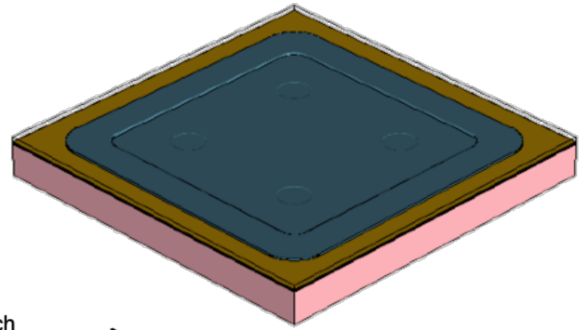
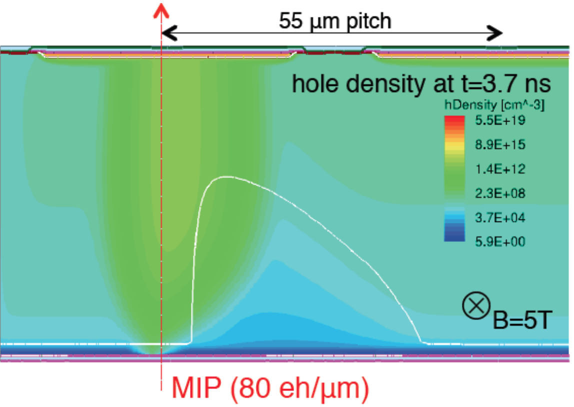
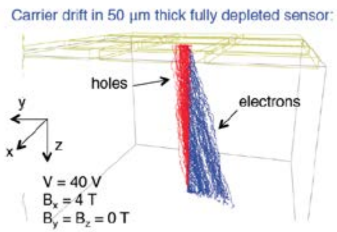
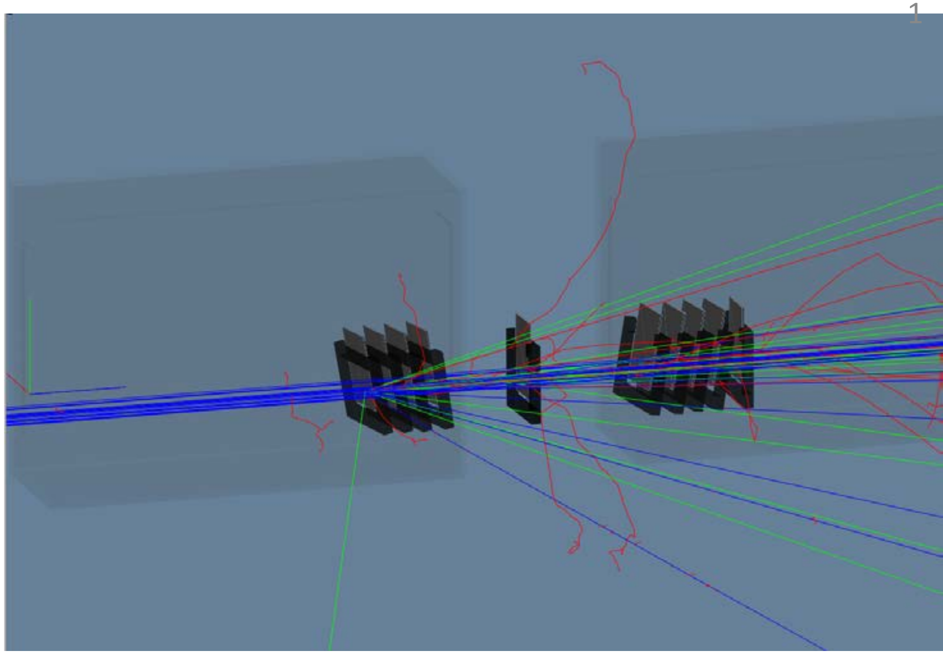








Simulation of Silicon detectors using TCAD and Monte-Carlo methods

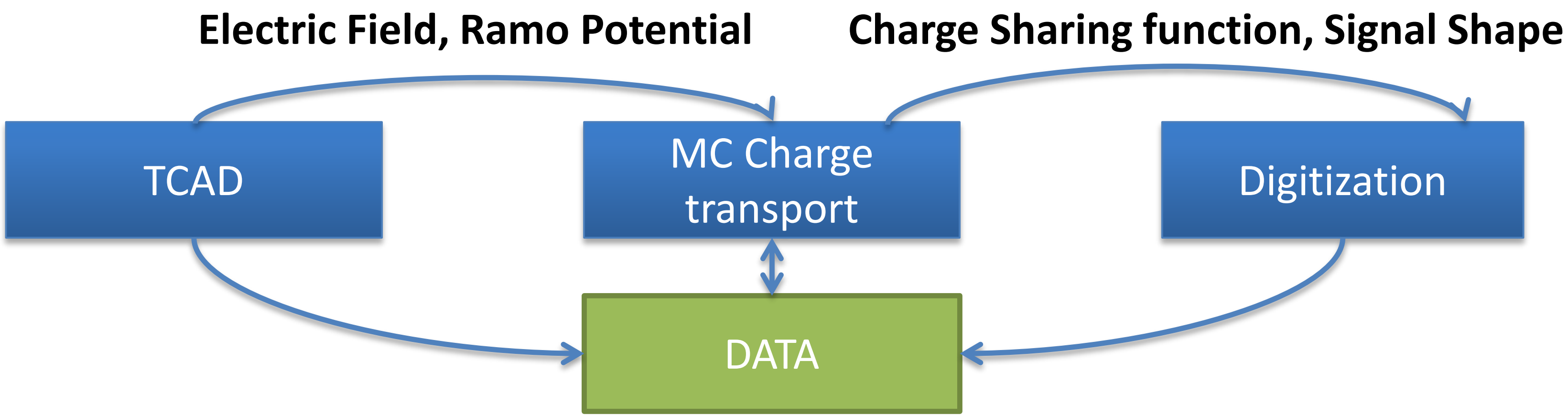
Mathieu Benoit

Outline

Warning this talk might contain spherical cows

- Introduction to detector simulation
  - Technology Computer-assisted design (TCAD)
  - GEANT4 and Monte-Carlo Charge transport
- Examples of TCAD Simulation use cases
  - Multi-Guard Ring structure in Planar sensors
  - Charge-Multiplication In heavily irradiated planar sensors
  - Field distribution in HV-CMOS sensors
- Monte-Carlo Charge transport use cases
  - Charge-sharing prediction for CdZnTe co-planar cross-strip sensors
  - Magnetic field effect on Cluster distribution in silicon pixel detectors

Sensor simulation flow



- First principle simulation
- Long simulation time (~hours per event)
- Detailed modeling of geometry

- Integration of TCAD Field and Ramo potential into simulation
- Faster (~s, min per event)
- Still computing intensive for large area detectors

- Parametric model
- Simple model
- Least computing intensive model (10-100/s)
- Include Readout ASIC effects
- Can be used for large area detectors

INTRODUCTION TO TCAD

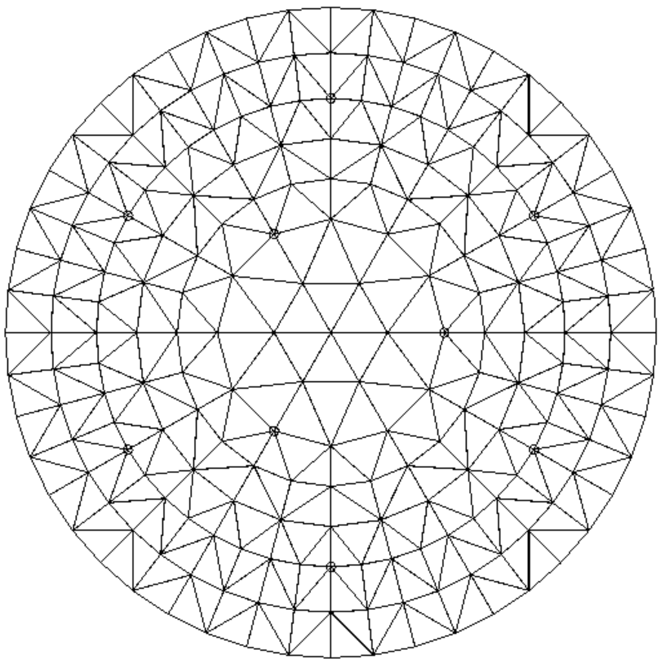
TCAD simulation principles

Discretization of the Domain

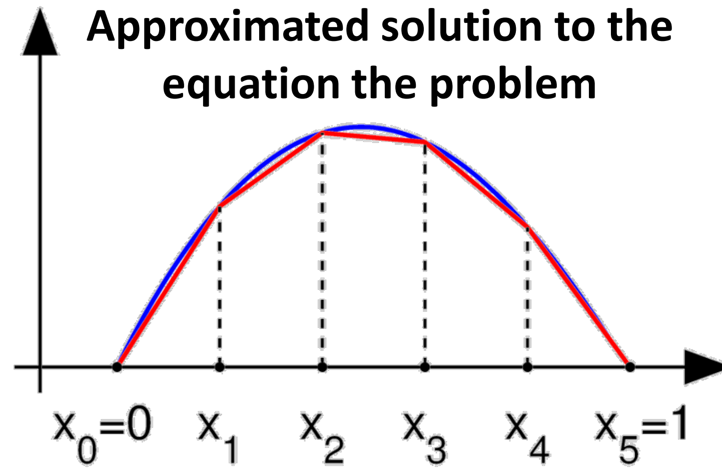
$MU_k = B$

$$q\frac{dn}{dt} = q\left[(G_n - R_n) + \nabla\cdot(n\mu_n\vec{E} + D_n\nabla n)\right]$$

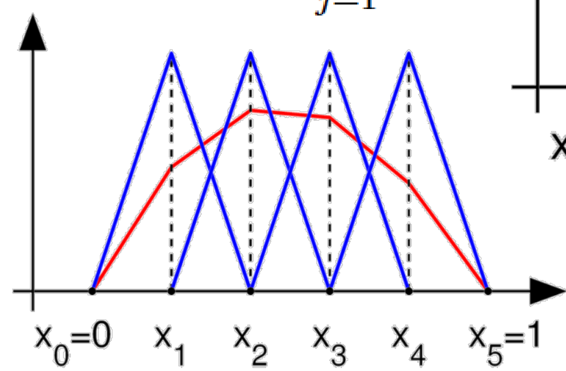
$$-\nabla(\varepsilon\cdot\nabla V) = q(c + p - n)$$



Approximated solution to the equation the problem



$$u_k = u_g + \sum_{j=1}^{n} u_j\phi_j$$



$U_k = M^{-1}B$

Approximation of the solution space using test function

TCAD simulation workflow

« Old-school » process simulation

- Hard-coded pixel geometry when defining processing steps
- Possibility for limited parametrization

Process Flow simulation

- Work with GDSII files provided by your favorite vendor
- Abstract description of the process

Simple description of the geometry and doping using an editor

- Define geometry (Shape,material)
- Define doping profile (parametric description)

Device Simulation Conditioning

- Reduce Complexity (symmetry, dead area removal)
- Remesh for Device simulation (reduce oxide/nitride mesh, increase bulk)

Device Simulation

- Electric Field, Ramo Potential
- Capacitance
- Transient Behavior
- Thermal/Mechanical Stress Simulation

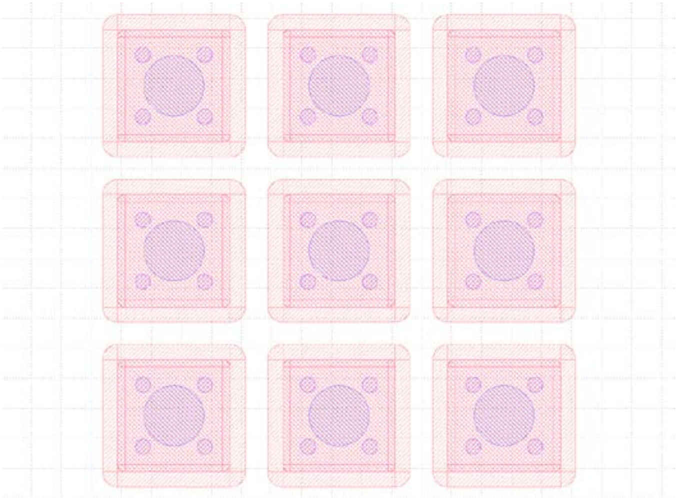
Post-Processing

- Extract Profiles (E(x,y,z) , etc)
- Extract Values (Breakdown, Depletion Potential)

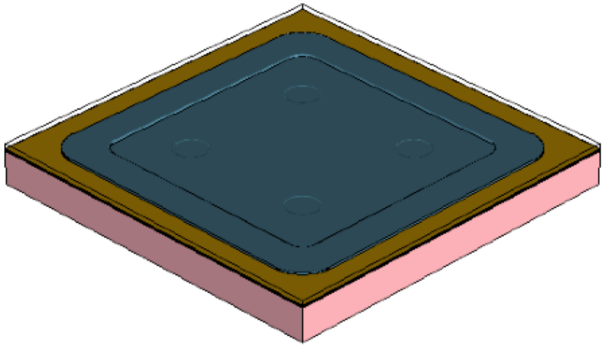
Process Flow Simulation

- Process Flow simulation allows for more automated studies of different geometries
  - Generate mask using your favorite software (pyGDS, Cadence, etc)
  - Use GDSII mask to define geometry
  - Use abstract and parametric description of the process
    - Implantation, lithography, deposits, annealing etc…
- Takes Advantage of multiplication of available CPU/RAM in the HEP Community
  - Chose a set of geometrical/Process/Electrical parameter to scan
  - Launch simulation in parallel using LSF Infrastructure (Synopsys Sentaurus @ CERN)

https://github.com/mathieubenoit/GDSII_Generator



Timepix 3x3 Pixel Mask set generated using pyGDS



Structure Generated using process Flow

Process Flow Simulation

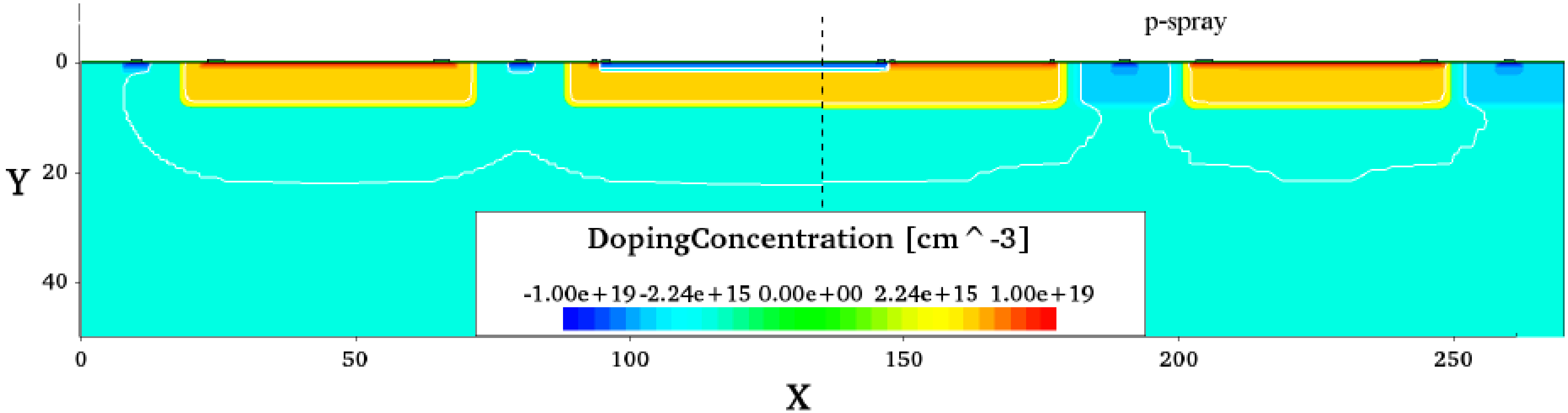
Variables & Macros | Flow | Unfolded Flow

Names	Arg	Value	Arg	Value	Arg	Value	Arg	Valu
Unfolded Flow								
#header								
insert	dios		sprocess	math coord.ucs	sde		tsuprem4	
environment	title	MPX3x3	save	true	grid	true	debug	false
substrate	material	Silicon	dopant	boron	concentration	0 /cm3	resistivity	5000 ohm
comment	text	Added process t						
insert	dios		sprocess	math numThread	sde		tsuprem4	
insert	dios		sprocess	#pdbSet Grid sM	sde		tsuprem4	
insert	dios		sprocess	grid remesh	sde		tsuprem4	
save	basename	After_first_mesh	format	plot	dios		sprocess	
#endheader								
deposit	material	Oxide	thickness	100 nm	dopant	default	concentration	/cm3
deposit	material	Nitride	thickness	200 nm	dopant	default	concentration	/cm3
implant	species	boron	dose	1e12 /cm2	energy	@PSPRAYENEF	tilt	0 deg
pattern	layer	IMPLANT	polarity	dark_field	thickness	0.1 um	side	front
save	basename	after_resist	format	plot	dios		sprocess	
insert	dios		sprocess	#etch type=anisi	sde		tsuprem4	
etch	material	Nitride	thickness	200 nm	etch_type	anisotropic	overetch	1
etch	material	Oxide	thickness	50 nm	etch_type	anisotropic	overetch	0
etch	material	Resist	thickness	default	etch_type	strip	overetch	0
implant	species	phosphorus	dose	@NDOSE@ /cm	energy	@NENERGY@ k	tilt	0 deg
save	basename	after_oxide_etch	format	dump	dios		sprocess	
pattern	layer	CONTACT	polarity	dark_field	thickness	0.1 um	side	front
etch	material	Oxide	thickness	default	etch_type	anisotropic	overetch	0
etch	material	Resist	thickness	default	etch_type	strip	overetch	0
save	basename	after_oxide_hole	format	plot	dios		sprocess	
deposit	material	Aluminum	thickness	300 nm	dopant	default	concentration	/cm3
pattern	layer	CANOD	polarity	light_field	thickness	0.1 um	side	front
etch	material	Aluminum	thickness	default	etch_type	anisotropic	overetch	0
etch	material	Resist	thickness	default	etch_type	strip	overetch	0
anneal	time	30 min	temperature	960 degC	pressure	1 atm	nitrogen	0 l/min
save	basename	top_n@node@	format	plot	dios		sprocess	
insert	dios		sprocess	paste direction=i	sde		tsuprem4	
insert	dios		sprocess	paste direction=l	sde		tsuprem4	
save	basename	one_per_three_r	format	plot	dios		sprocess	

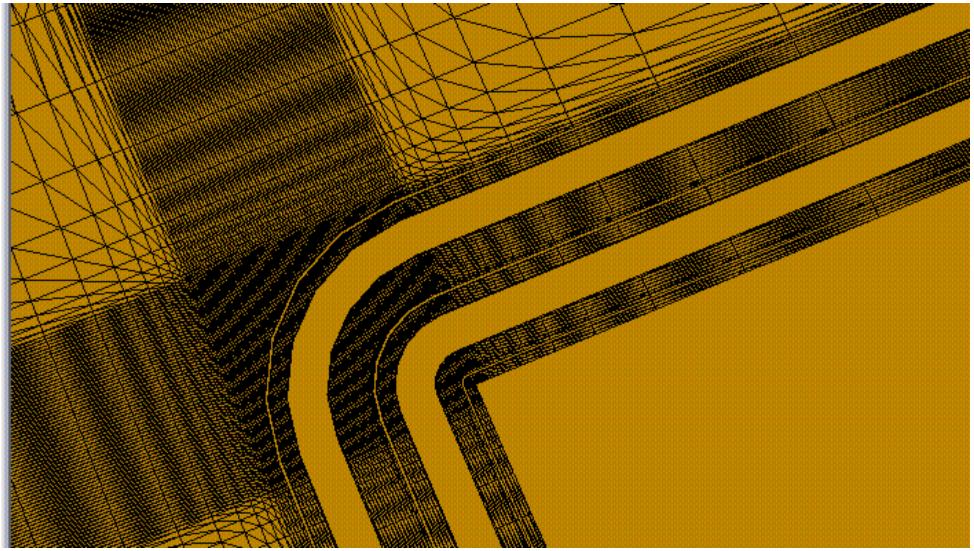
Process Simulation

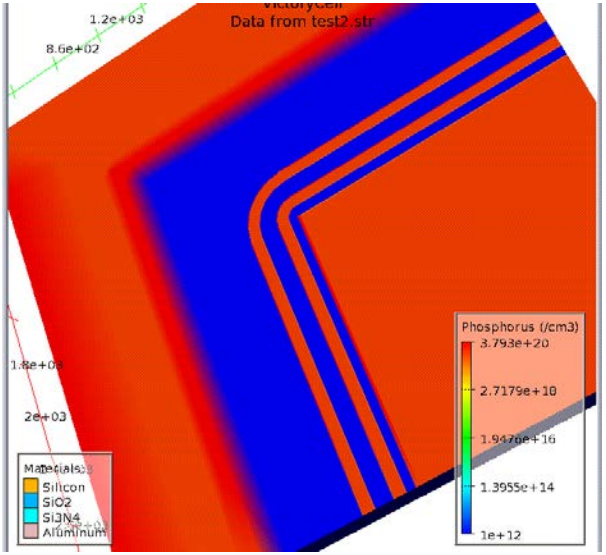
Process Simulation allow to define the bulk properties of the device to simulate

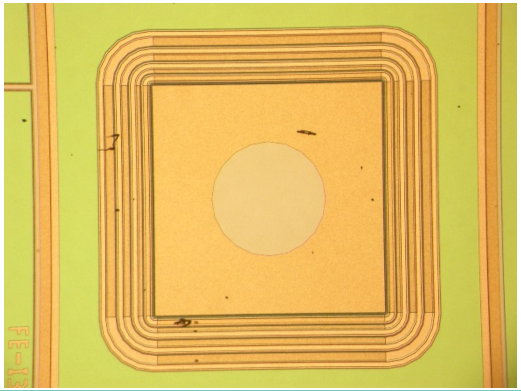
- Doping concentration
- Electrode position and contact surface
- Oxide surfaces
- Traps and defect concentration
- Well defined Mesh



Importance of meshing properly







- Meshing in the **first main problem you will encounter when doing TCAD simulation**
- Determination of the perfect mesh is not an exact science (a lot of trial and error !)
  - Upper limit of mesh size set by device feature size (implants , electrodes)
  - Lower limit of mesh size set by computational limits (RAM, computing time)
  - Meshing algorithm available in software packages also have internal limitation (!!!)

TCAD simulation principles : Beyond the standard model !

