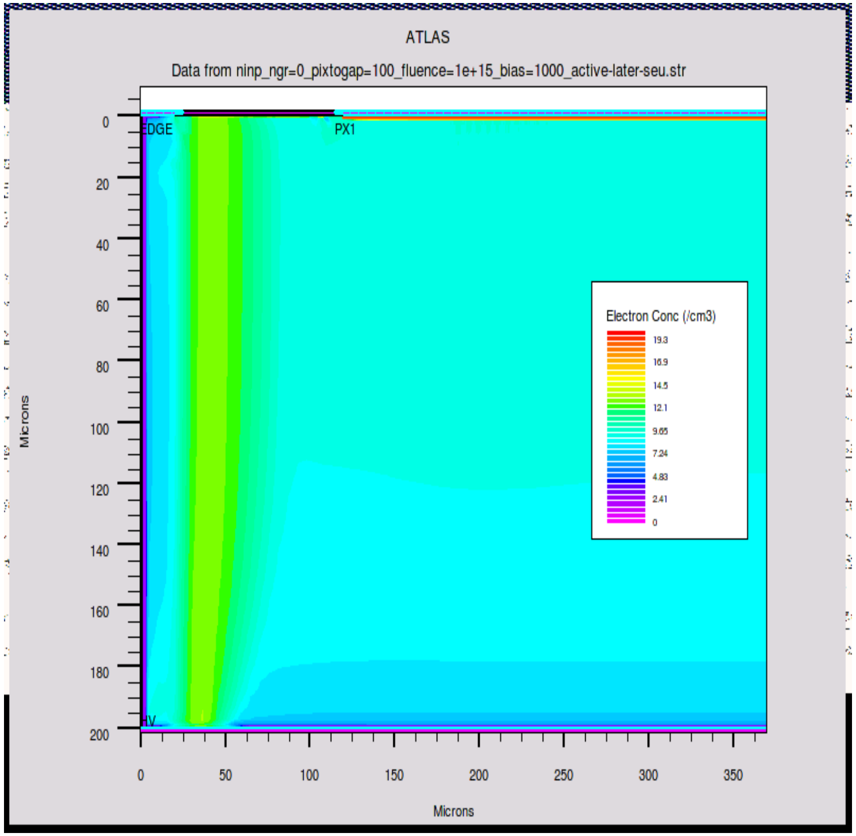


Holes

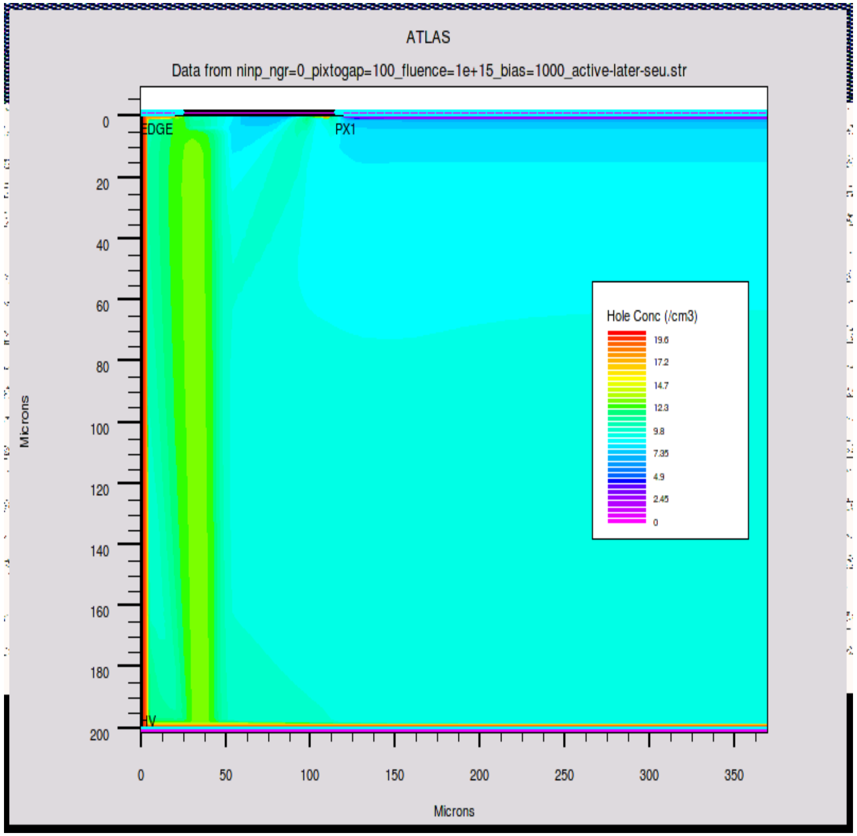


80 ps after particle hit

Electrons

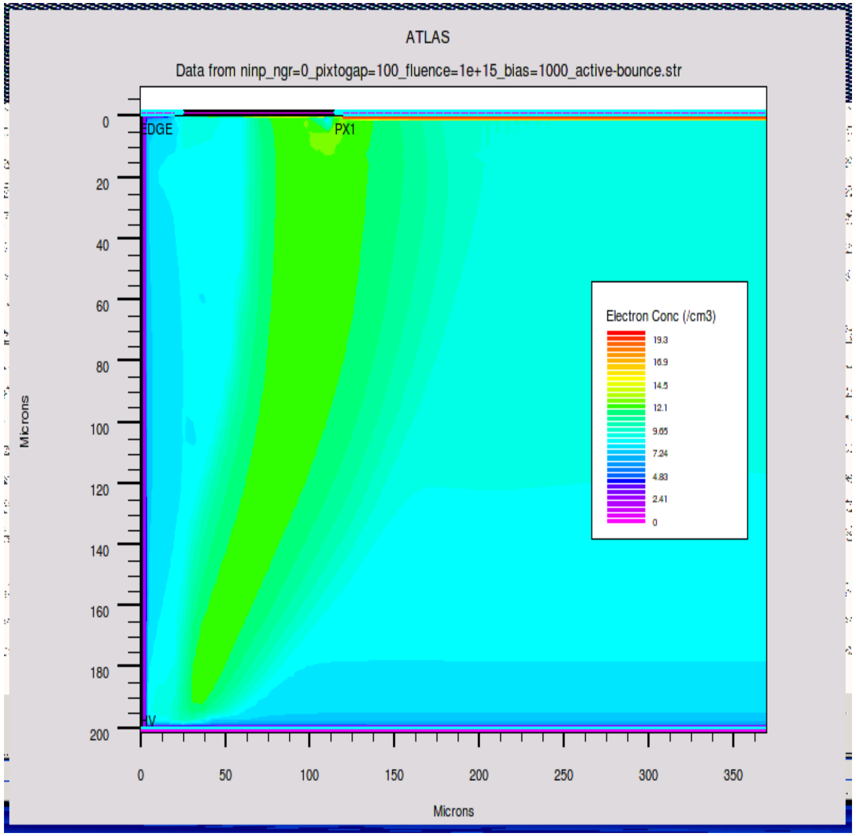


Holes

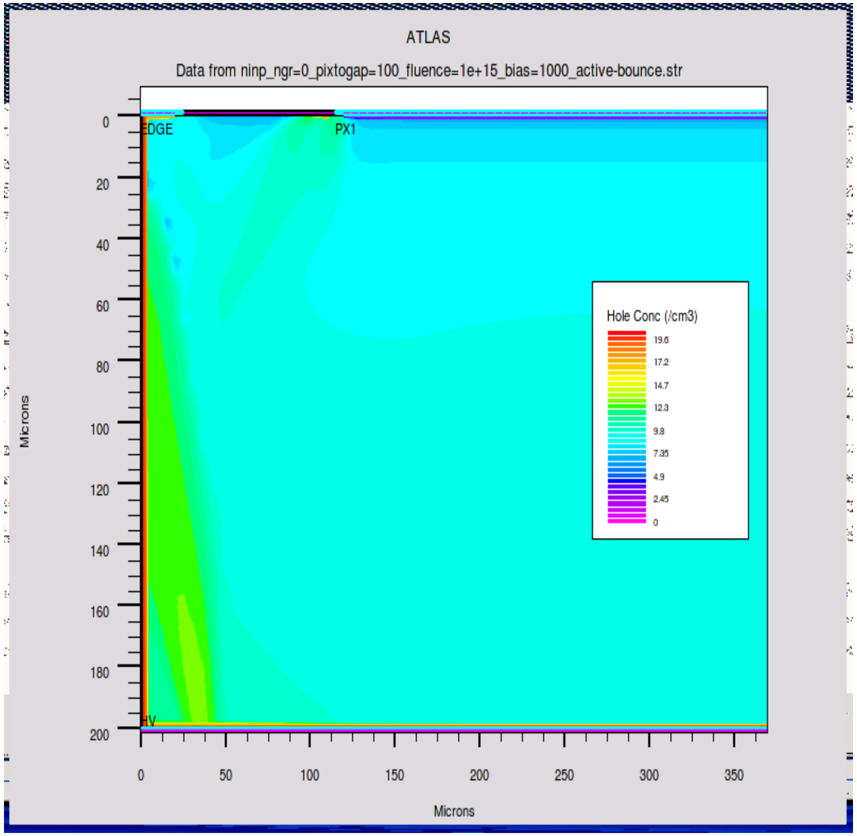


780 ps after particle hit