It is possible for the main TCAD simulation to perform simulation at higher orders of Boltzmann Transport Equation :

The thermodynamic model

- Continuity equation only
- Maxwell-Boltzmann Statistics expected
- Take into account thermal gradients
- Transport Time >> Energy Relaxation time

$$\vec{J}_n = -nq\mu_n(\nabla\Phi_n + P_n\nabla T)$$

$$\vec{J}_p = -pq\mu_p(\nabla\Phi_p + P_p\nabla T)$$

Carrier current Equations

The hydrodynamic model

- Energy balance taken into account
- Modelize Carrier Heating, Velocity overshoot
- Transport Time ~ Energy Relaxation time
- Full Thermal treatment possible

$$\vec{J}_n = q\mu_n\left(n\nabla E_C + kT_n\nabla n - nkT_n\nabla\ln\gamma_n + \lambda_n f_n^{td} kn\nabla T_n - 1.5nkT_n\nabla\ln m_n\right)$$

$$\vec{J}_p = q\mu_p\left(p\nabla E_V - kT_p\nabla p + pkT_p\nabla\ln\gamma_p - \lambda_p f_p^{td} kp\nabla T_p - 1.5pkT_p\nabla\ln m_p\right)$$

Physics List (Device Simulation)

Physics	Models
Mobility	Concentration-dependent mobility (fit to experimental data), Parallel field dependent mobility (fit to experimental saturation velocities)
Generation recombination and trapping	Modified concentration dependent Shockley-Read-Hall Generation/recombination (for treatment of defects)
Impact ionization	Selberherr's Impact ionization model
Tunneling	Band-to-band tunnelling, Trap-Assisted tunneling
Oxide physics	Fowler-Nordheim tunnelling, interface charge accumulation

$$q\frac{dn}{dt} = q\left[(G_n - R_n) + \nabla\cdot\,(n\mu_n\vec{E} + D_n\nabla n)\right]$$

$$-\nabla(\varepsilon\cdot\,\nabla V) = q(c + p - n)$$

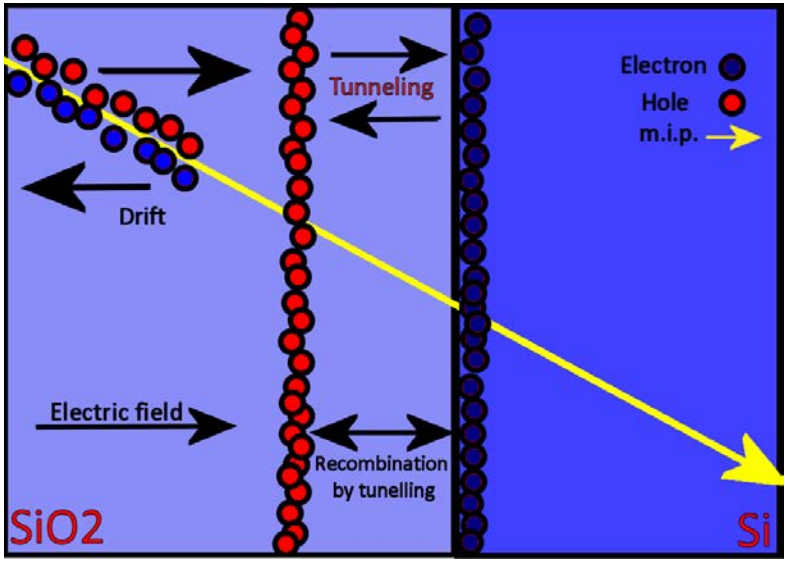
Radiation damage

Non-ionizing Energy loss

P-TYPE RADIATION DAMAGE MODEL

Defect's energy (eV)	Introduction rate (cm^{-1})	Electron capture cross-section (cm^{-2})	Hole capture cross-section (cm^{-2})
$E_c - 0.42$	1.613	2.e-15	2e-14
$E_c - 0.46$	0.9	5e-15	5e-14
$E_c - 0.10$	100	2e-15	2.5e-15
$E_v + 0.36$	0.9	2.5e-14	2.5e-15

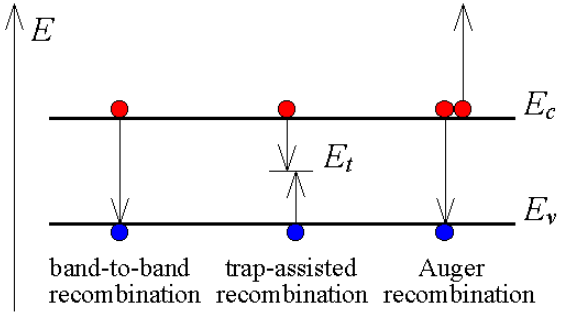
Ionizing Energy loss



Good recent progress on obtaining quantitative models for radiation damage modeling, See [RD50: simulation of radiation-induced defects](), T. Hannu Tapani Peltola, Vertex15

Generation/Recombination

- Modified Shockley-Read-Hall G/R
  - A sum of SRH contribution by each trap
  - Γ is the degeneracy of the trap, n_i the intrinsic concentration of carriers



$$R_{n,p} = \sum R_i$$

$$R_i = \frac{pn - n_i^{\;2}}{\tau_{ni}\left(p + \Gamma n_i e^{(Ef - Ei)/kT}\right) + \tau_{pi}\left(n + \frac{n_i e^{(Ei - Ef)/kT}}{\Gamma}\right)}$$

Generation/Recombination

- Transient behaviour of traps

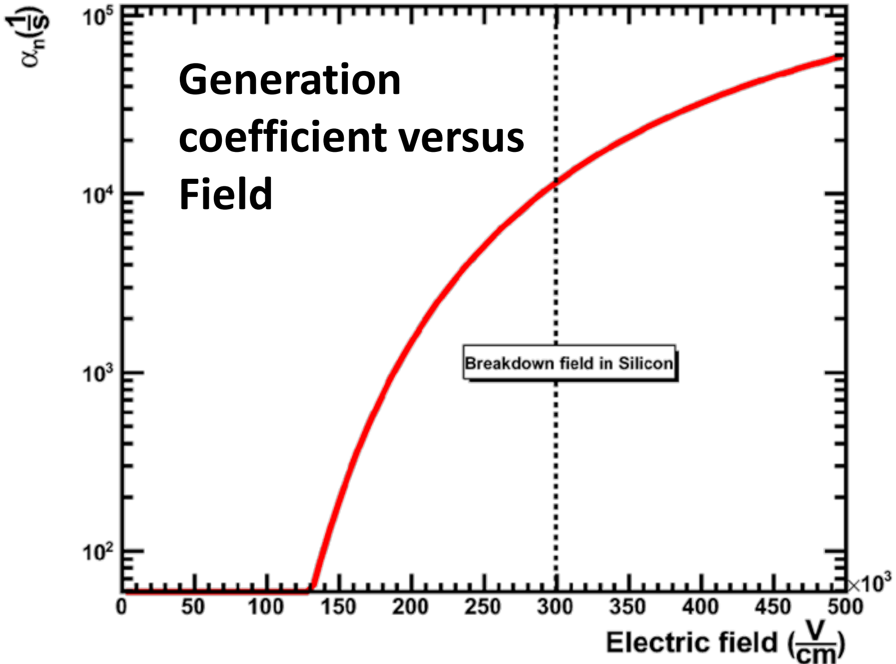
$$\frac{dN_{tD}^{+}}{dt} = \rho_t \left\{ \overbrace{v_p \sigma_p \left(p(1-F_{tD})\right.}^{\text{hole capture}} \overbrace{- F_{tD} n_i \Gamma e^{\frac{E_i - E_t}{kT}}}^{\text{hole emmision}} \left.\right) - v_n \sigma_n \left(\overbrace{n F_{tD}}^{\text{electron capture}} \overbrace{- \frac{(1-F_{tD}) n_i}{\Gamma} e^{\frac{E_t - E_i}{kT}}}^{\text{electron emmision}} \right) \right\}$$

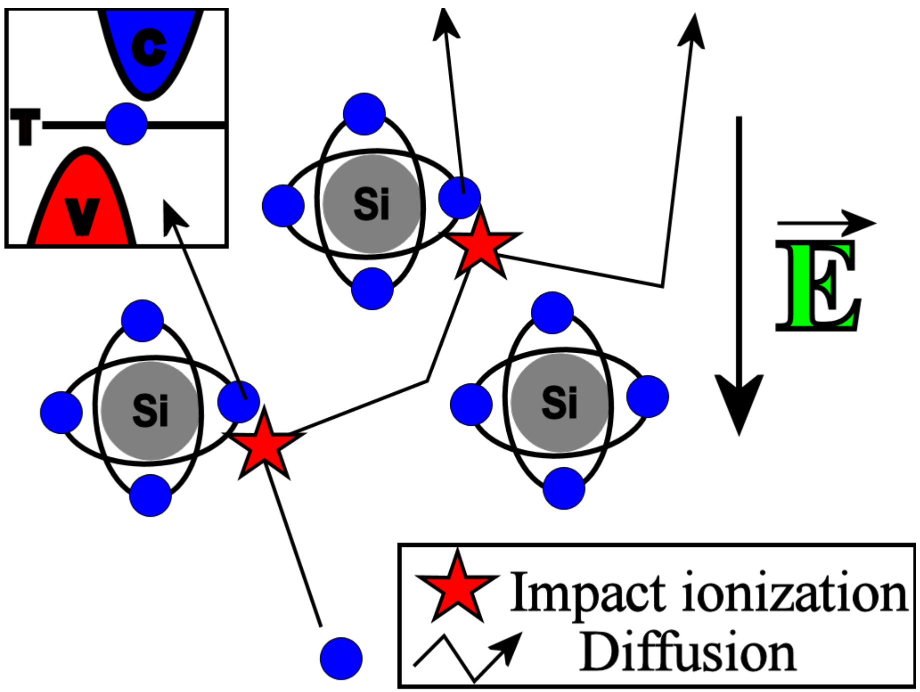
$$\frac{dN_{tA}^{-}}{dt} = \rho_t \left\{ \underbrace{v_n \sigma_n \left(n(1-F_{tA})\right.}_{\text{Electron capture}} \underbrace{- F_{tA} n_i \Gamma e^{\frac{E_t - E_i}{kT}}}_{\text{Electron emmision}} \left.\right) - v_p \sigma_p \left(\underbrace{p F_{tA}}_{\text{Hole capture}} \underbrace{- \frac{(1-F_{tA}) n_i}{\Gamma} e^{\frac{E_i - E_t}{kT}}}_{\text{Hole emmision}} \right) \right\}$$

$\sigma_{n,p}$ is trap capture cross-section
$v_{n,p}$ is thermal velocity
n_i is intrinsic concentration
$F_{tA,TD}$ the probability of ionization
$N_{tA,TD}$ space charge density

$$\sigma_n = \frac{1}{\rho_{trap} \tau_n v_n} \quad \sigma_p = \frac{1}{\rho_{trap} \tau_p v_p}$$

Impact ionization





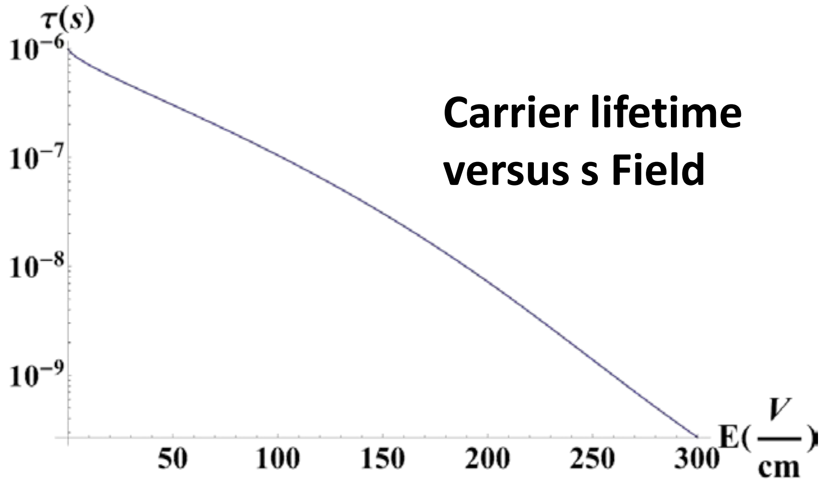
$$G = \alpha_n(E)J_n + \alpha_p(E)J_p$$

$$\alpha_n = A_n e^{-(B_n/E)^{\beta_n}}$$

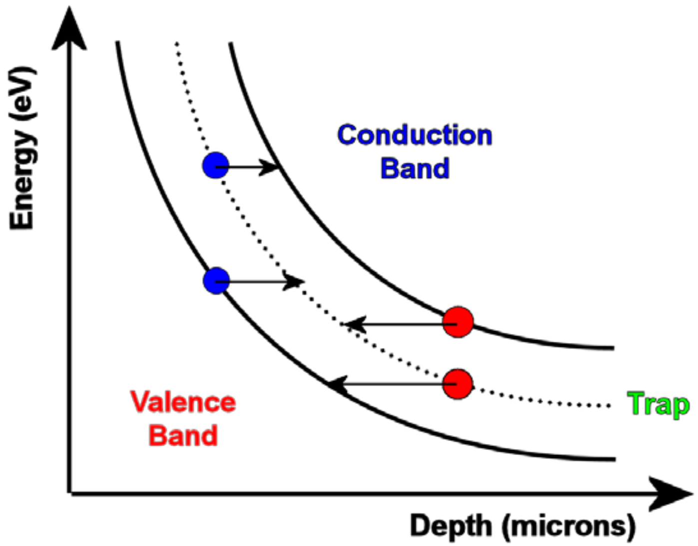
$$\alpha_p = A_p e^{-(B_p/E)^{\beta_p}}$$

Selberherr, S., **"Analysis and Simulation of Semiconductor Devices"**, Springer-Verlag Wien New York, ISBN 3-211-81800-6, 1984.

Phonon-assisted trap-to-band tunnelling



Carrier lifetime versus s Field



$$R_i = \frac{pn - n_i^2}{\frac{\tau_{n0}}{1+\Gamma_n^{DIRAC}}(p + \Gamma n_i e^{(Ef-Ei)/kT}) + \frac{\tau_{p0}}{1+\Gamma_p^{DIRAC}}(n + \frac{n_i e^{(Ei-Ef)/kT}}{\Gamma})}$$

$$\Gamma_n^{DIRAC} = \frac{\Delta E_n}{kT_L}\int_0^1 e^{(\frac{\Delta E_n}{kT_L}u - K_n u^{3/2})}du \qquad K_n = \frac{4}{3}\frac{\sqrt{2m_0 m_{tunnel}\Delta E_n{}^3}}{3q\hbar|E|}$$

$$\Gamma_p^{DIRAC} = \frac{\Delta E_p}{kT_L}\int_0^1 e^{(\frac{\Delta E_p}{kT_L}u - K_p u^{3/2})}du \qquad K_p = \frac{4}{3}\frac{\sqrt{2m_0 m_{tunnel}\Delta E_p{}^3}}{3q\hbar|E|}$$

Hurkx, G.A.M., D.B.M. Klaasen, M.P.G. Knuvers, and F.G. O'Hara, **"A New Recombination Model Describing Heavy-Doping Effects and Low Temperature Behaviour",** *IEDM Technical Digest(1989): 307-310.*

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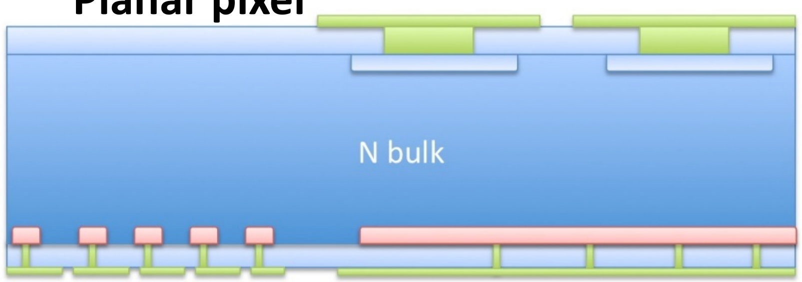
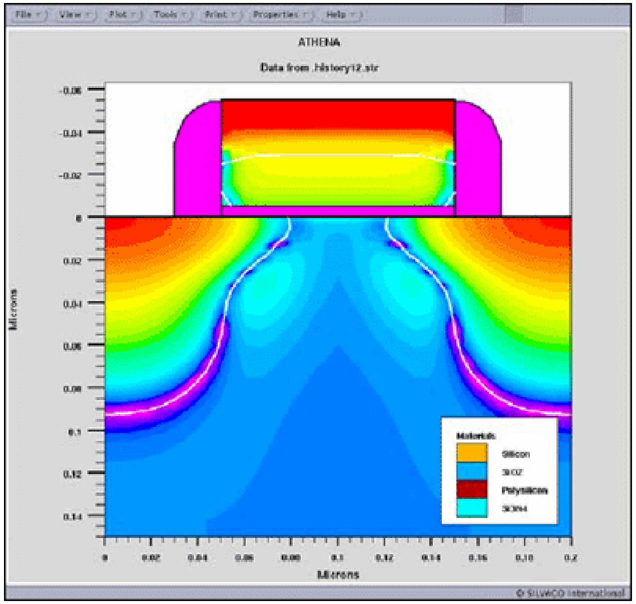
Boundary Conditions

- To define the problem to solve, we must identify the type of boundary in the geometry
  - Ohmic contact (Voltage=X or Current=Y)
  - Floating contact (Voltage=? or Current=0)
  - MOS Floating Contact or gate (Voltage=X, Charge =Q)
  - Insulator (Current = 0, Charge = X)
  - Schottky Barrier
  - Thermal boundaries (Power = X or Temperature = X)
  - Spice circuit element or other TCAD model link
  - Mix of the above

Planar pixel



Transistor



Numerical methods and convergence

- The second major issue you will encounter when doing TCAD simulation is convergence
  - In practice most problems will have large non-linearities due to the model used for G/R -> Newton method
  - More complex solver must be used to obtain solution in practice
  - A good initial solution is needed for all practical purposes
  - The solution is obtained by an iterative process and is driven by the boundary conditions of the problem

$$MX + B = R$$

$$M(X - R/M) + B = R2$$

(...) Convergence criteria

$$M(X - R/M - R2/M - (...)) + B = \in$$

Poisson Equation solution at Vbias=0 (Linear)

↓

Poisson Equation + n/p solution at Vbias=0

↓

Poisson Equation + n,p solution at Vbias=0

↓

Poisson Equation + n,p solution at Vbias=dV

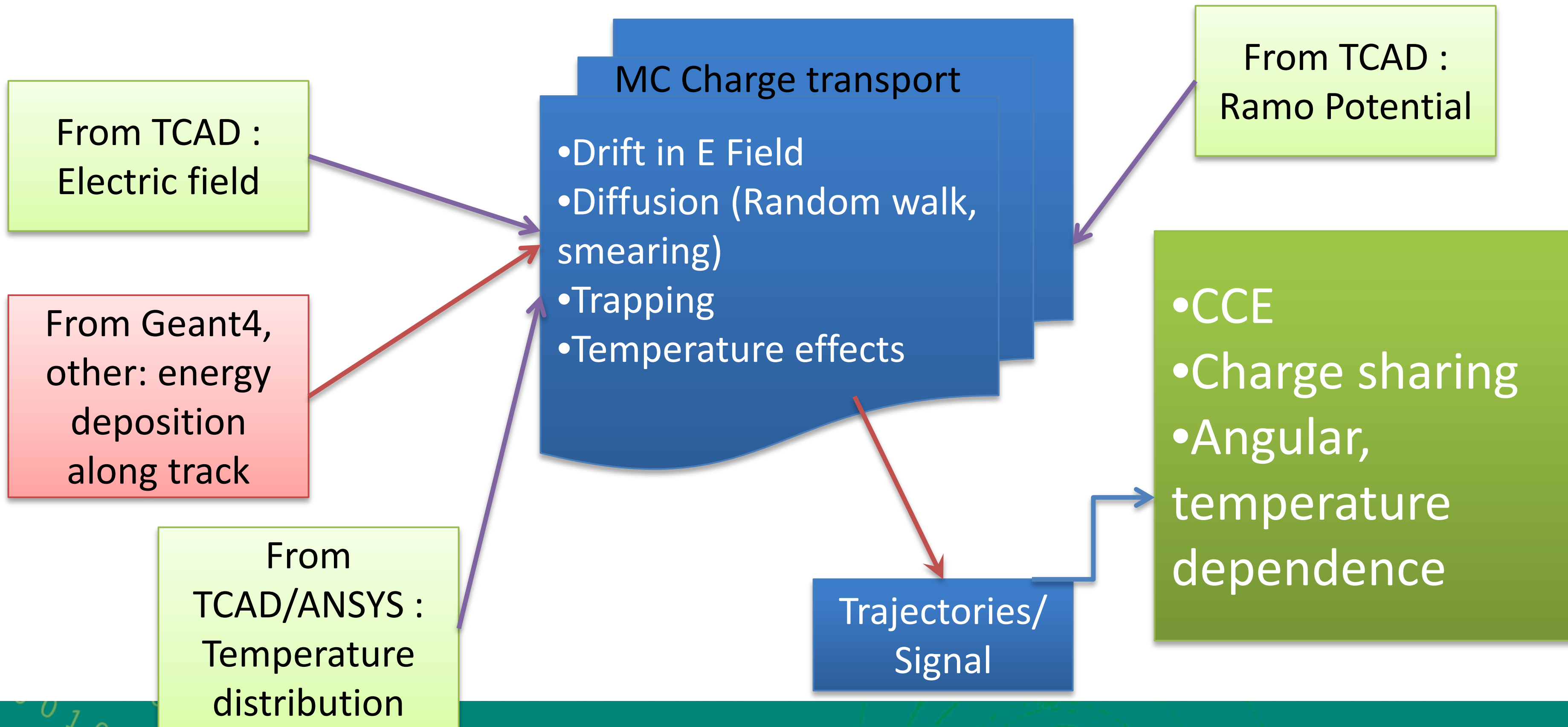
(...)

Poisson Equation + n&p solution at Vbias=Vfinal

INTRODUCTION MC CHARGE TRANSPORT

Simulation of detector behaviour : **MC Charge Transport**

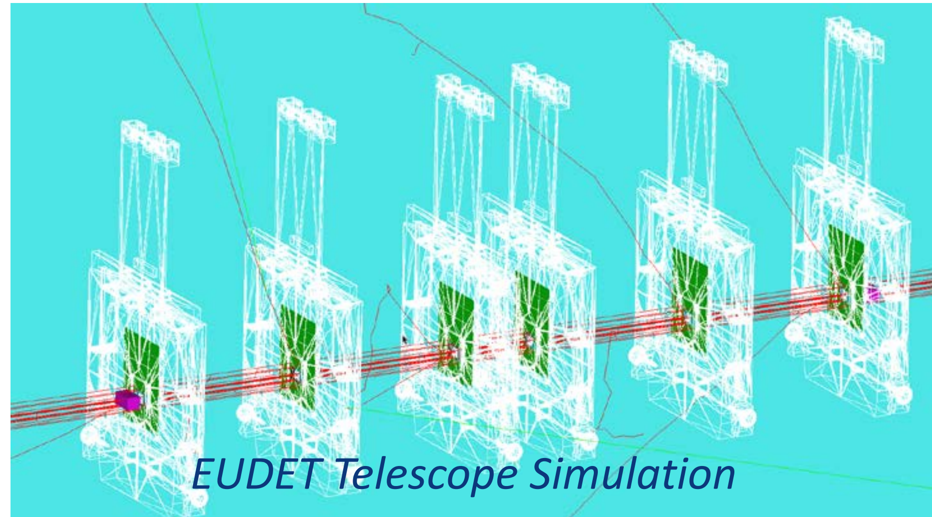
- Monte-Carlo approach to simulation of charge transport of e/h in Silicon
- https://github.com/mathieubenoit/clicmctsi



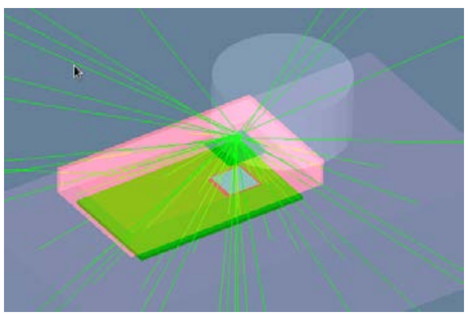
GEANT4 Simulation of Sensors

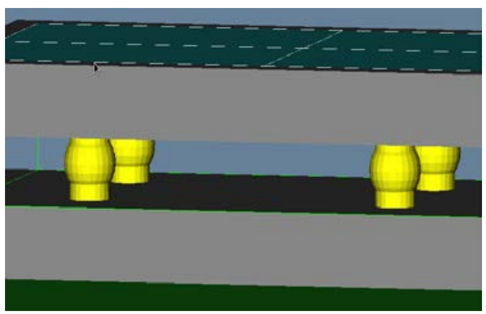
The **AllPix Simulation framework** allow for simulation of generic pixelated detectors

- Outputs data in EUTelescope data format allowing for telescope simulation reconstruction
- Geometry fully customizable
    - Thicknesses, bumps geometry, materials
- Used as a Digitizer test bench for ATLAS and CLICdp
- Use as a cluster topology generator tool for the RD53 collaboration (65nm ASIC for HL-LHC) in dev
- So Simple it is even use by CERN@SchoolHigh School students !