Electrons

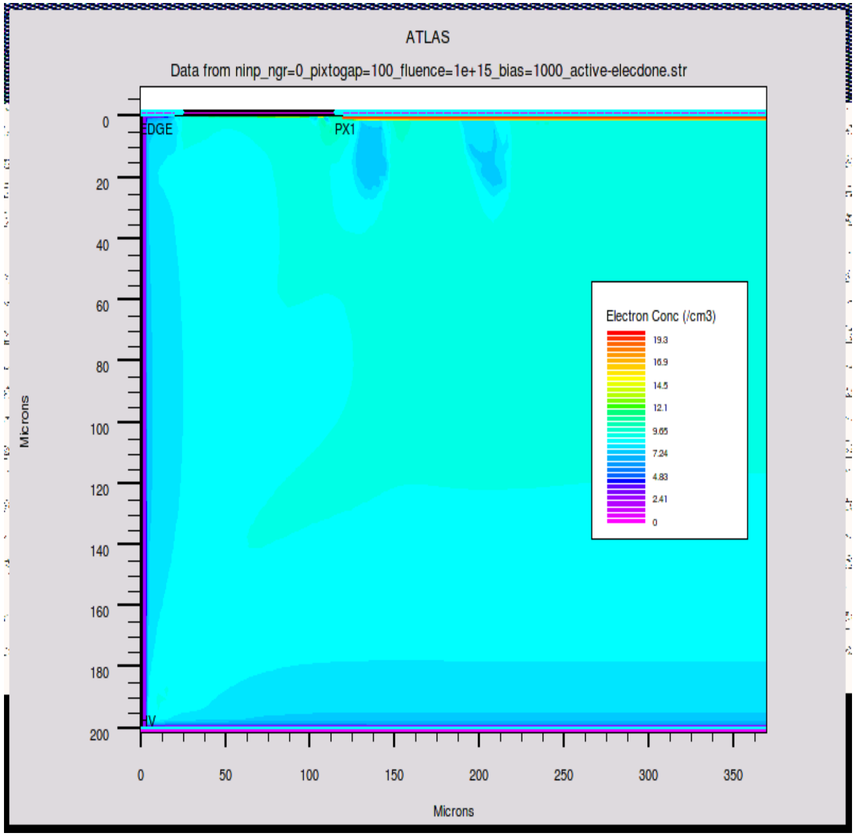


Holes

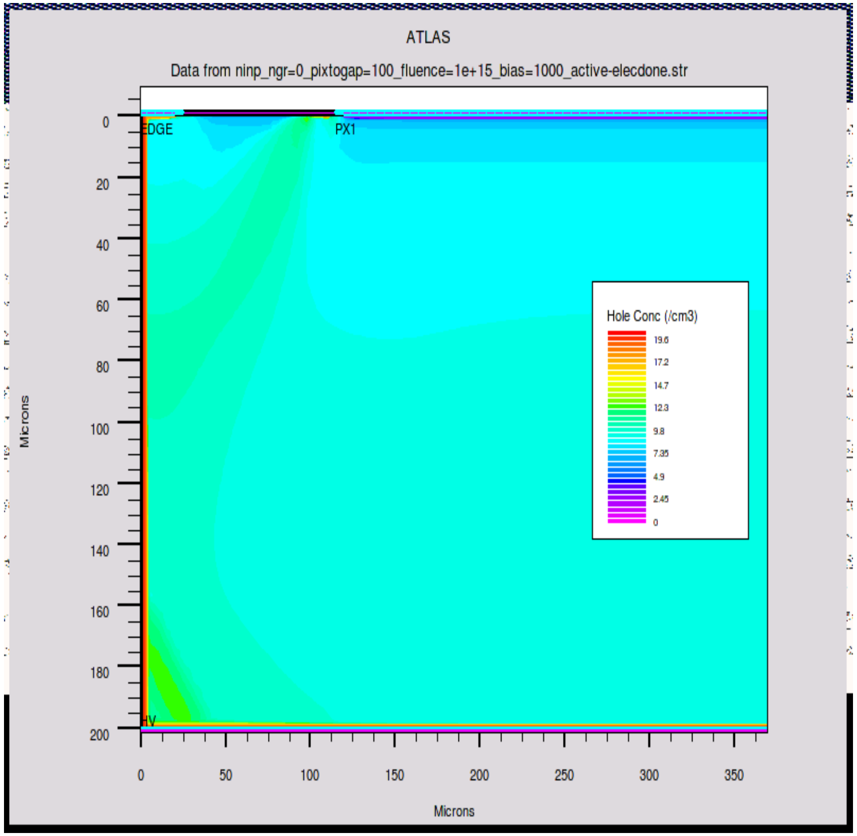