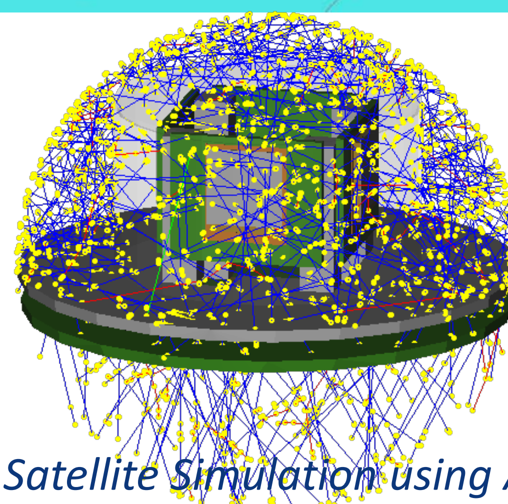


EUDET Telescope Simulation





https://twiki.cern.ch/twiki/bin/view/Main/AllPix
https://github.com/ALLPix/allpix



LUCID Satellite Simulation using AllPix

GEANT4 Simulation of Sensors

- Generic pixel simulation description
  - Specify pitch pitch, array size, bump size etc.. In a XML file
  - Use digitisation model provided by AllPix
    - MIMOSA26,Timepix,FEI3,MCTruth
  - Easily implement new digitizer using template generated by helper script
  - Implement dead material using GEANT4 primitive or GDML models (example provided)

- Simulation scenario using simple GEANT Script
  - Position sensors in geometry using x,y,z,angles
  - Position appliances in the geometry
  - Define beam type and statistics, geometry
  - Visualize the results (with a bit of effort ;))

- Output raw and digitized hits in a ROOT file for post-processing
  - EUTELESCOPE, Timepix, Judith data format available
  - Can be analysed standalone using MAFALDA :https://twiki.cern.ch/twiki/bin/view/Main/MAFalda

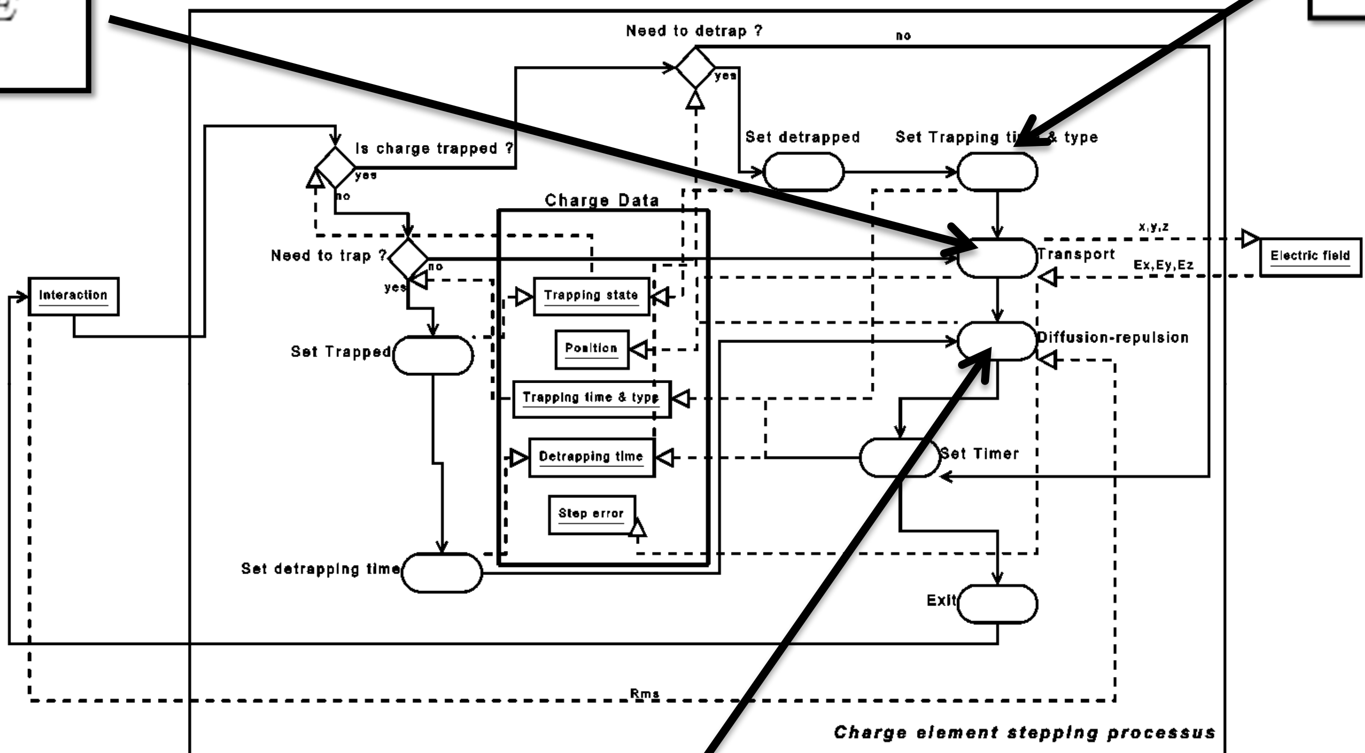
Charge Transport algorithm

$$\frac{d\vec{r}}{dt} = \mu\vec{E}$$

Drift

$$P(t) = \frac{1}{\tau_i} \exp \frac{t}{\tau_i}$$

Trapping



Diffusion
+
Repulsion

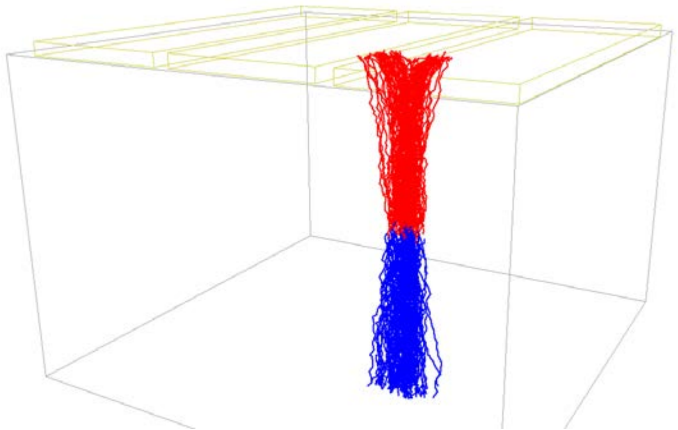
$$\vec{D} = \left(D + \frac{\sigma_x e N \mu}{20\sqrt{5}\sigma_y\sigma_z\pi\epsilon_0\epsilon_r}, D + \frac{\sigma_y e N \mu}{20\sqrt{5}\sigma_x\sigma_z\pi\epsilon_0\epsilon_r}, D + \frac{\sigma_z e N \mu}{20\sqrt{5}\sigma_x\sigma_y\pi\epsilon_0\epsilon_r}\right)$$

$$\rho(r,t) = \frac{N}{8(\pi D t)^{3/2}} \exp\left(-\frac{r^2}{4Dt}\right)$$

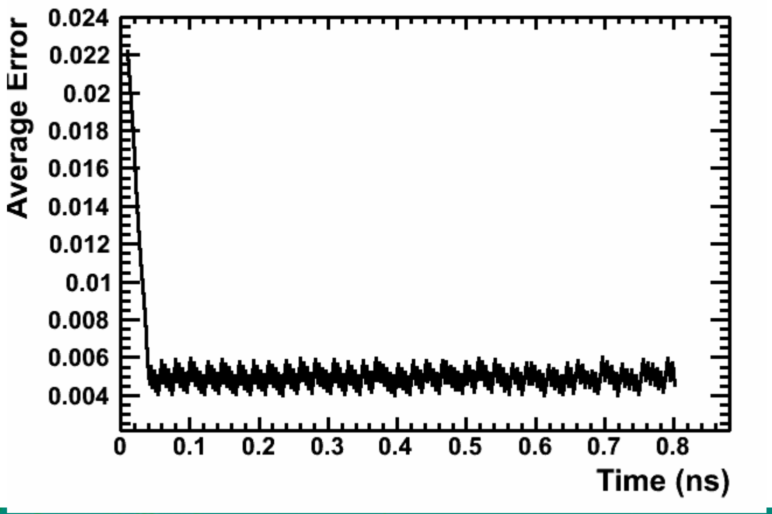
MC Charge transport

The main challenge in Charge Transport **Simulation is to write the proper propagator** that takes into account all the effects present in your device

- Trapping, De-trapping, Recombination
- Drift in Electric Field
- Lorentz Force
- Diffusion
- Charge multiplication



Each Charge element (e/h pairs) is propagated following these effects. Error propagation is important to obtain proper results. For example, **a good integration algorithm is RKF5**



$$\Delta x_{ordre\,5} = A*(K1+K2+K3+K4+K5)\Delta t$$

$$\Delta x_{ordre\,4} = B*(K1+K2+K3+K4)\Delta t$$

$$E = \frac{\Delta x_{ordre\,5} - \Delta x_{ordre\,4}}{\Delta x_{ordre\,5}}$$

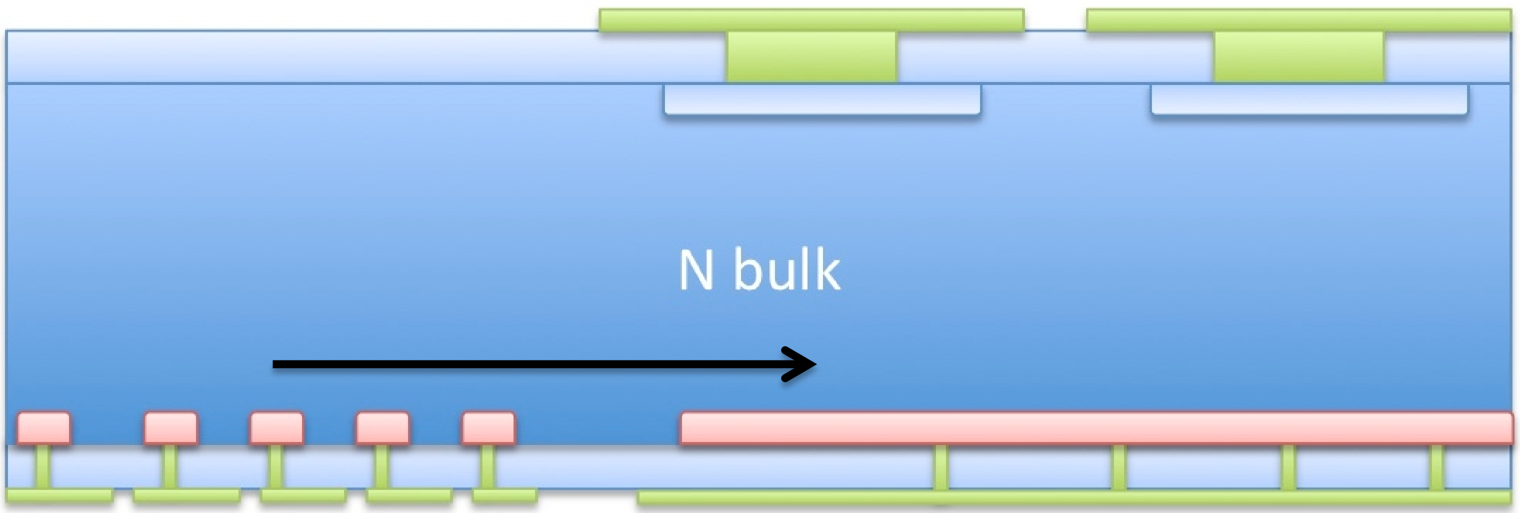
TCAD SIMULATION EXAMPLES

TCAD Simulation capabilities

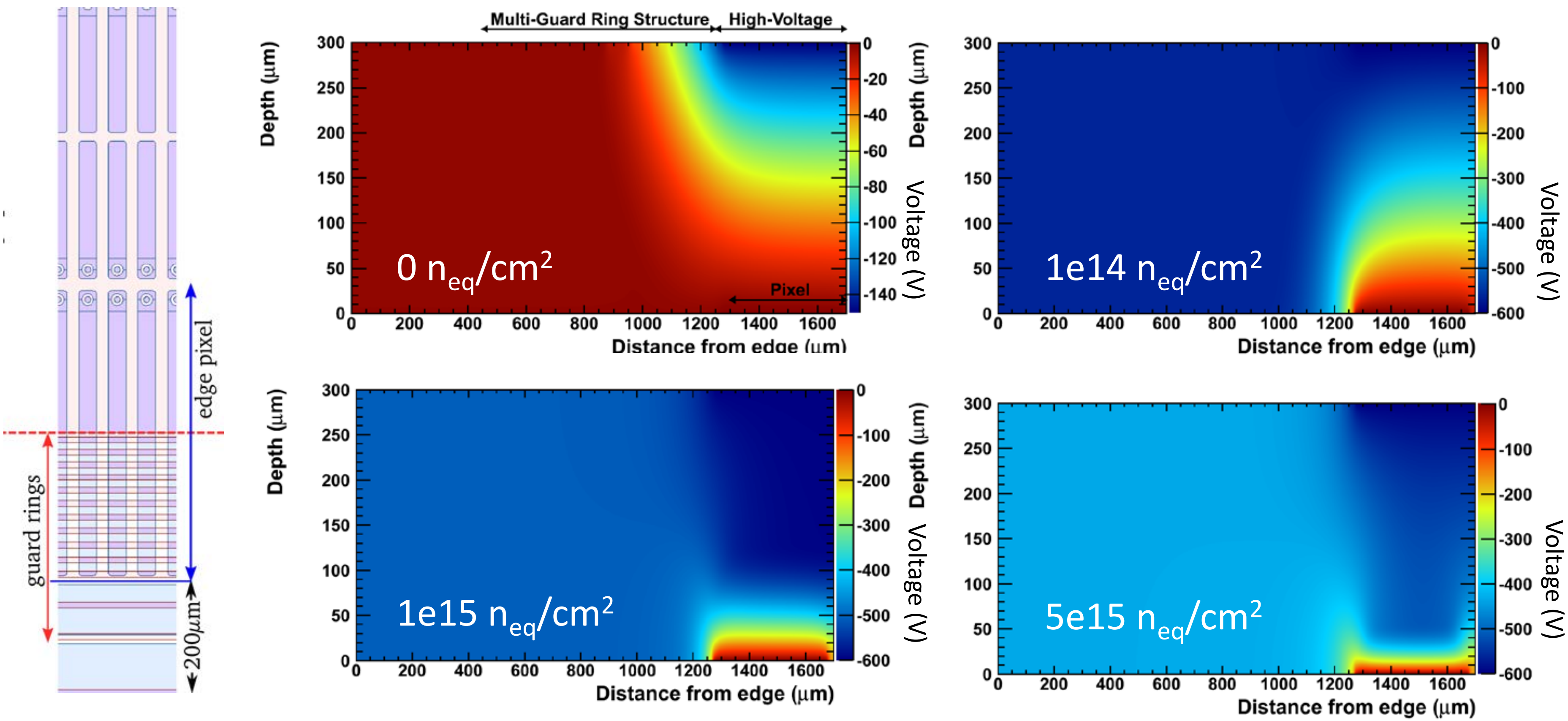
- TCAD is suitable for simulation of complex structure
  - Guard rings , punch-trough
  - E-Field distribution in presence of complex doping profiles
- Transient simulation
  - Voltage/Current changes, Particles
- AC Analysis (CV Curves, inter-pixel/strip capacitance)

ATLAS IBL Guard Ring structure

To reduce IBL sensor inactive edge, the idea was to push them under the pixel

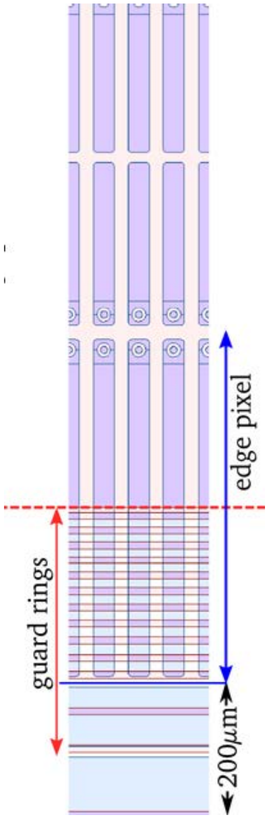


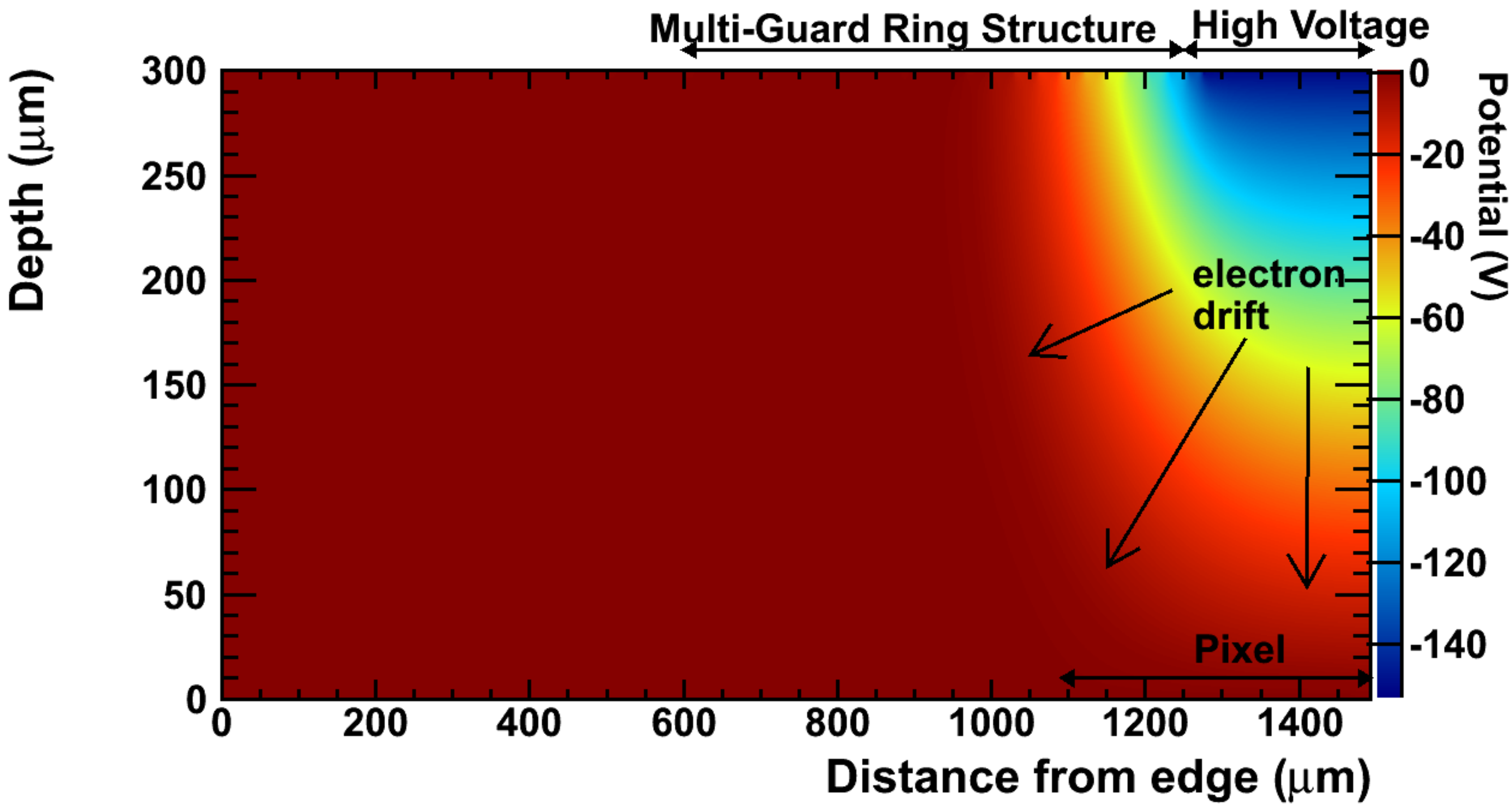
ATLAS Guard Ring Simulation and Space-Charge Sign Inversion (SCSI)



Simulation of Radiation Damage Effects on Planar Pixel Guard Ring Structure for ATLAS Inner Detector Upgrade
by: M. Benoit, A. Lounis, N. Dinu
Nuclear Science, IEEE Transactions on, Vol. 56, No. 6. (08 December 2009), pp. 3236-3243,
doi:10.1109/TNS.2009.2034002

ATLAS Guard Ring Simulation and Space-Charge Sign inversion (SCSI)





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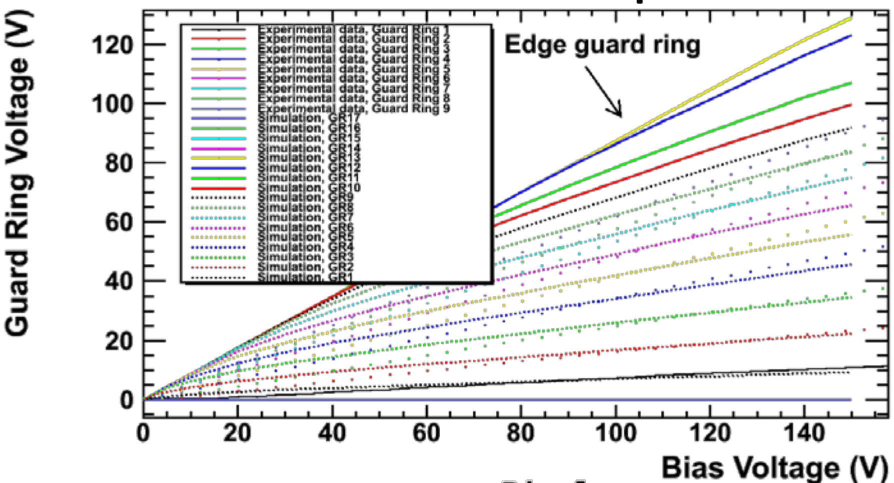
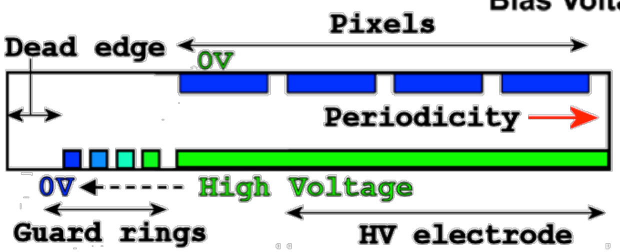
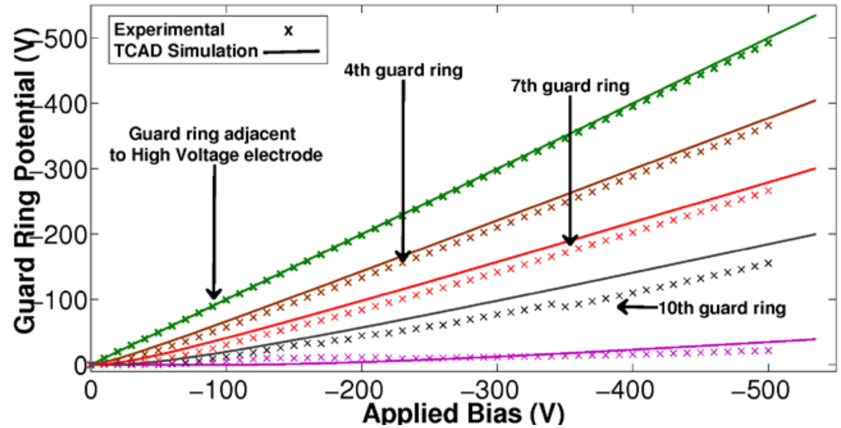
ATLAS GR : Measurement vs Simulation

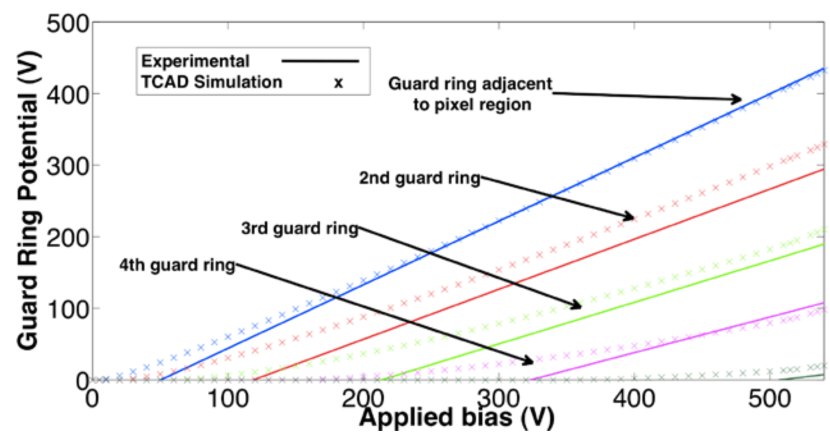
small GR n-in-p







n-in-n

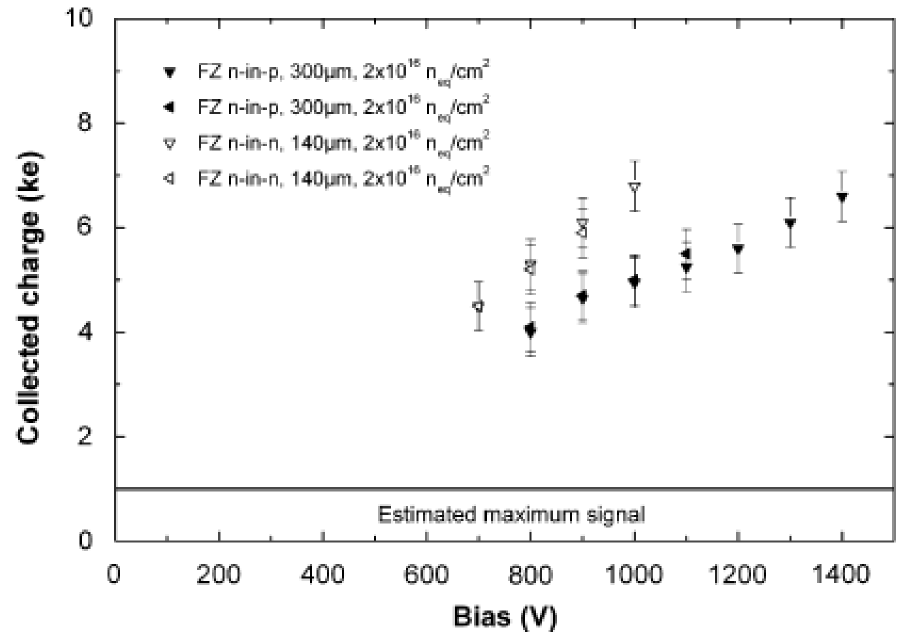


Very good agreement between simulation and data when using adequate technological parameters!

Large GR n-in-p

Charge multiplication in silicon planar sensors

- Measurements performed on diodes irradiated to sLHC fluence show anomalous charge collection
- The idea has been to use the radiation damage model in TCAD and include the impact ionization and trap-to-band tunnelling into the simulation to see if these physical effects can reproduce the observed behavior



G. Casse and al., “Evidence of enhanced signal response at high bias voltages in planar silicon detectors irradiated up to 2.2x10e16 neq cm-2,” Nucl. Instrum. Meth. A , j.nima.2010.04.085,, vol. In Press, Corrected Proof, pp. –, 2010.

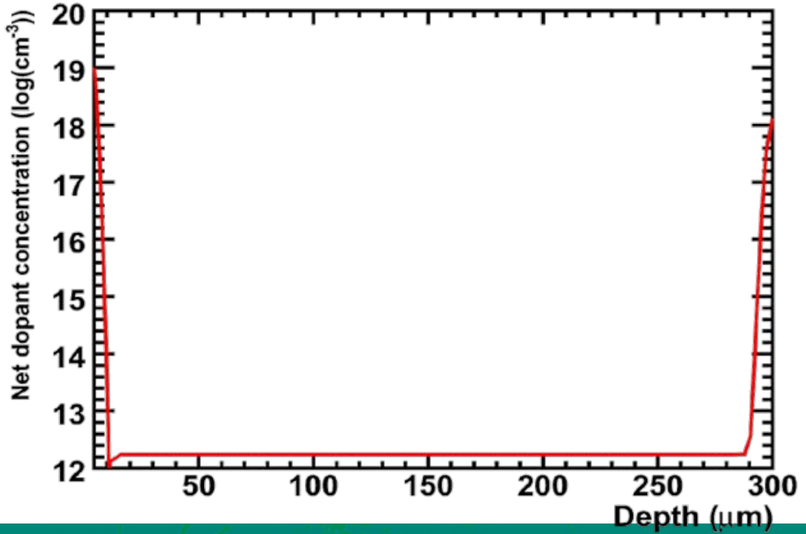
M. Mikuz, V. Cindro, G. Kramberger, I. Mandic, and M. Zavrtanik, “Study of anomalous charge collection efficiency in heavily irradiated silicon strip detectors,–,j.nima, 2010.