4 ns after particle hit

Electrons

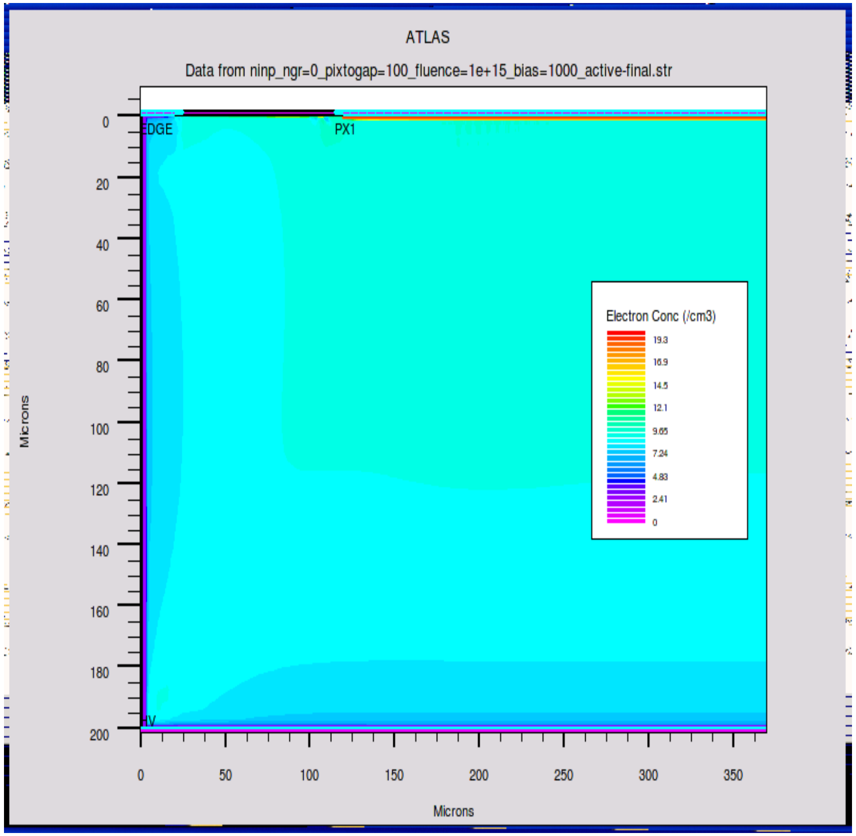


Holes



100 ns after particle hit

Electrons



Holes