An example : 1D heavily irradiated n-in-p diode

- A simple 1D p-type diode, n readout
- Neff = 1.74e12/cm3
- 140 and 300 microns thickness
- 2KΩcm resistivity, high implant peak concentration (1e18-19/cm3)

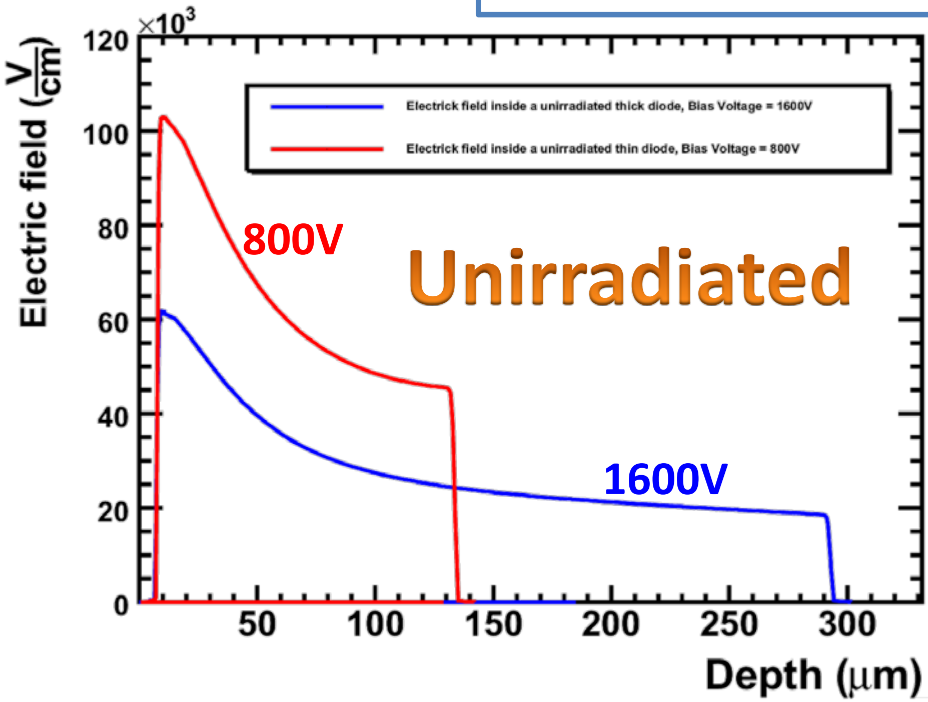
To simulate the CCE curve of the irradiated detector, We:

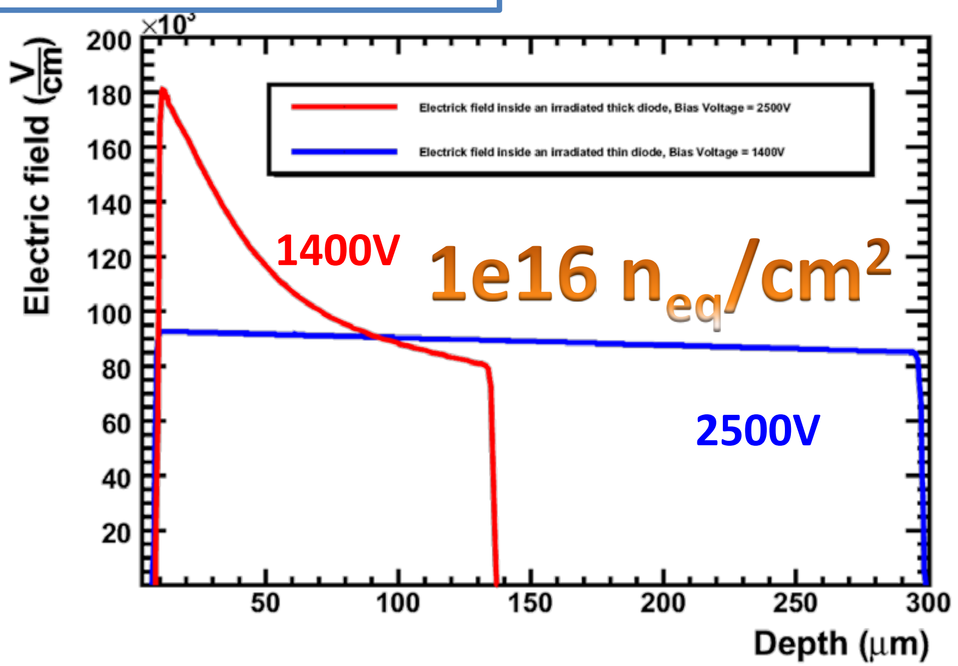
- **1. Generate a mip-like charge distribution with a 1060nm laser, 0.05W/cm2**
- **2. Perform transient simulation over 25ns for each bias**
- **3. Numerical integration of resulting current minus pedestal**
- **4. Numerical integration of available photocurrent**
- **5. CCE= Qpulse / Qphotocurrent**



Electric field profiles

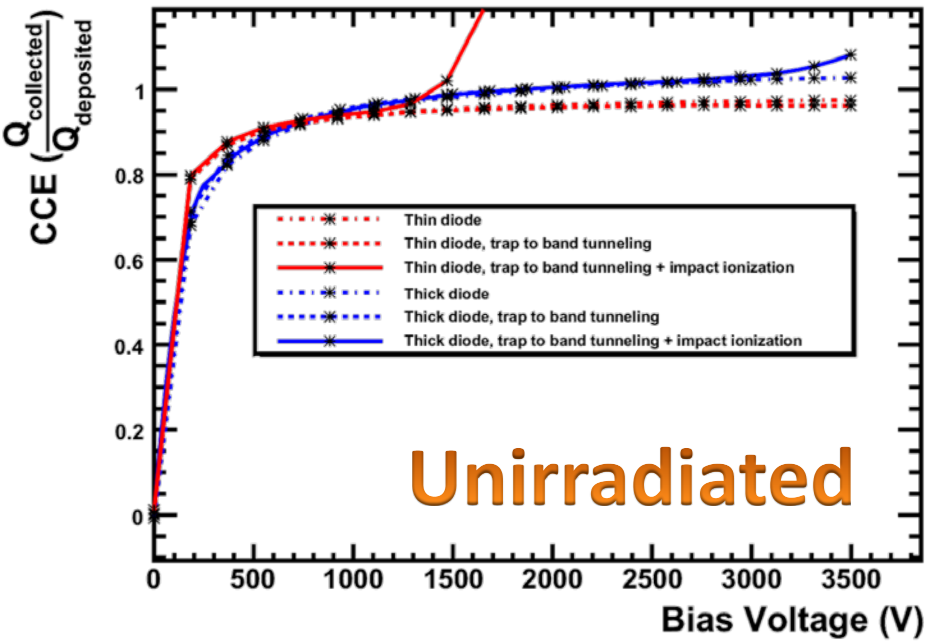
Electric field before hard junction breakdown.

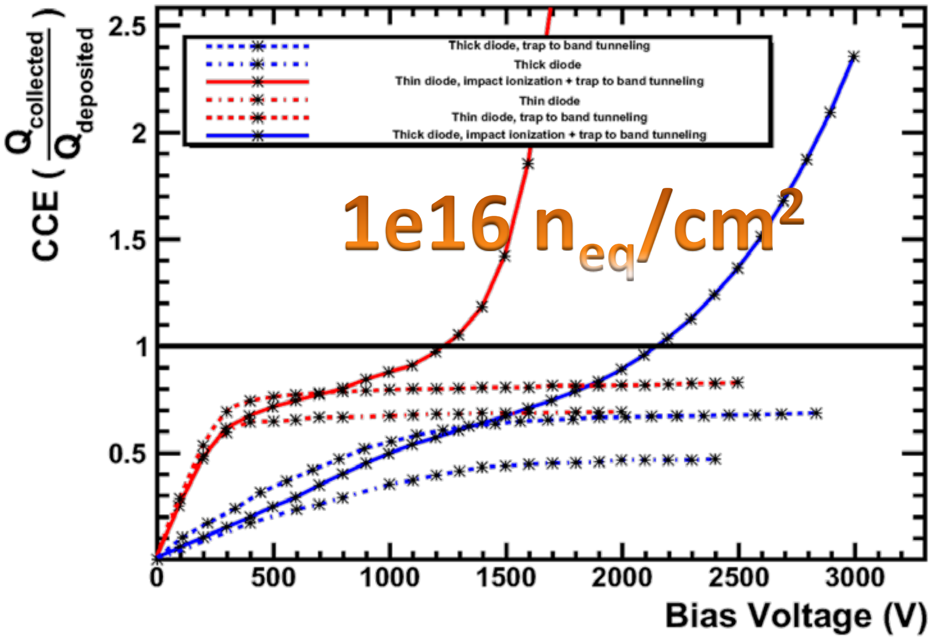




Sensor can be biased to HV after irradiation without reaching hard breakdown allowing multiplication in the high electric field produced by this bias

Charge collection efficiency

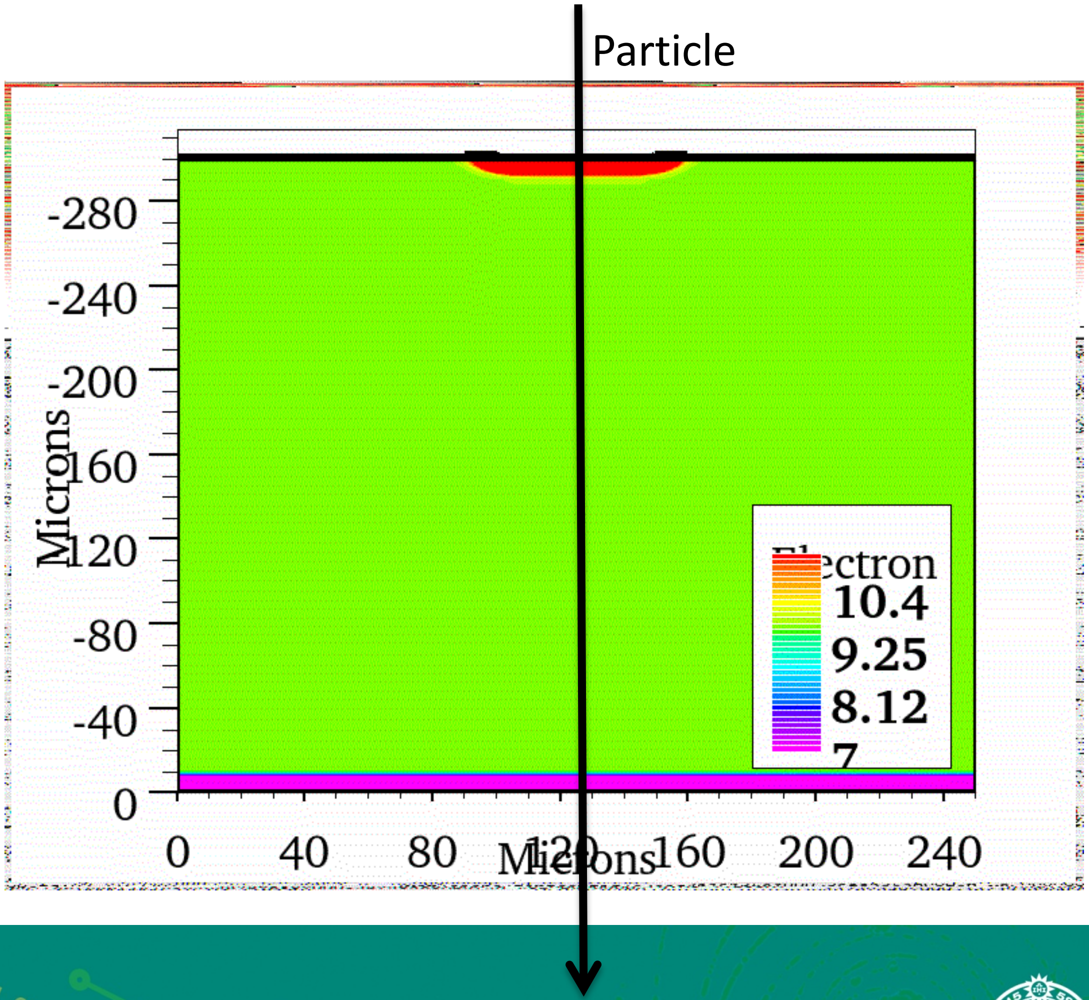




Unirradiated diode unaffected by TTBT and II are off. However, they both contribute to CCE after irradiation because of the presence of the > 200kV/cm field

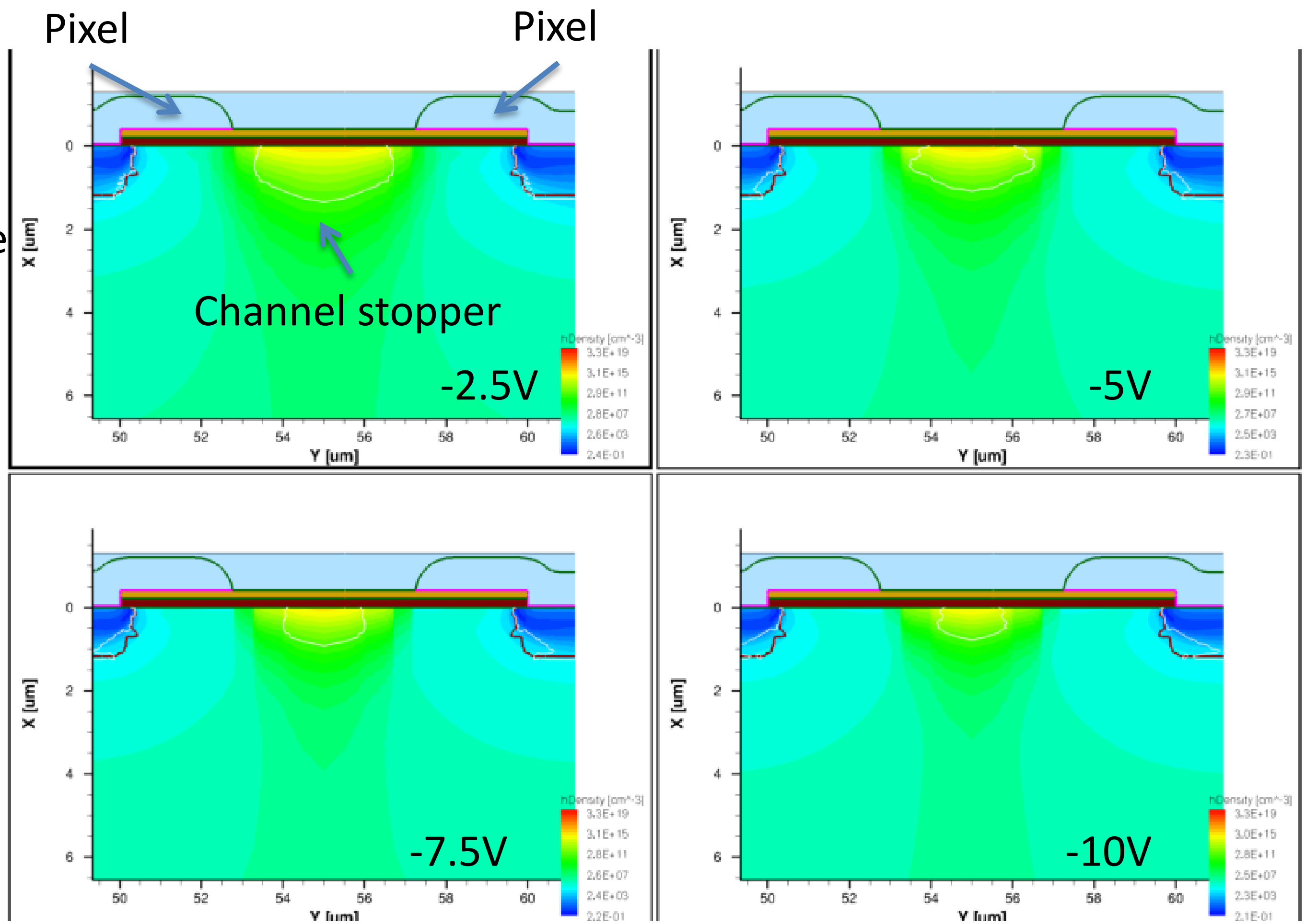
Simulation of charge multiplication and trap-assisted tunneling in irradiated planar pixel sensors
by: M. Benoit, A. Lounis, N. Dinu
In IEEE Nuclear Science Symposuim & Medical Imaging Conference (October 2010), pp. 612-616, doi:10.1109/NSSMIC.2010.5873832

Charge multiplication in silicon planar sensors

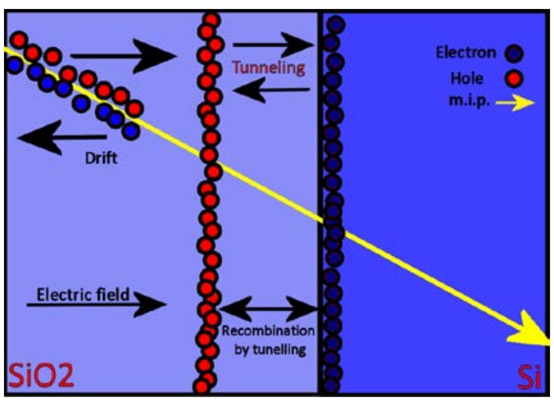


P-spray insulation

P-Spray (or p-stop, moderated p-spray) is an important parameter in the design of radiation hard sensors. TCAD can be used to optimize process parameters to maximize insulation while keeping breakdown high (E< 300kV/cm at Channel stopper junction).

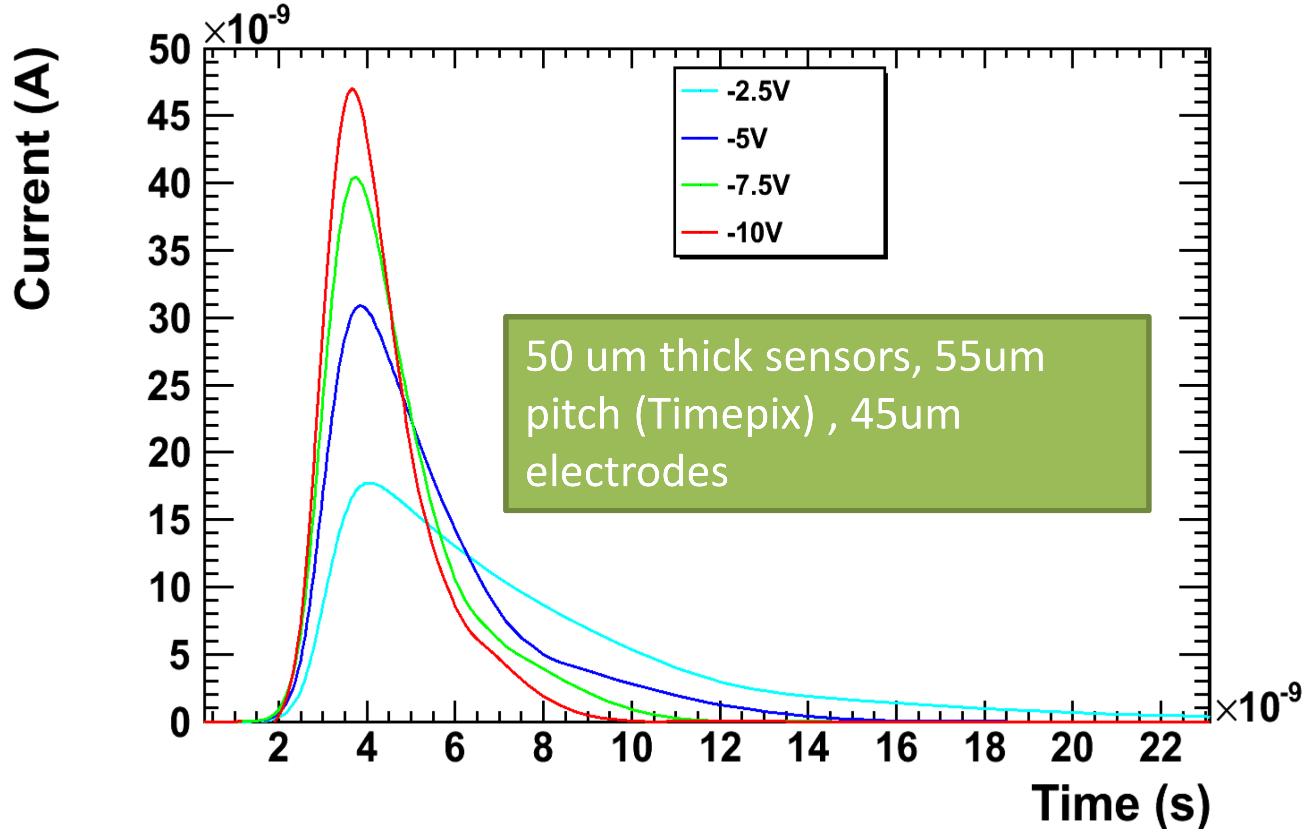


Channel stopper in n-in-p Timepix Pixel sensor for various biasing conditions (Hole Concentration represented)



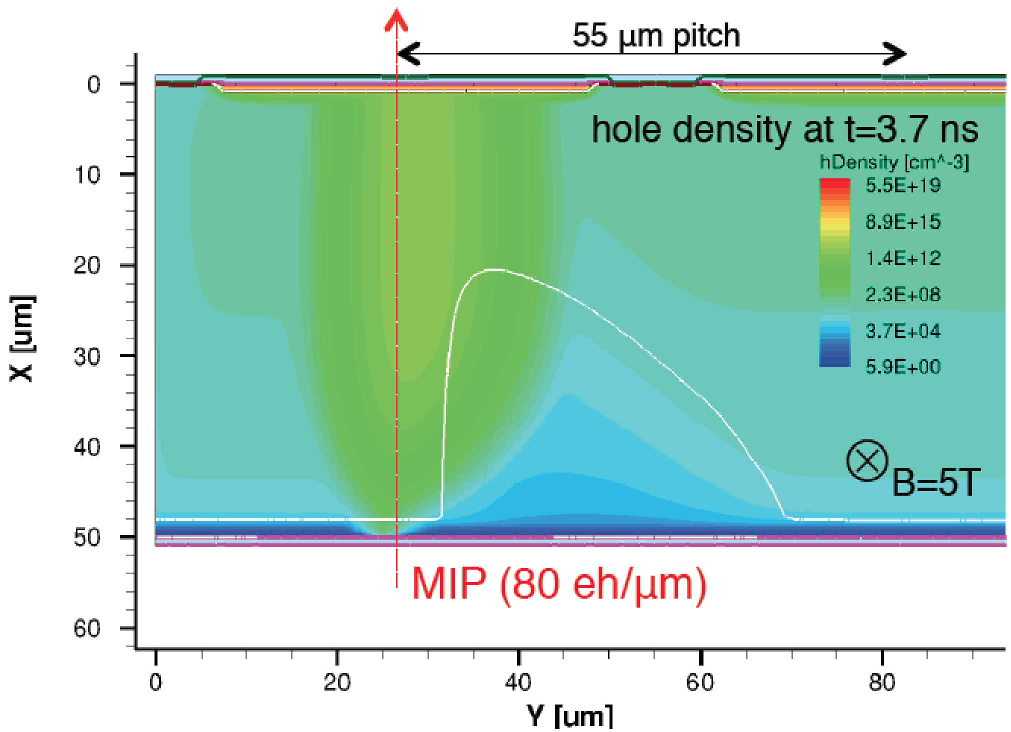
Pulse Shape and Rise time

Pulse shape and rise time can be of interest for chip designers We used Transient TCAD simulation for 50um thin sensors to investigate pulse shape and rise time in sensor foreseen for CLIC Vertex detectors

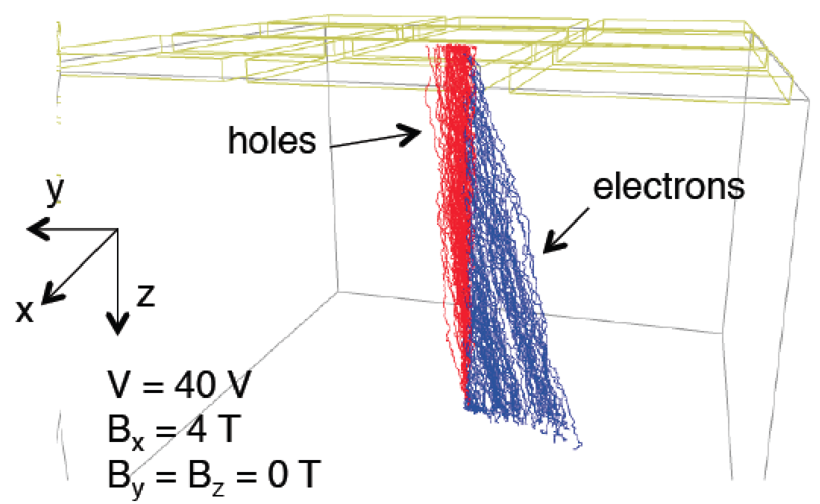


Magnetic Field Effects

spread of charge cloud in p-on-n sensor with B field:



Carrier drift in 50 µm thick fully depleted sensor:



In CLIC, combination of high Magnetic Field and thin sensors can lead to large Lorentz angle , TCAD was used to estimate the magnitude of these effects for various operation condition. Monte-Carlo Charge transport combined with Electric field obtained from TCAD was used to estimate clustersize and shapes

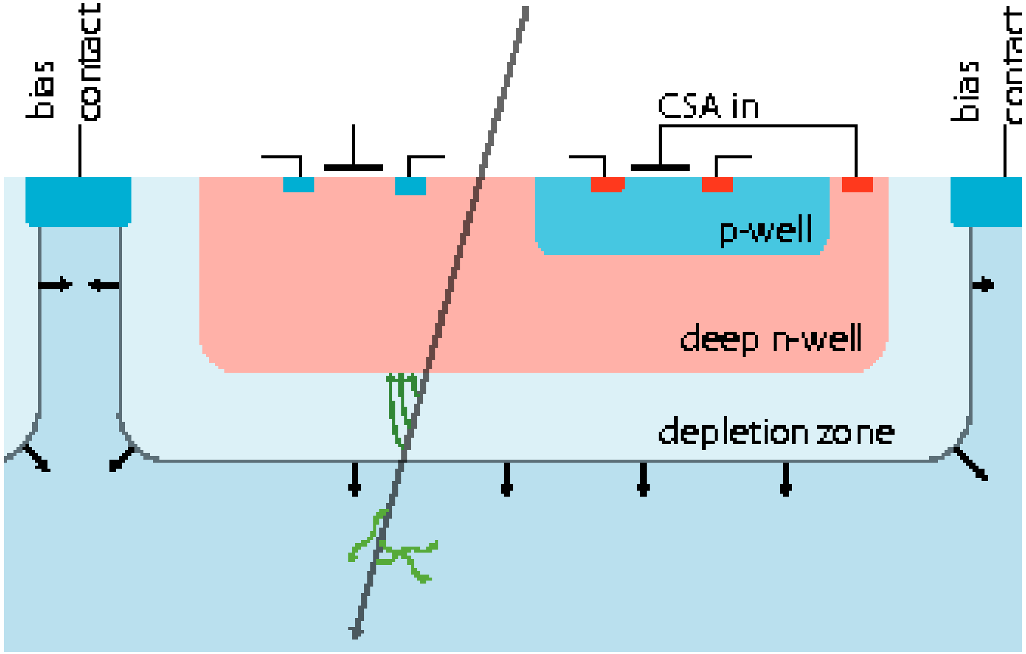
HV/HR-CMOS Pixel sensors

HV-CMOS process can be used for particle detection

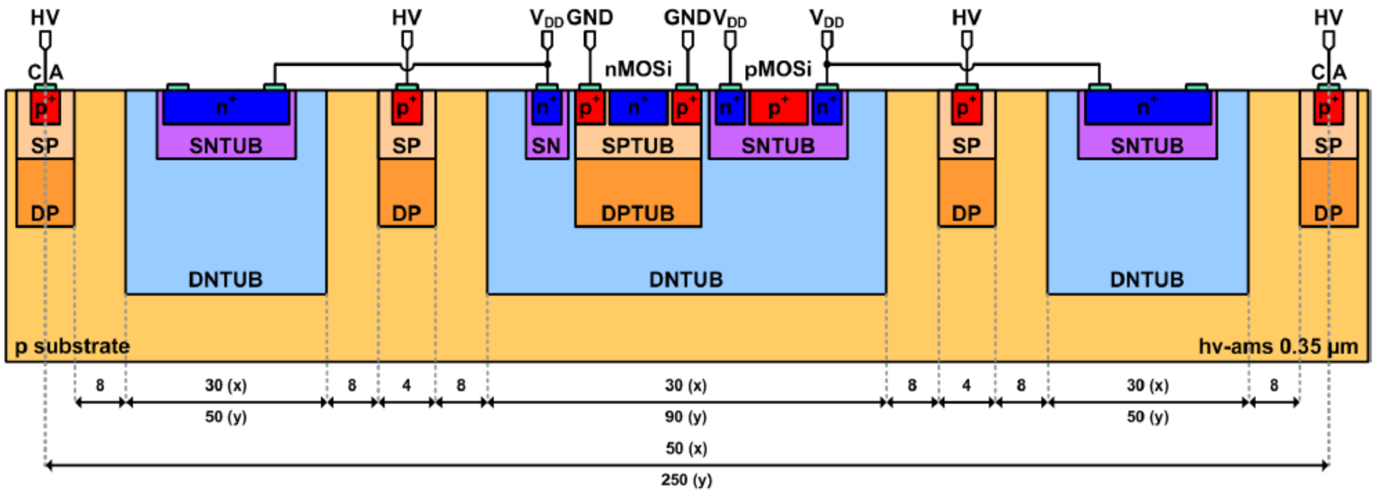
- Large-scale production capabilities
- Electronics can be integrated in the pixels
- Bias is usually applied from the top
- Typically low-resistivity substrate but high-resistivity is possible

This pose new challenge in terms of TCAD simulation

- More complex geometry
- Possibility to optimize important parameters such a capacitance and signal speed



HV/HR-CMOS Pixel sensors



Eva Vilella-Figueras, https://indico.cern.ch/event/361445

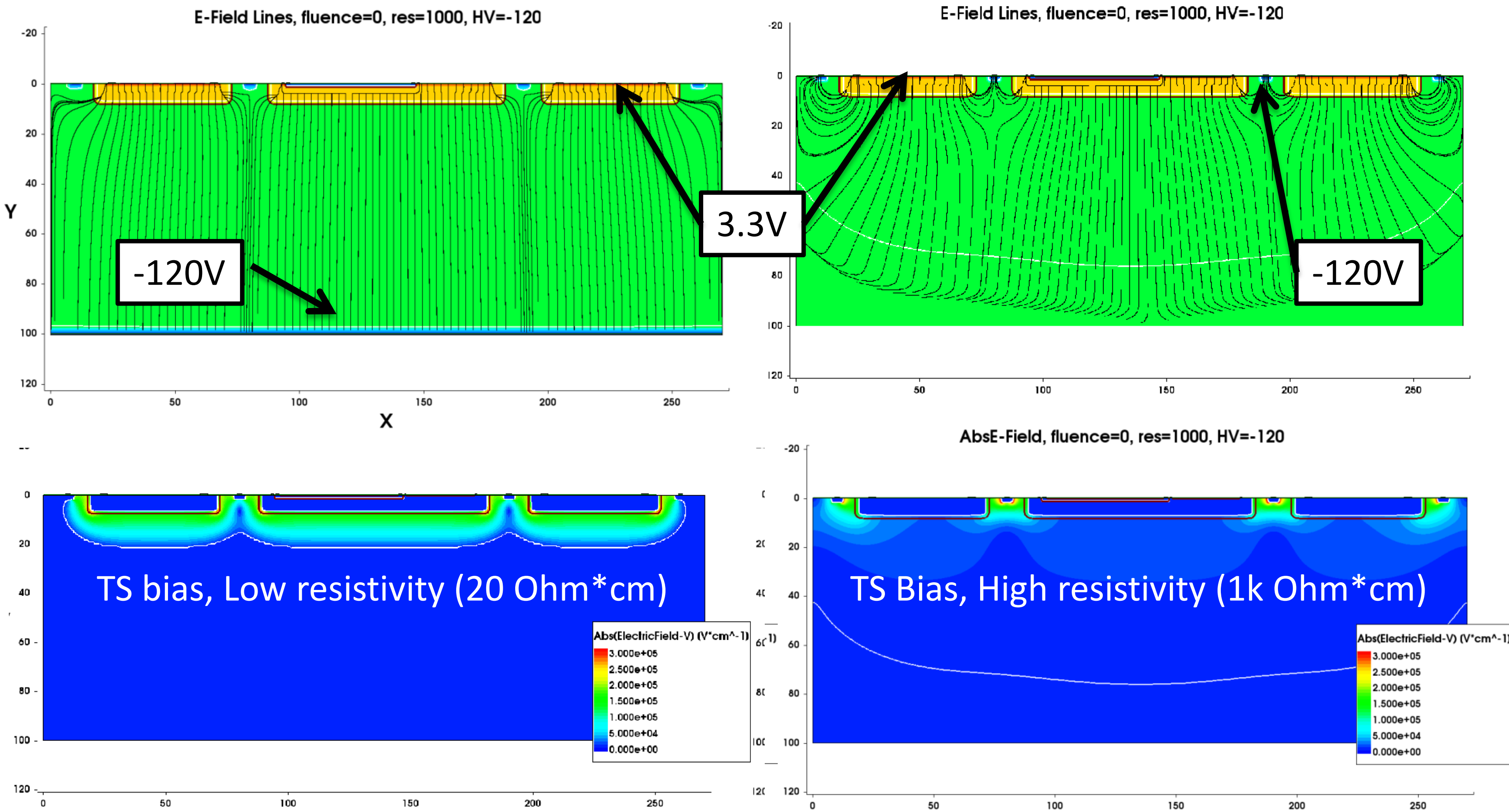
- VSS: 0.0 V
- VDD: 3.3 V
- HV: 0 – -200 V
- Resistivity: 20, 80, 200, 1000 Ωcm
- Top bias without back process
- Back bias with floating top contacts

Extra deep p-well

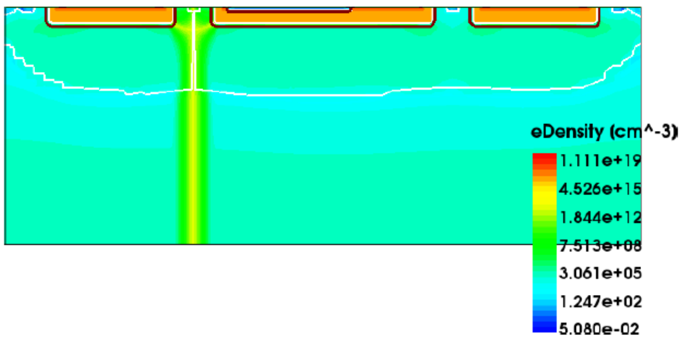
(M. Benoit in comm. with AMS)

- Inverting DNTUB mask
- Same doping concentration as DNTUB

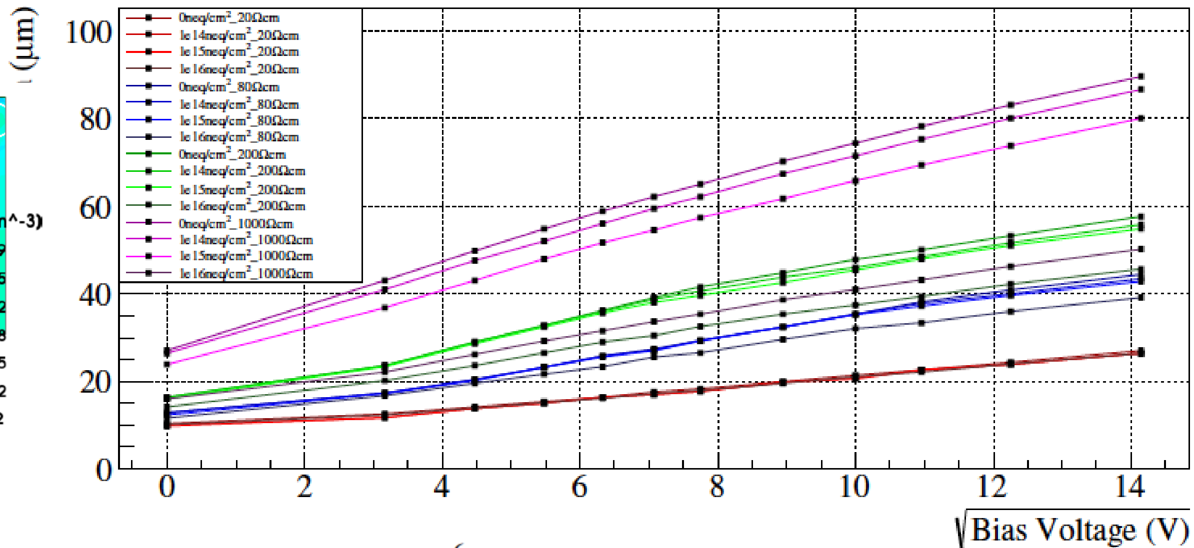
Back-side versus top biasing

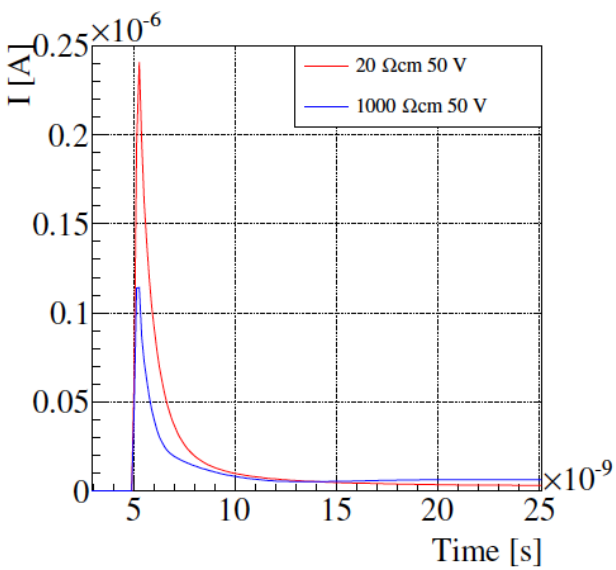


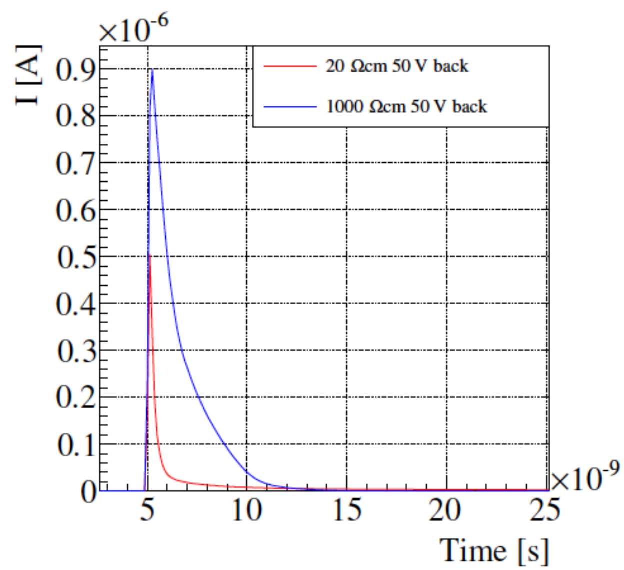
HV/HR-CMOS Pixel sensors



F. Di Bello



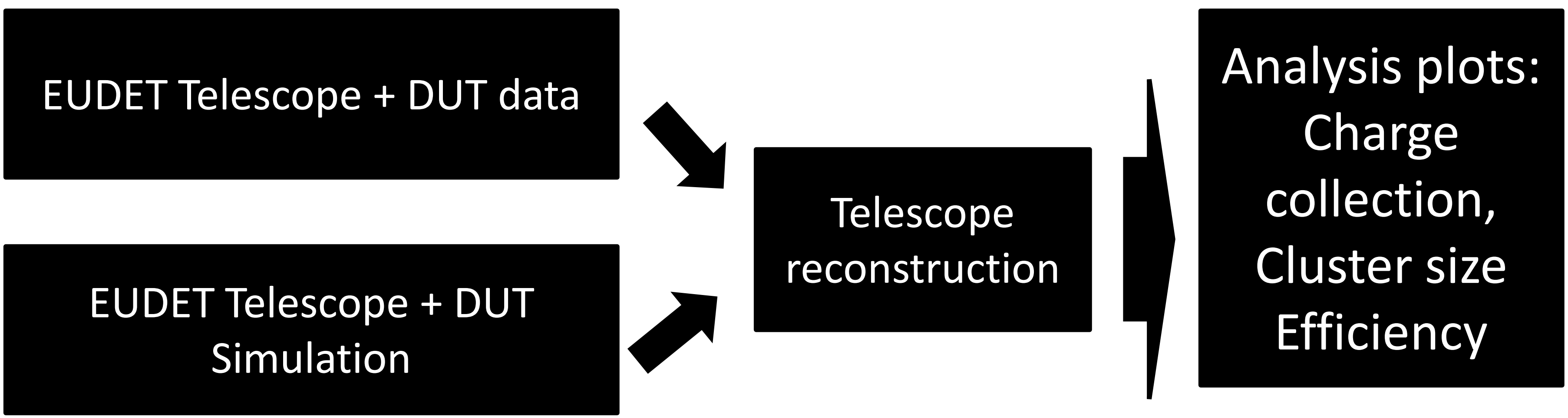




MC CHARGE TRANSPORT AND GEANT4 SIMULATION EXAMPLE

Simulation of detector behaviour : GEANT4 simulation and digitization calibration

- Using a detailed GEANT4 framework **reproducing a well know telescope setup (EUDET)**, we can **compare and tune the digitizer** to represent well prototype behaviour by comparing real data and simulation in the reconstruction and analysis framework of the telescope

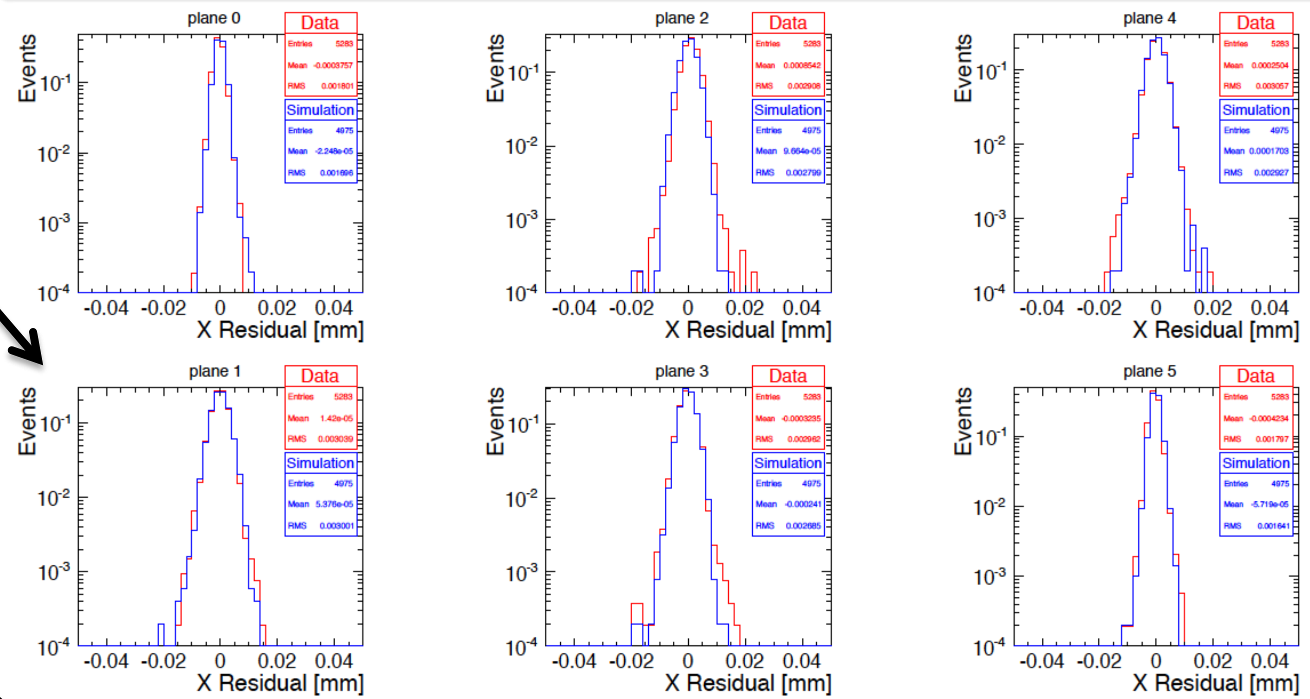


Simulation of detector behaviour : GEANT4 simulation and digitization calibration

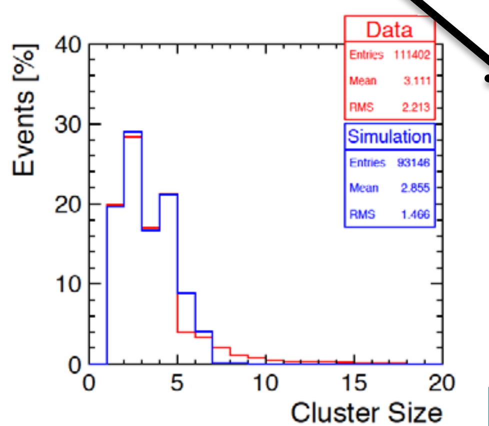
- The final goal of the simulation is **to produce a fast digitizer reproducing well the behaviour of prototypes,** usable in full detector simulation
- Use Test Beam telescope data to **compare real DUT and Simulated DUT** to validate the digitizer
- **Incorporate chip effects into the simulation** at this level
  - Counter accuracy
  - timing accuracy
  - Noise, jitter of the DAC
  - Threshold
  - Crosstalk
  - Non-linearity in the analog acquisition chain
  - Inefficiency in the Digital buffers etc
- Telescope (sim and data) are a good benchmark **for clustering algorithm**

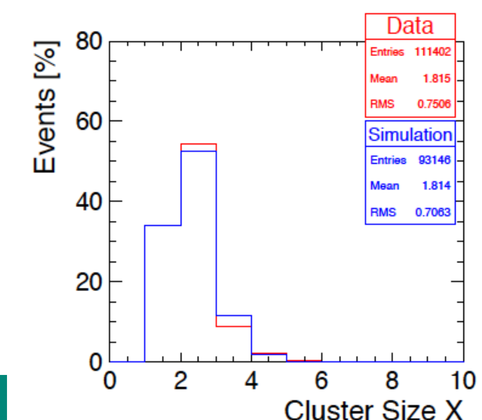
GEANT4 Simulation and digitization studies

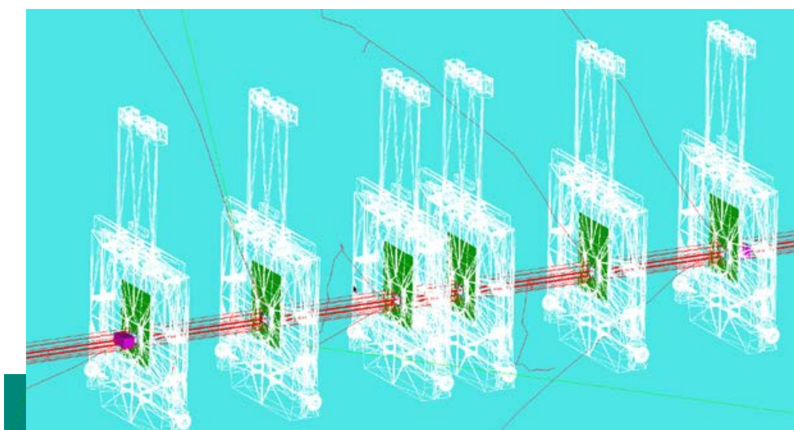
MIMOSA26 Telescope simulated and real residuals using AllPix digitization model



Cluster size distribution







Magnetic Field and Biasing conditions effects on charge transport in Thin depleted Silicon Detectors

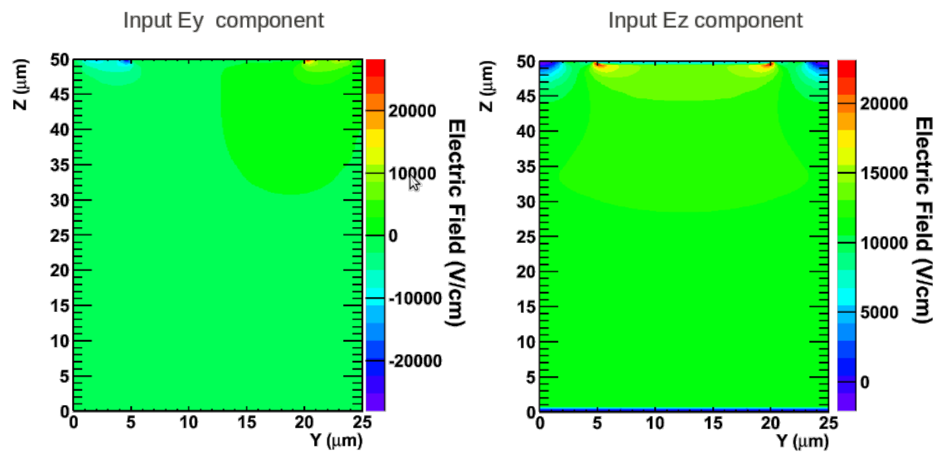
https://edms.cern.ch/document/1240445/

Thin sensors (~50 um) are depleted at very low voltage (1-10 V) leading to **larger Lorentz angle** in the drift of carriers

Signal Rise time in various condition must meet the vertex detector **timing requirements (~10ns)**

A set of simulation was performed to study these effects in pixel sensors

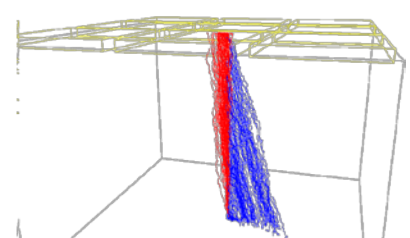
- **TCAD simulation of thin pixel sensors**. Slow approach but allow to solve the full system of equation, useful for tuning of simpler models
- **Monte-Carlo Charge Transport coupled to Static TCAD simulation**. Allow for larger statistics, can be coupled to GEANT4
- **Geant4 simulation and Digitization model**



$$J_n = q\mu_n n \mathrm{E}_{eff}(\mathrm{B}) + q\mathrm{D}_n \nabla n + \frac{q}{\tau_n}$$

$$J_p = q\mu_p p \mathrm{E}_{eff}(\mathrm{B}) + q\mathrm{D}_p \nabla p + \frac{q}{\tau_p}$$

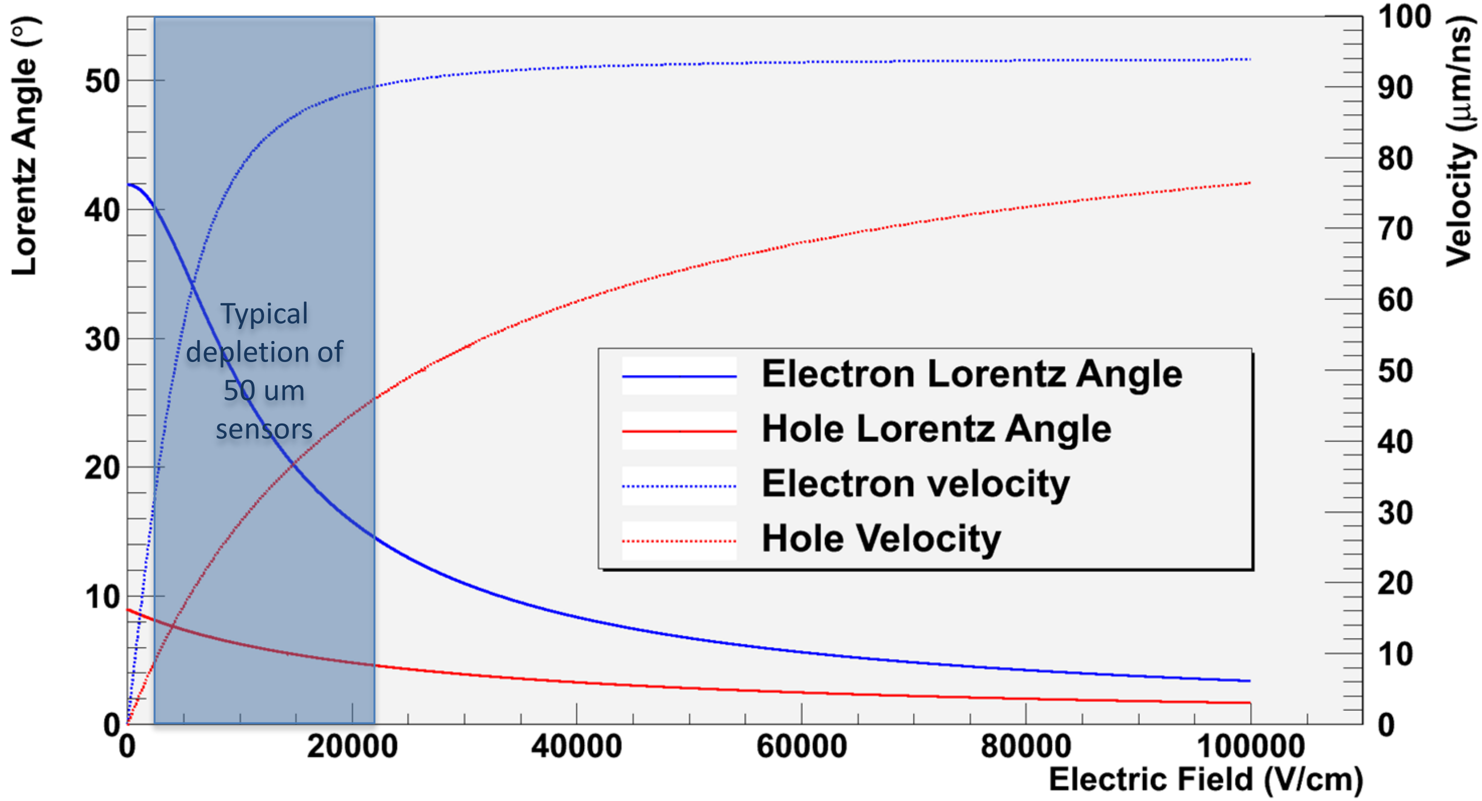
$$d = |E|\mu t$$
$$L = |E + E_B|\mu t$$
$$\tan(\theta_L) = \mu_{eff} B$$
$$\vec{E} \cdot \vec{E}_B = 0$$
$$\vec{E}_B \cdot \vec{B} = 0$$



Carrier drift in a 50 um thick fully depleted sensor

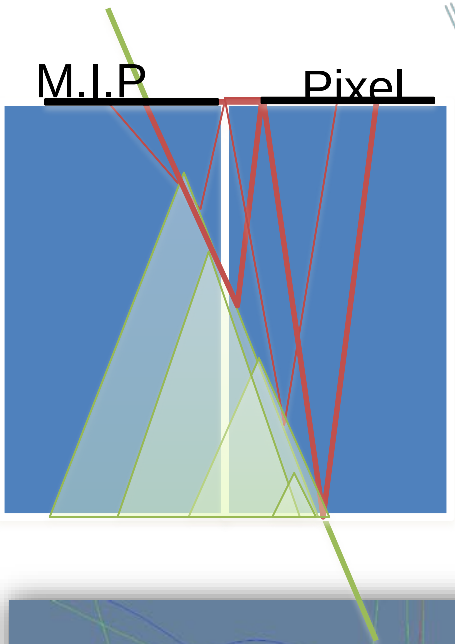
Magnetic Field and Biasing conditions effects on charge transport in Thin depleted Silicon Detectors

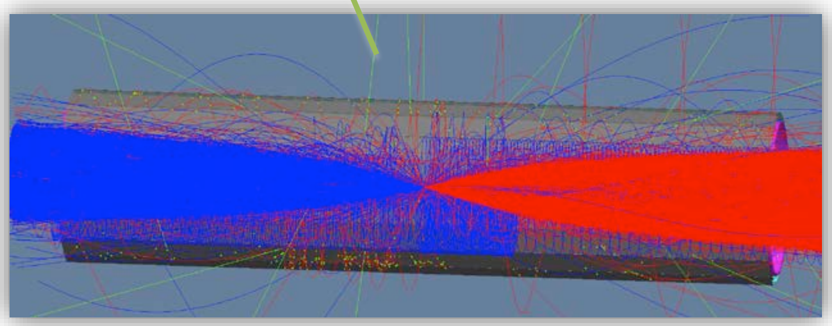
- Monte-Carlo Simulation, coupled with TCAD, lead to an estimation of the Lorentz angle in a typical Thin Silicon Sensor



Magnetic Field and Biasing conditions effects on charge transport in Thin depleted Silicon Detectors

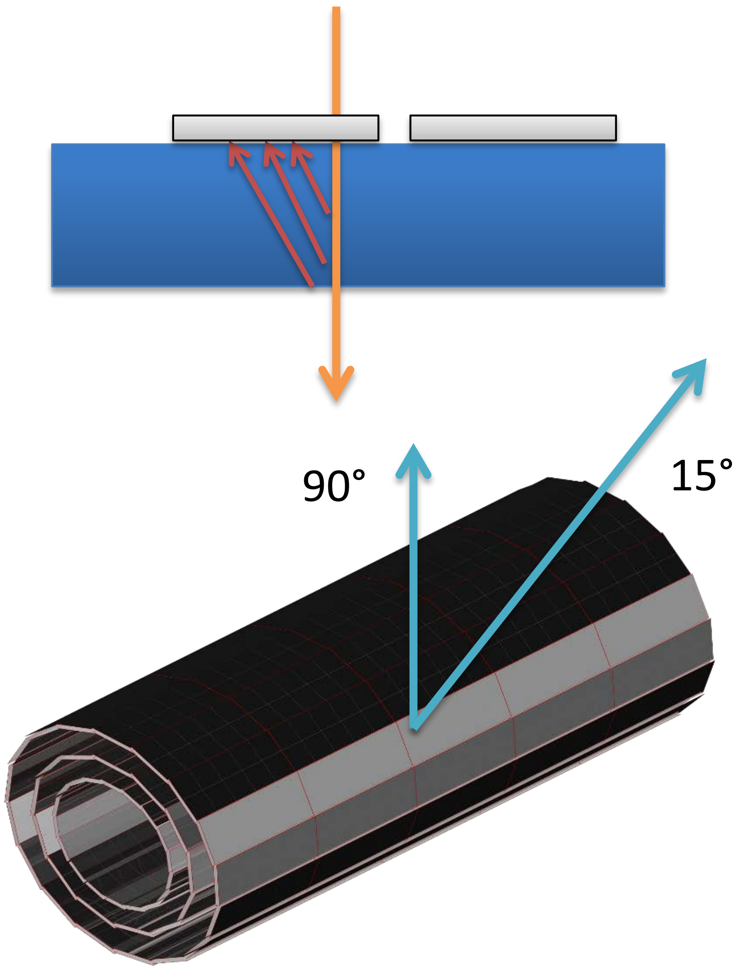
- Large Lorentz angle in the Vertex Sensors will lead to higher hit multiplicity
  - **Possibility to tilt sensor along the Z-Axis to enhance or reduce this effect**
- A Fast Balistic Digitization Model was developped to reproduce Lorentz angle effects in GEANT4 Simulation of the detector
- Drift, Diffusion and Lorentz for taken into account
- Calibrated to Monte-Carlo and TCAD Results
- Compared to TestBeam data with Timepix detectors
- This model was used to evaluate the modification to the Original layout in terms of occupancy and compare to original CDR numbers

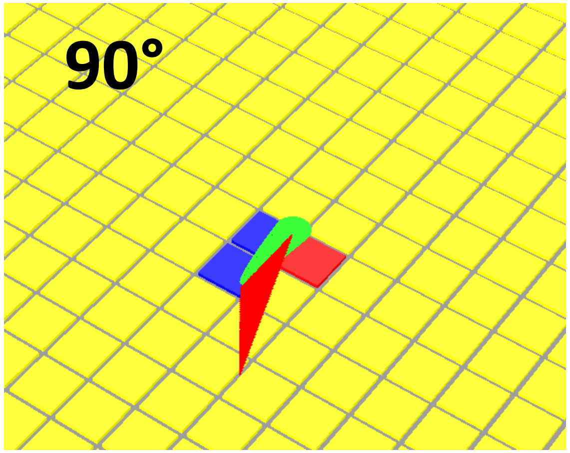


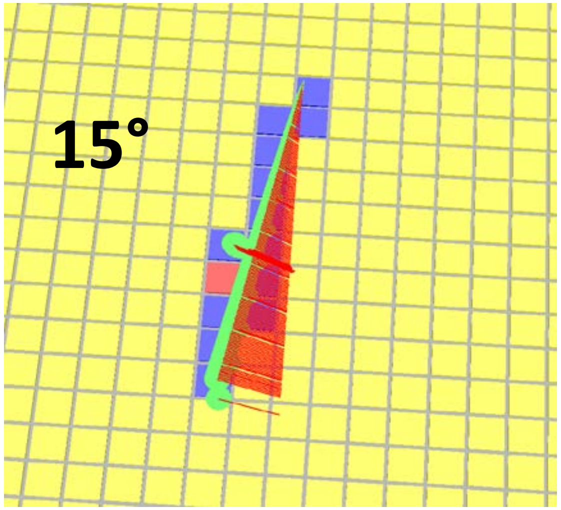


GEANT4 simulation Beam Background in CLIC vertex detector using our tuned digitizer

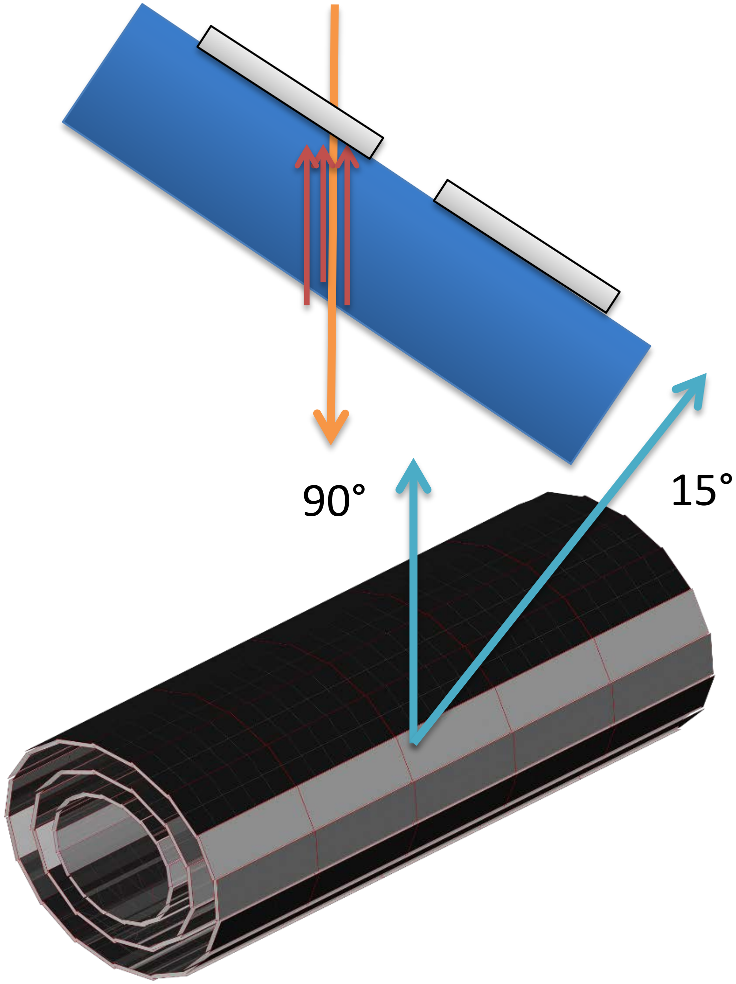
Lorentz angle effects (0 degrees incidence, B=4T)

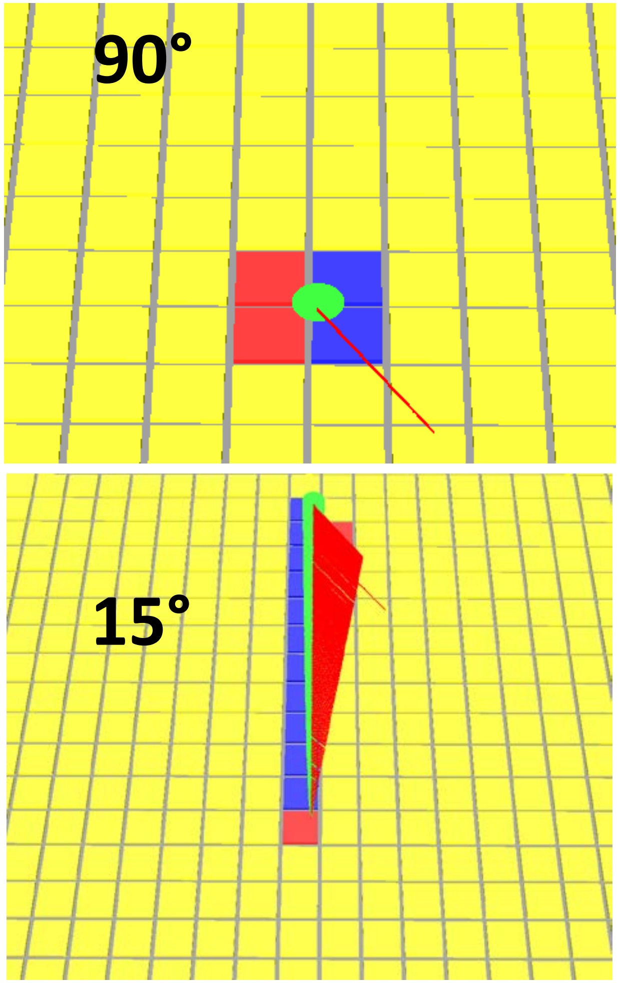




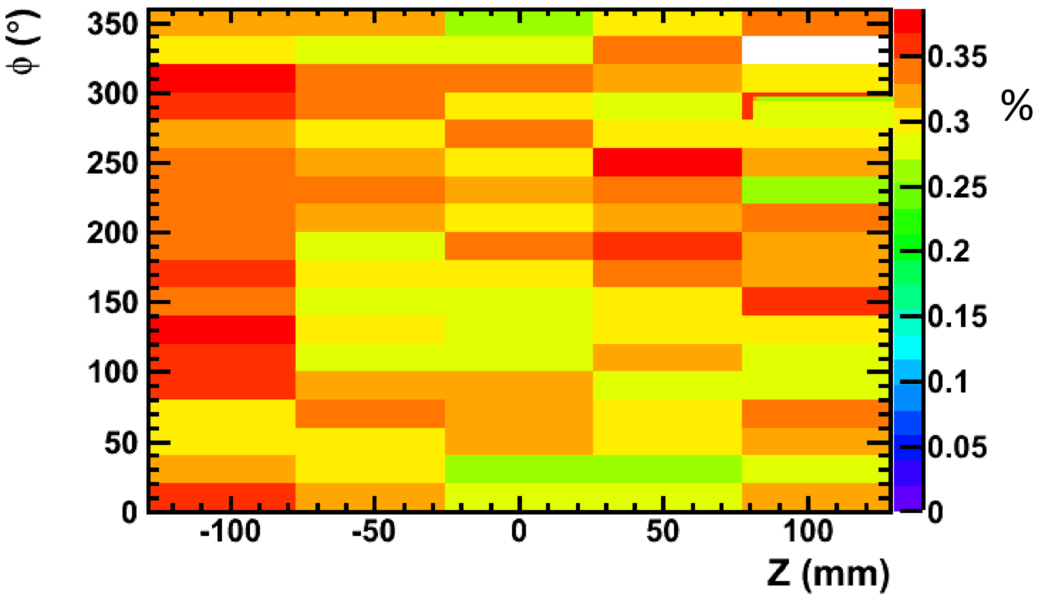


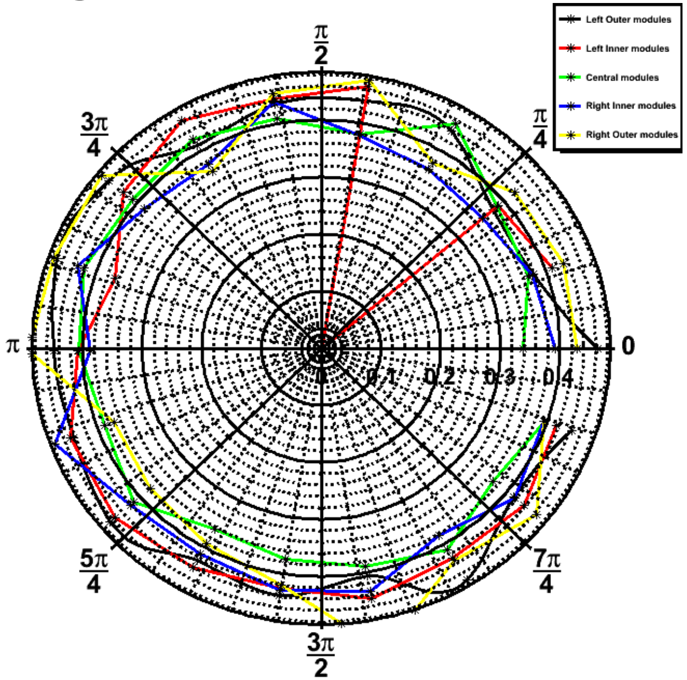
Lorentz angle effects (0 degrees incidence, B=4T)





Occupancy simulation using a realistic digitization model





Full Detector simulation using MC Charge transport can be computing intensive, but on a small scale, it can provide with validation for simpler models and provide more solid numbers for the design in terms of occupancy, buffers, data rate , etc …

M. Benoit, L.A. Hamel / Nuclear Instruments and Methods in Physics Research A 606 (2009) 508–516

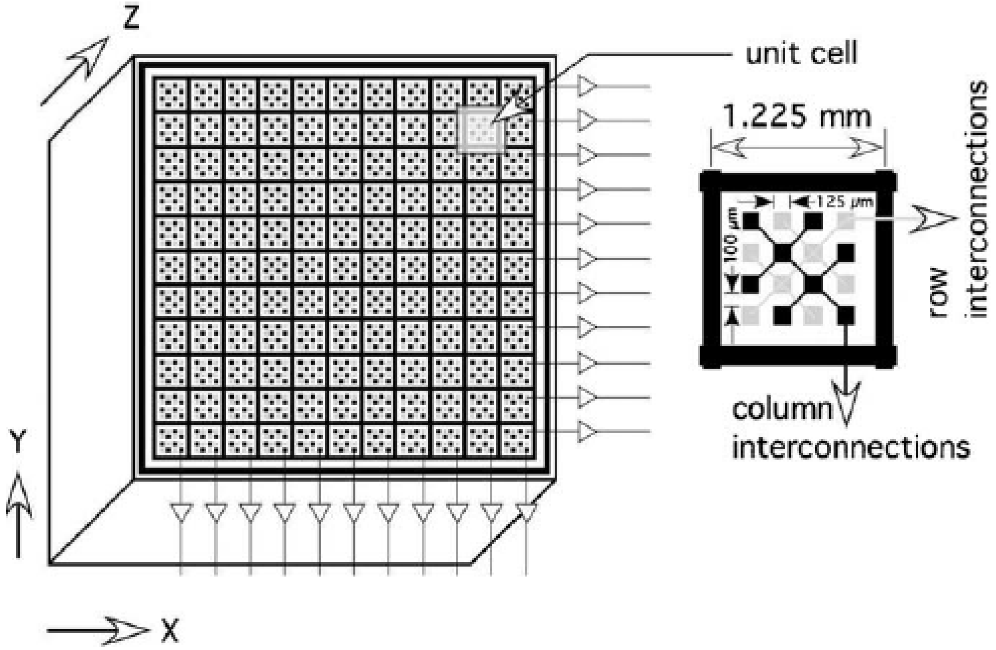
Charge Transport in CdZnTe Pixel sensors

CdZnTe is a heavy semiconductor used for high efficiency of gamma rays

They exhibit:

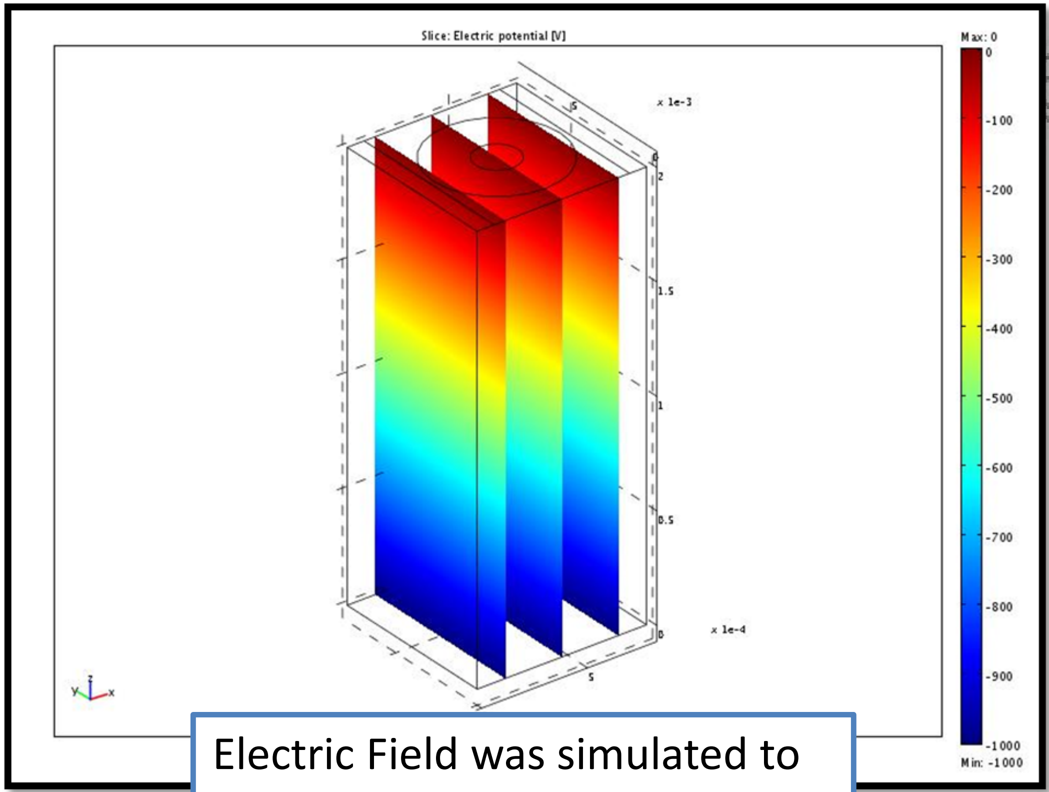
- high level of trapping
- Very slow hole signal
- Defect like Tellurium precipitate

Commonly used in space, medical and homeland security applications nowadays

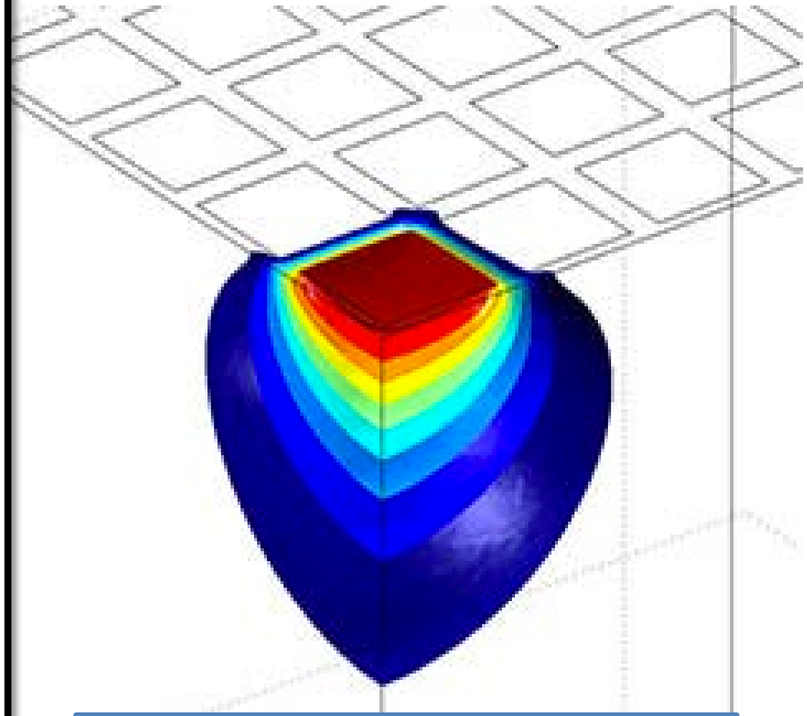


Single-Sided Cross-Strip detectors were investigated in CdZnTe as low-channel count method to obtain 2D information about the interaction. Charge sharing needed to be evaluated to calculate the necessary pixel size to allow enough signal in each channel

Charge Transport in CdZnTe Pixel sensors

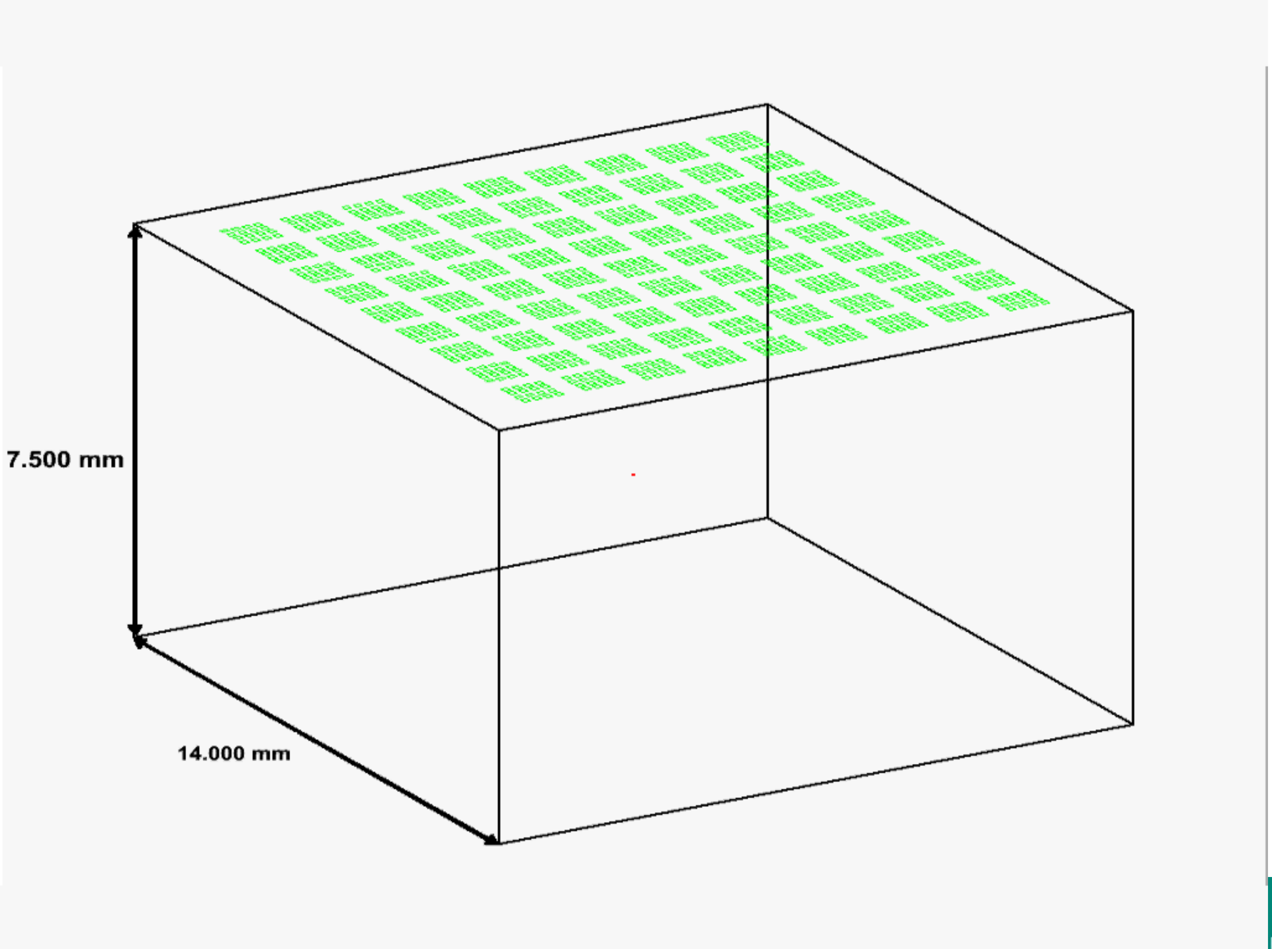


Electric Field was simulated to calculate charge carriers trajectory



Ramo Potential was calculated to evaluate charge induction

Charge Transport in CdZnTe Pixel sensors



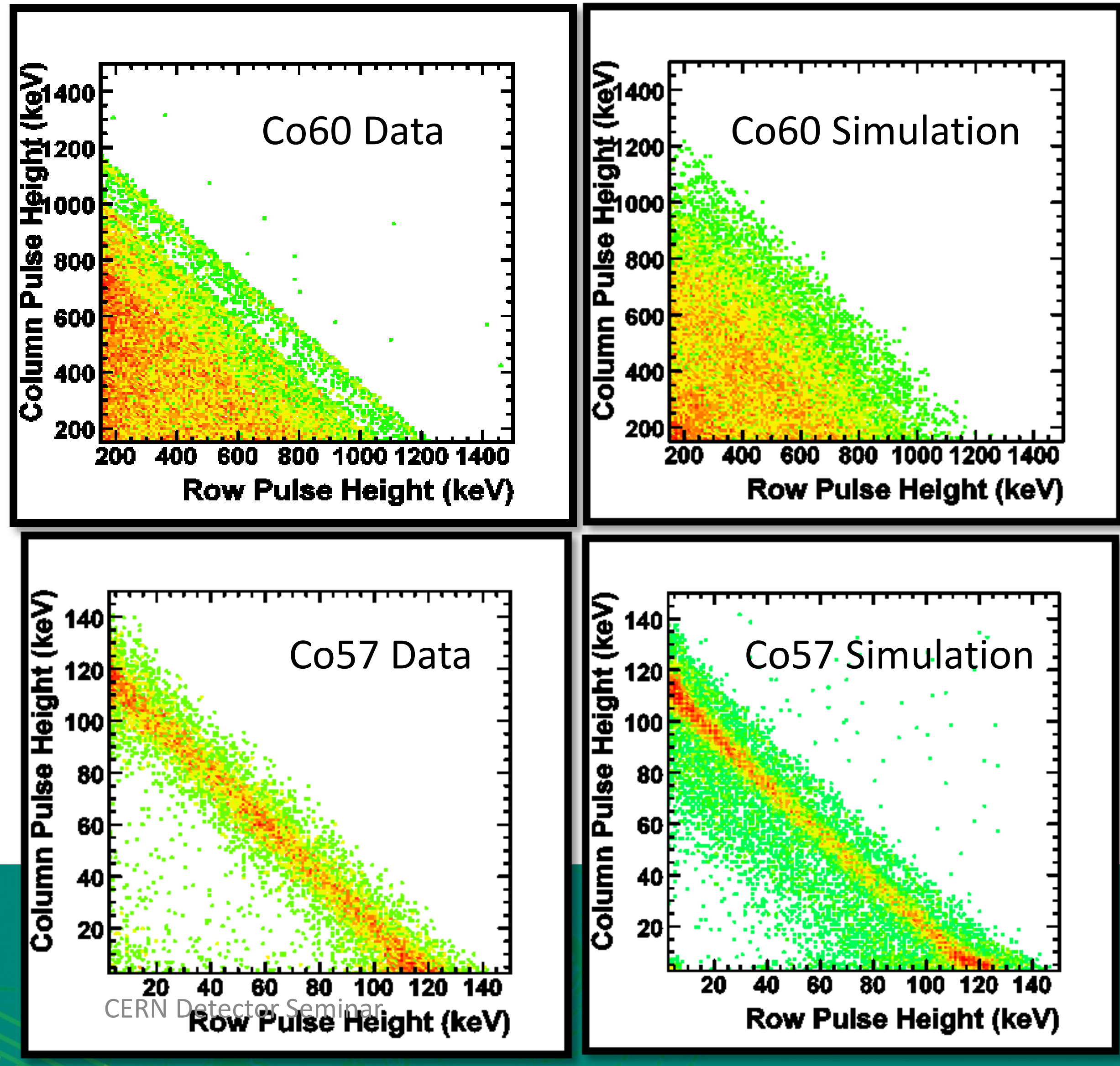
Charge Transport in CdZnTe Pixel sensors

After including all effects :

- Field and Ramo potential from TCAD
- Trapping and detrapping of electrons
- Diffusion
- Electrostatic repulsion

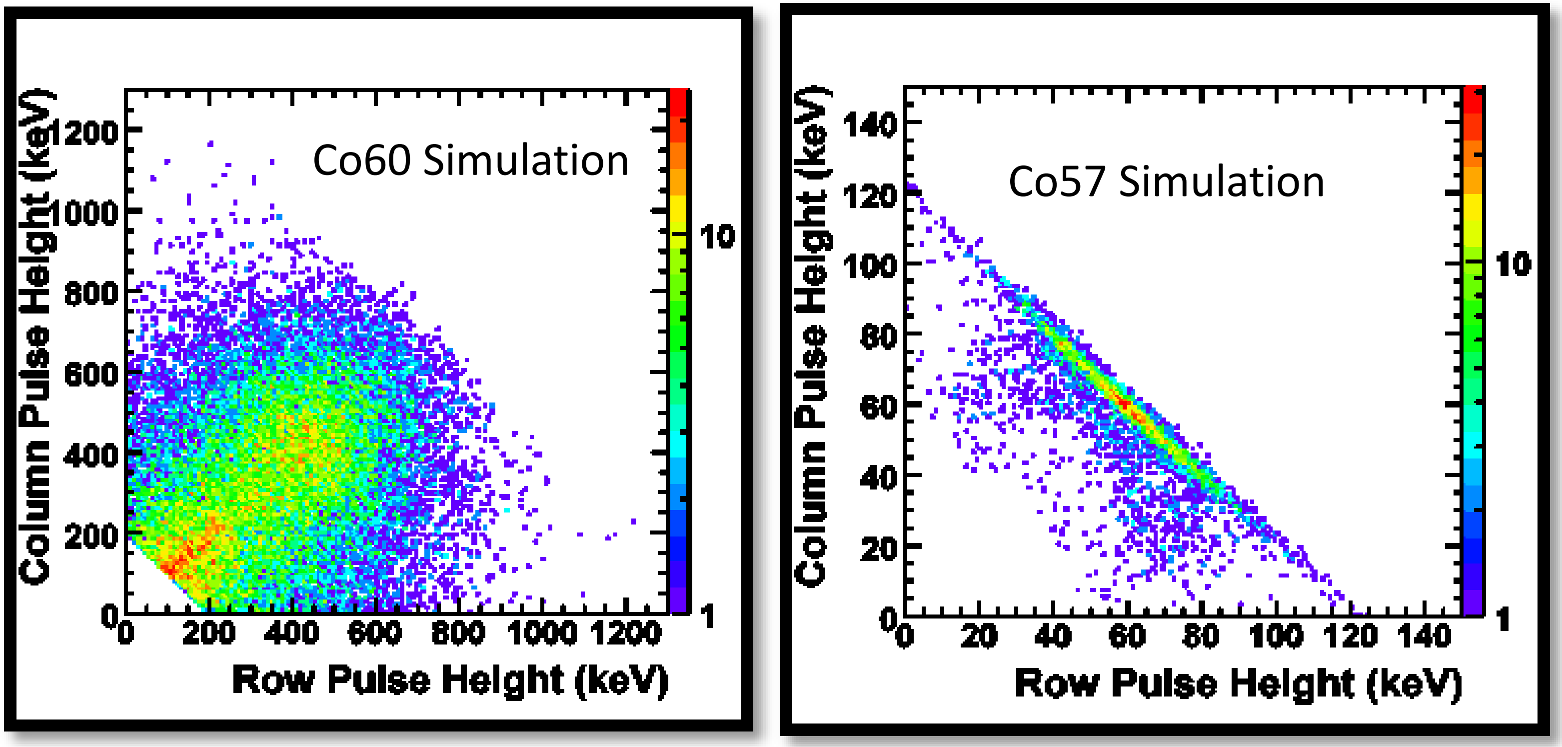
We obtain a good agreement between data and simulation. It is clear in this case (225um pixels) , that charge sharing is insufficient to get good detection efficiency in both channel

X Energy VS Y Energy (keV)



Charge Transport in CdZnTe Pixel sensors

X Energy VS Y Energy (keV)



Having gained confidence in our model, we can make prediction on the optimal pixel pitch to use (biggest possible size giving sufficient charge sharing). Here represented, 150um pixels

Available software and documentation

- GDSII Generator
  - https://github.com/mathieubenoit/GDSII_Generator
- Example code for MC Charge transport
  - https://github.com/mathieubenoit/clicmctsi
- Charge Transport in CdZnTe
  - M. Benoit, L.A. Hamel / Nuclear Instruments and Methods in Physics Research A 606 (2009) 508–516
- Note on B Field Iterator equation
  - https://edms.cern.ch/document/1240445/
- AllPix
  - https://twiki.cern.ch/twiki/bin/view/Main/AllPix
  - https://github.com/ALLPix/allpix
- AllPix to EUTELescope converter
  - https://github.com/mathieubenoit/FEI4Telescope2SLCIO

Conclusion

I Hope to have demonstrated that TCAD and Monte-Carlo Simulation of detectors can be useful tools that can affect real life detectors

However not everything is perfect and improvement are needed to become more quantitative

- 3D Modeling is very computing intensive
- Radiation damage model need to be validated on a large range of substrate and devices
- MC Models must integrate these improvement on the radiation damage modeling

TCAD Simulation Suite Synopsys Sentaurus available in limited quantities at CERN. User base is booming 5- <25 in the last two years ! We need more licences !

Many MC Charge transport model are available, mostly home code, no complete commercial product, but have a look to find one that fits your need, or write your own !

This is why experimental scientists hate theoretical scientists.

Credits : SMBC

Thank you for your attention !

Credits

- AMS TCAD Enthusiast for TCAD Material on HVCMOS
  - Lingxin Meng, Matthew Buckland, Mahmoud Tavassoli, Vagelis Gkougkousis
- TCAD of ATLAS IBL Sensors
  - Nicoleta Dinu and Abdenour Lounis
- Original idea for Allpix
  - John Iddaraga
- CdZnTe Simulation
  - Louis-André Hamel
- Timepix and Telescope simulation
  - PH-LCD group @ CERN and Timepix Collaboration

Publications

[1] M. Benoit, A. Lounis, and N. Dinu, "Simulation of charge multiplication and trap-assisted tunneling in irradiated planar pixel sensors," in IEEE Nuclear Science Symposuim & Medical Imaging Conference. IEEE, Oct. 2010, pp. 612–616. [Online]. Available: http://dx.doi.org/10.1109/NSSMIC.2010.5873832

[2] J. Weingarten, S. Altenheiner, M. Beimforde, M. Benoit, M. Bomben, G. Calderini, C. Gallrapp, M. George, S. Gibson, S. Grinstein, Z. Janoska, J. Jentzsch, O. Jinnouchi, T. Kishida, A. La Rosa, V. Libov, A. Macchiolo, G. Marchiori, D. Münstermann, R. Nagai, G. Piacquadio, B. Ristic, I. Rubinskiy, A. Rummler, Y. Takubo, G. Troska, S. Tsiskaridtze, I. Tsurin, Y. Unno, P. Weigel, and T. Wittig, "Planar pixel sensors for the ATLAS upgrade: Beam tests results," Apr. 2012. [Online]. Available: http://arxiv.org/abs/1204.1266

[3] M. Benoit, J. Märk, P. Weiss, D. Benoit, J. C. Clemens, D. Fougeron, B. Janvier, M. Jevaud, S. Karkar, M. Menouni, F. Pain, L. Pinot, C. Morel, and P. Laniece, "New concept of a submillimetric pixellated silicon detector for intracerebral application," Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, Aug. 2011. [Online]. Available: http://dx.doi.org/10.1016/j.nima.2011.08.027

[4] G. Calderini, M. Benoit, N. Dinu, A. Lounis, and G. Marchiori, "Simulations of planar pixel sensors for the ATLAS high luminosity upgrade," Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, Apr. 2010. [Online]. Available: http://dx.doi.org/10.1016/j.nima.2010.04.082

[5] M. Benoit, A. Lounis, and N. Dinu, "Simulation of charge multiplication and trap-assisted tunneling in irradiated planar pixel sensors," CERN, Geneva, Tech. Rep. ATL-UPGRADE-INT-2010-002, Oct. 2010.

[6] ——, "Simulation of radiation damage effects on planar pixel guard ring structure for ATLAS inner detector upgrade," Nuclear Science, IEEE Transactions on, vol. 56, no. 6, pp. 3236–3243, Dec. 2009. [Online]. Available: http://dx.doi.org/10.1109/TNS.2009.2034002

[7] L. A. Hamel, M. Benoit, B. Donmez, J. R. Macri, M. L. McConnell, T. Narita, and J. M. Ryan, "Optimization of Single-Sided Charge-Sharing strip detectors," in Nuclear Science Symposium Conference Record, 2006. IEEE, vol. 6, Nov. 2006, pp. 3759–3761. [Online]. Available: http://dx.doi.org/10.1109/NSSMIC.2006.353811

[8] A. Lounis, D. Martinot, G. Calderini, G. Marchiori, M. Benoit, and N. Dinu, "TCAD simulations of ATLAS pixel guard ring and edge structure for SLHC upgrade," CERN, Geneva, Tech. Rep. ATL-COM-UPGRADE-2009-013, Oct. 2009.

[9] M. Benoit and L. A. Hamel, "Simulation of charge collection processes in semiconductor CdZnTe -ray detectors," Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, vol. 606, no. 3, pp. 508–516, Jul. 2009. [Online]. Available: http://dx.doi.org/10.1016/j.nima.2009.04.019

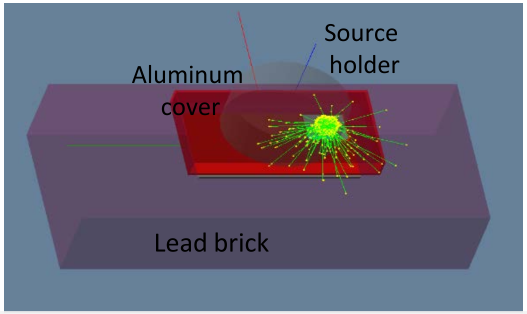
[10] M. Benoit, A. Lounis, and N. Dinu, "Simulation of guard ring influence on the performance of ATLAS pixel detectors for inner layer replacement," J. Inst., vol. 4, no. 03, 2009. [Online]. Available: http://www.iop.org/EJ/abstract/-search=66292014.1/1748-0221/4/03/P03025

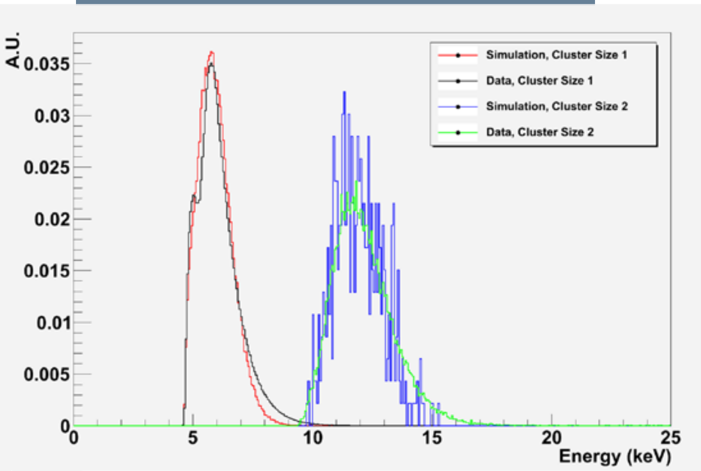
Thesis (in english) :Étude des détecteurs planaires pixels durcis aux radiations pour la mise à jour du détecteur de vertex d'ATLAS

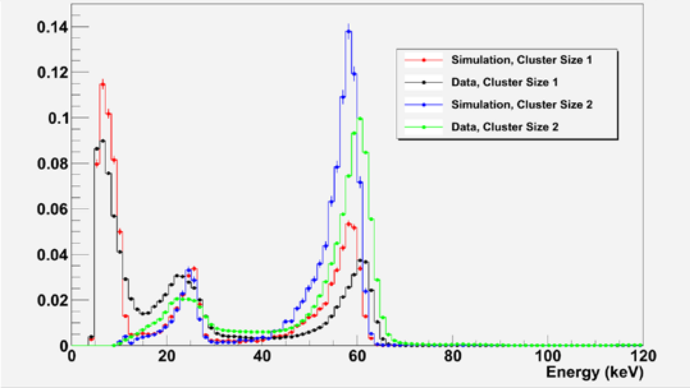
Backup

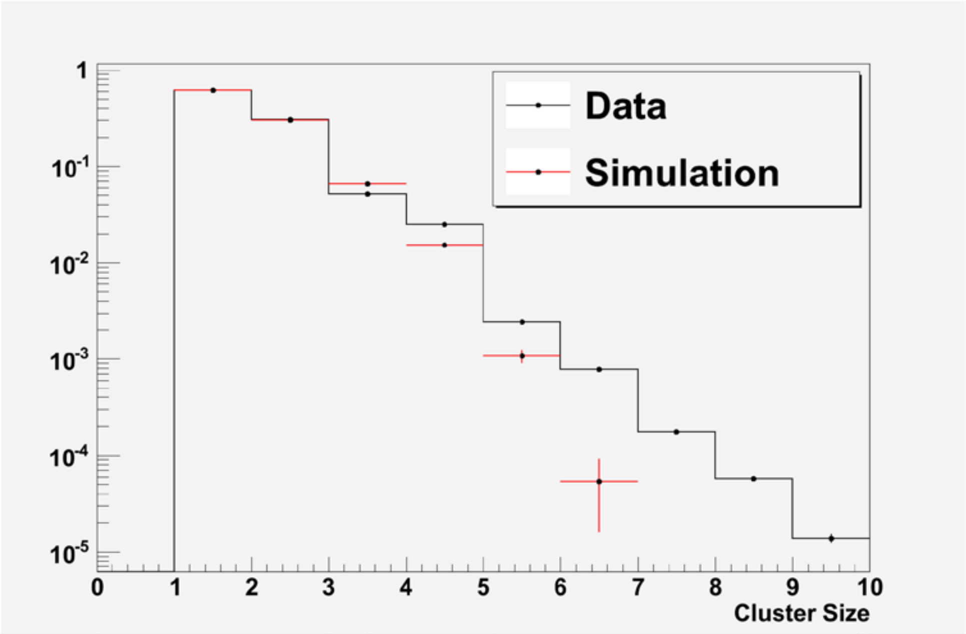
Timepix calibration and digitization tuning

- Experimental data were compared to a GEANT4 simulation of the setup
  - To calibrate the simulation using the ballistic model we need to include Chip effect on the measurement (noise , crosstalk)
  - We calibrate by trying to reproduce Cluster Size distribution and Energy resolution of the timepix sensor



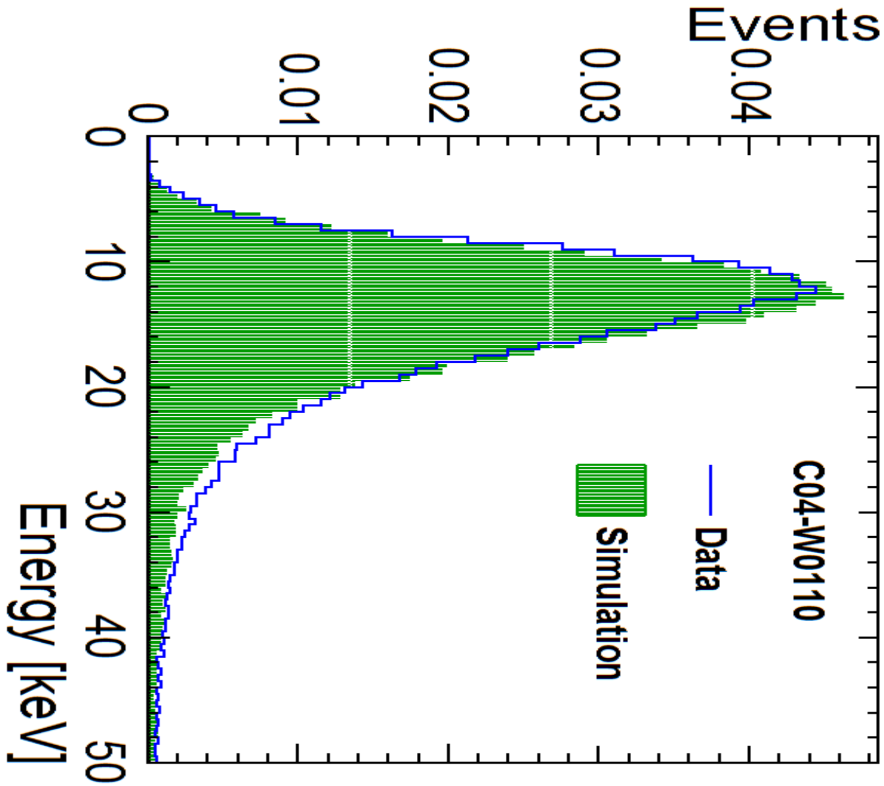






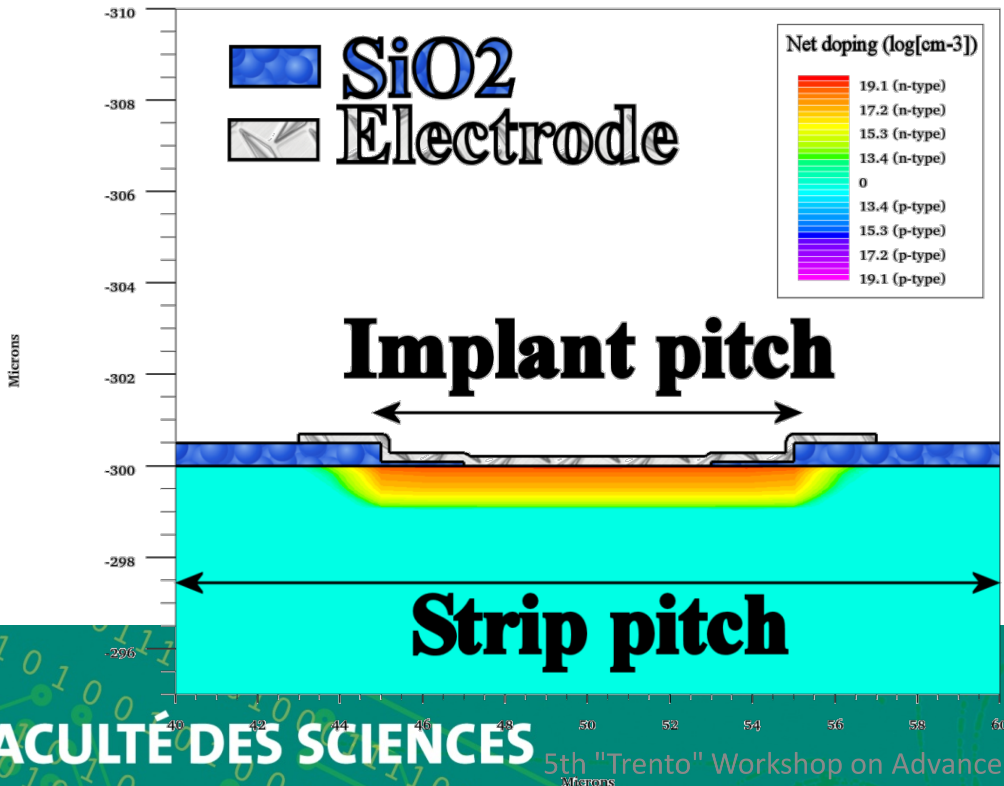
Simulation validation

- Validation of energy deposition in thin silicon sensor: 50 um planar sensor
  - Data:
    - Timepix readout chip: calibrated with radioactive/X-ray sources. Pixel-by-pixel calibration used to compensate for the differences across the whole matrix.
    - All clusters considered
  - Geant4 PAI (Photo absorption ionization) model describes well the MPV and width of the energy loss distribution and 2keV gaussian noise.
  - Perfect agreement between data and Geant4.



2D simulation : Strips with various doping profile and geometry

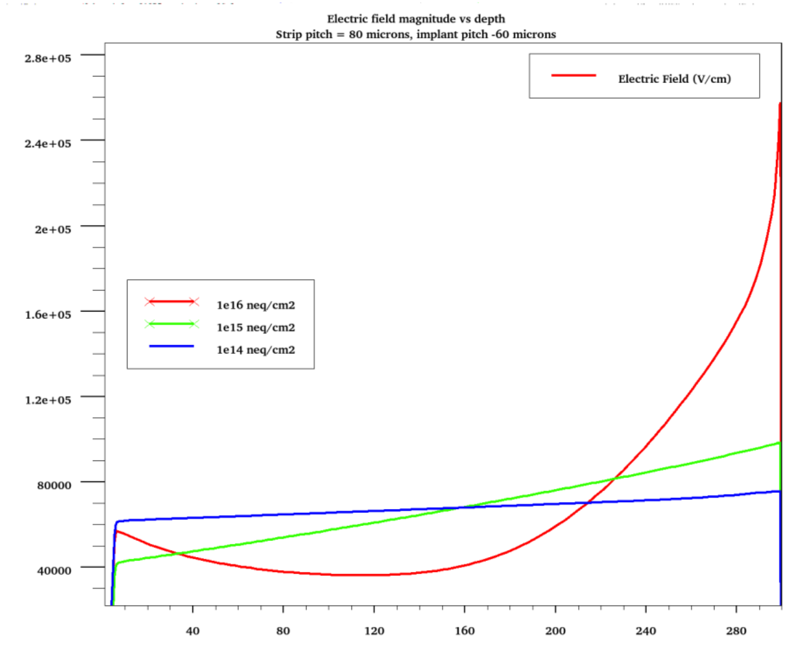
- A set of n-in-p strip sensor with different strip and implant pitch , and with different intermediate strip pitch was studied

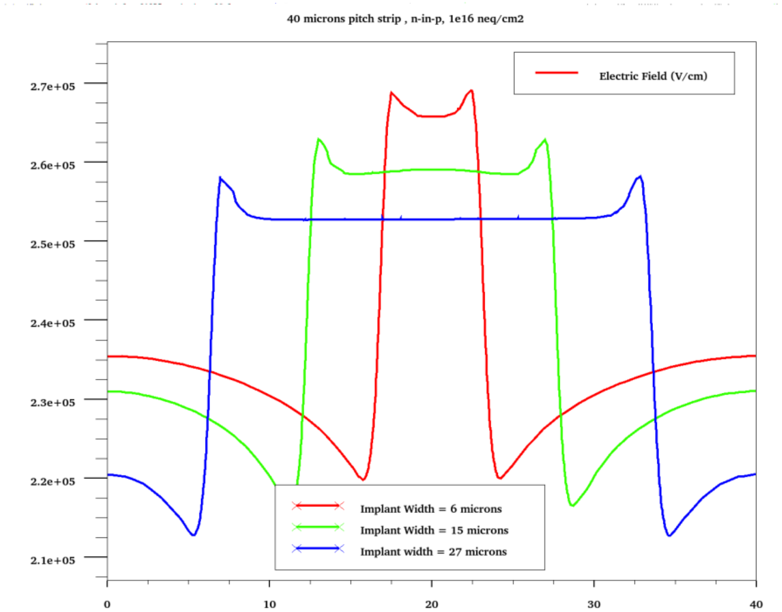


Strip pitch (μm)	Implant width (μm)
80	60
80	25
80	6
100	70
100	33
100	10
40	27
40	15
40	6

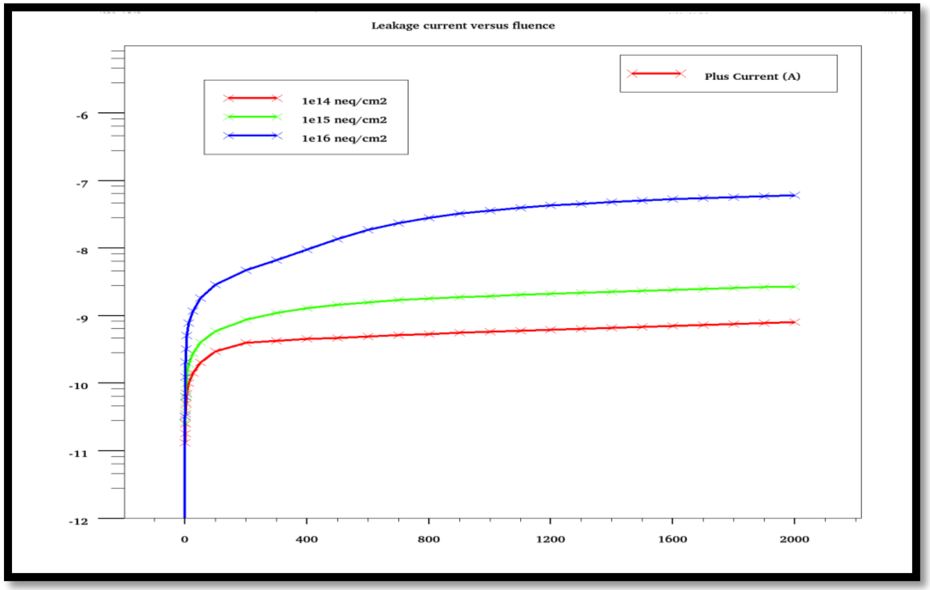
2D simulation : Strips with various doping profile an

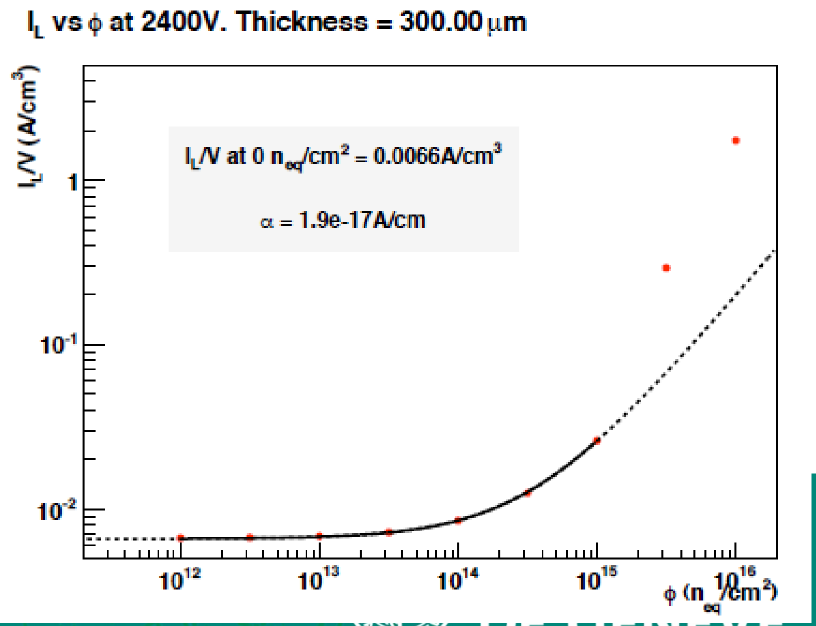
- Each sensor was biased at 2000V, and simulated for a fluence of $10^{14,15,16}$ n_{eq}/cm^2
- Moderate p-spray insulation between strips
- Classical implantation for n strip implant
- Drive-in 100 min @ 900C





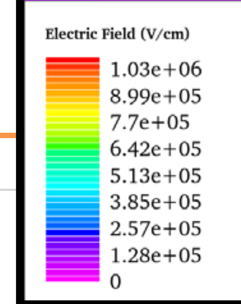
2D simulation : Leakage current

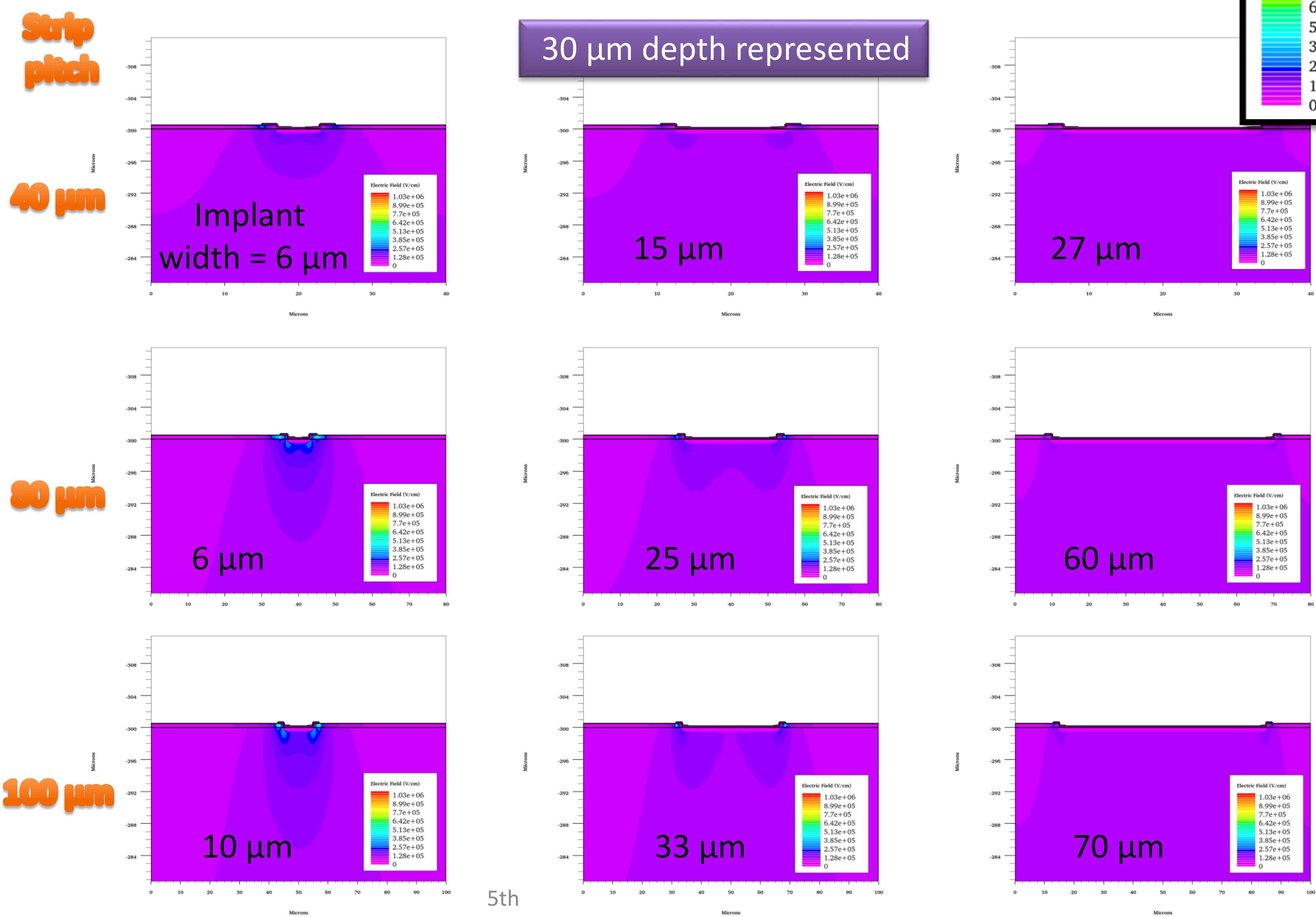




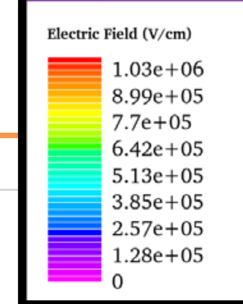
- Leakage from different strip pitch not influenced by the pitch
- Hard breakdown of the junction at the strip extremity lower for small implant pitch/ strip pitch ratio
- α =1.9e-17A/cm
- Contribution from Trap-to-band tunelling and impact ionization visible in leakage current about 1e15 n_{eq}/cm^2

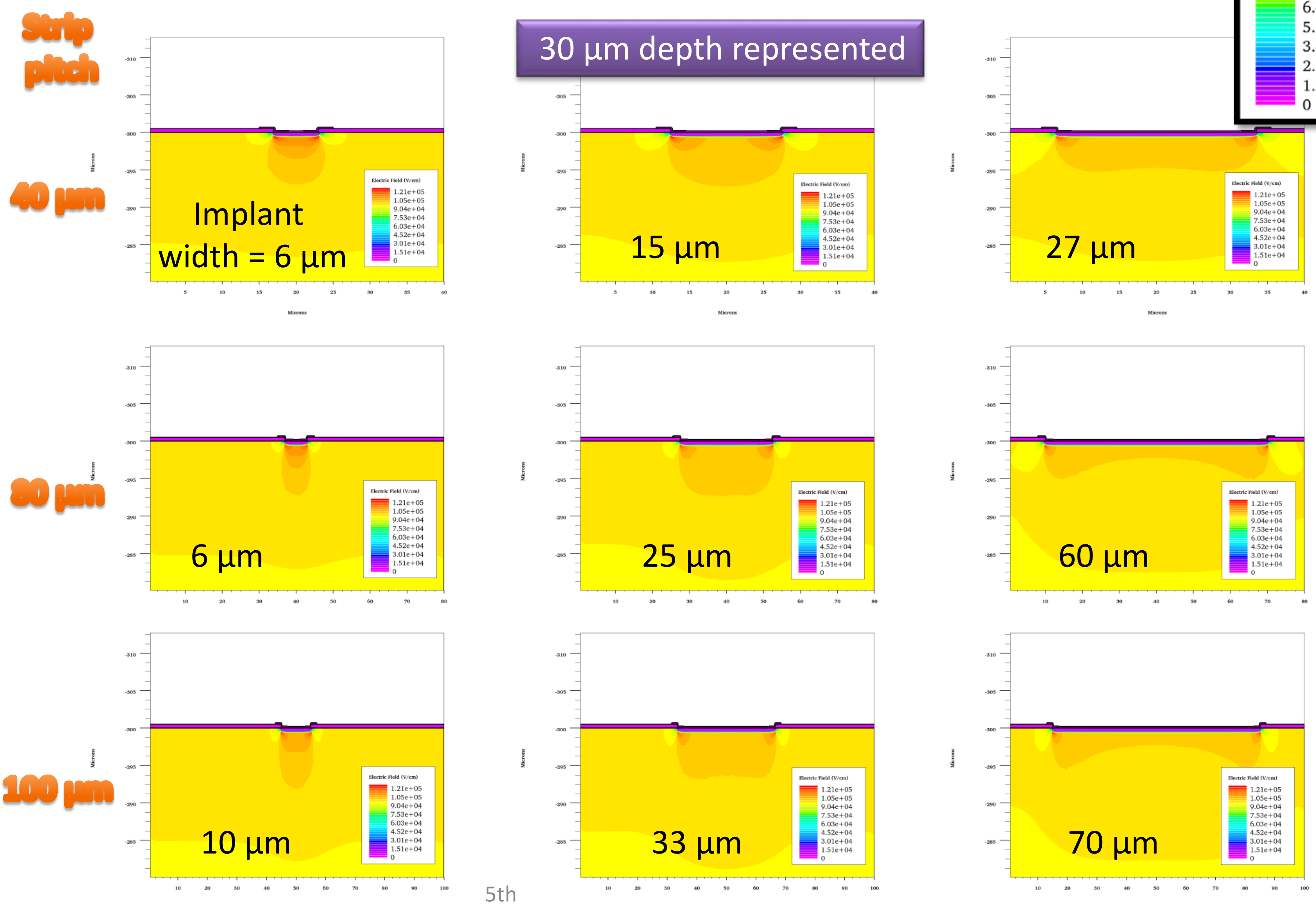
2D simulation : Electric field (at 10^{14} n_{eq}/cm^2)



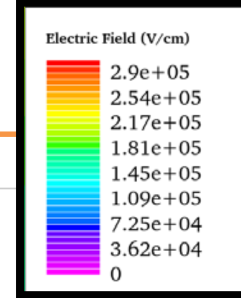


2D simulation : Electric field (at 10^{15} n_{eq}/cm^2)



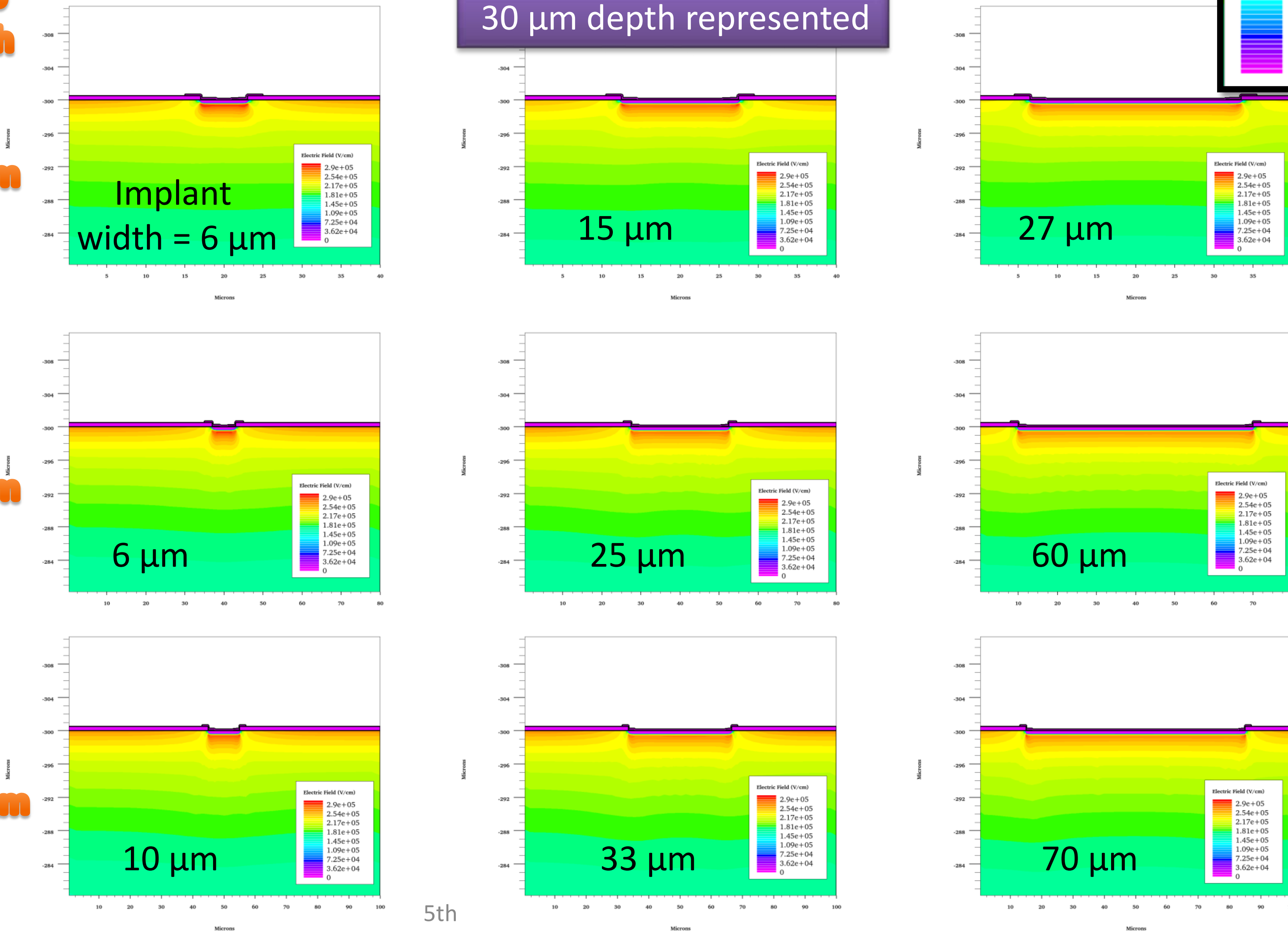


2D simulation : Electric field (at 10^{16} n_{eq}/cm^2)



30 µm depth represented

Strip pitch



Comparison of main commercial TCAD software packages

SILVACO TCAD Suite	Sentaurus TCAD Suite
http://www.silvaco.com/ Silvaco Data Systems was founded in 1984 by Dr. Ivan Pesic. The initial product, UTMOST, quickly became the industry standard for parameter extraction, device characterization and modeling. In 1985 Silvaco entered the SPICE circuit simulation market with SmartSpice. In 1987 Silvaco entered into the technology computer aided design (TCAD) market. By 1992 Silvaco became the dominant TCAD supplier with the ATHENA process simulator and ATLAS device simulator. Educational prices available on request from Silvaco	http://www.synopsys.com/Tools/TCAD/Pages/default.aspx Formely ISE TCAD, bought by Synopsis Synopsys is a world leader in electronic design automation (EDA), supplying the global electronics market with the software, IP and services used in semiconductor design and manufacturing. Synopsys' comprehensive, integrated portfolio of implementation, verification, IP, manufacturing and FPGA solutions helps address the key challenges designers and manufacturers face today, such as power and yield management, system-to-silicon verification and time-to-results. These technology-leading solutions help give Synopsys customers a competitive edge in bringing the best products to market quickly while reducing costs and schedule risk. Synopsys is headquartered in Mountain View, California, and has more than 60 offices located throughout North America, Europe, Japan, Asia and India. Available from EUROPractice

Disclaimer : I do not have any link with any of the company producing TCAD software. Recommandation here are strictly personal based on my experience with both software during my work in HEP

Comparison of main commercial TCAD software packages

SILVACO	Sentaurus
Athena : 2D SSUPREM4 based process simulator	Sprocess : 2D/3D SSUPREM4 based process simulation
ATLAS : 2D (and basic 3D) device simulation	Sdevice : 2D and 3D device simulation
VICTORYCELL : GDS based 3D process simulation	SnMesh : Adaptativ meshing tool for process and device simulation
VICTORYPROCESS : 3D Process simulation	Swb : Sentaurus WorkBench, GUI controling simulation process flow, parametrization etc..
VICTORY DEVICE : 3D device simulation	
Virtual Wafer Fab : wrapper of the different tool in a GUI	

SENTAURUS (Synopsys)

• Advantages	Inconvenients

• 3D Simulation built-in
  • Seemless transition from 2D to 3D
 	
• Excellent user interface
 	
• Support for LSF (lxbatch !!!)
 	
• Parallel 3D solver (takes advantage of modern multi-core CPU)
 	
• Adaptative meshing and clever 3D meshing algorithm
	• User support very slow
	  • ~1-2 months for an answer
	
	• Syntax of the simulation protocol is a bit more tedious than for equivalence in the competitor (learning curve steeper)
	
	• Set of example smaller and less relevant for HEP than the competitor

SILVACO

Advantages	Inconvenients

• Simple scripting language make it easy to start real work within a short time
• Extensive litterature supporting the validity of the software
• Very responsive user support:
  • Email exchange directly with the engineers
  • Custom patches produced following our needs
	• More complex parametric simulation planification (Design-Of-Experiment)
	• GUI rather old and in need of a rejuvenation
	• No parallel solver for 3D device simulation
	• No 3D process simulation without the purchase of an expensive supplementary licence
	• Meshing methods not adapted to 3D simulation

Common aspects

- The physics included in both simulation software are very similar :
  - Both software based on the same open-source base programs.
    - Syntax, outputs in most case identical
    - Models are based on same publications
  - Solving methods essentially the same
    - Matrix handling however differ between software
  - Both, unsurprisingly, claim to be the best on the market !

Common aspects

- Both software allow for redefinition of any constants, input parameters of the models used , ex :
  - Lifetime, cross-section , bandgap, impact ionization coefficient etc…
- Many (not all) models can be redefined using the internal C interpreter, ex :
  - Redefined impact ionization coefficient variation with electric field
  - Redefined mobility dependence on $T,E,N_{A/D}$

TCAD simulation as a black box (1)

- Both software are sold as compiled software with no access to source code, however :
  - Both software are extensively used in the industry with a lot of success translating in a major contribution to the improvement of the microelectronics
  - Both software are extensively documented with references provided :
    - SILVACO ATLAS Manual -> 898 pages
    - SENTAURUS DEVICE Manual -> 1284 pages

TCAD simulation as a black box (2)

- The benefit of using a commercial software w.r.t Home-Made solution are :
  - to benefit from a large user base (debugging, feedback and new features) ☺
  - Less focus on mathematics and coding more focus on physics ☺ (physicist can't do everything, we should stick to what we know best !)
    - Ex: Writing a Navier-Stokes solver for a 2D very specific geometry (given a receipe and all equation and numerical methods) ~ 1-2 months for a master student

TCAD simulation as a black box (3)

- FEM is commonly use to provide reliable simulation for design of the plane that flew you here , or the cooling system of your laptop

- Simulation of non-irradiated semiconductor device has reached a similar level or reliability

- A lot of work from the RD50 collaboration could very much bring the simulation of irradiated sensors to the same state !